Reacting Flow

Simcenter STAR-CCM+ provides a selection of models that you can use to simulate a wide range of reacting flow applications.

In Simcenter STAR-CCM+, there are two specific categories of reacting flow models, Flamelet, and Reacting Species Transport. Whenever applicable, you use the flamelet models, otherwise, you use the reacting species transport models. To decide on a modeling approach, it is important to consider the relation between the rate at which species react and the rate at which species mix (the chemistry time-scales and turbulence time-scales).

You can create simple chemical mechanisms in Simcenter STAR-CCM+ either manually or using the flamelet table generators, or you can import more complex chemical mechanisms from another source, such as DARS. A selection of ignitors are also available to use with most combustion models in Simcenter STAR-CCM+.

Simcenter STAR-CCM+ provides the option to use the Adaptive Mesh model in conjunction with a combustion model. This combination improves the ability of the volume mesh to resolve the internal flame structure by adapting the cell sizes within the existing mesh according to a scalar range that is specified for a selected variable, such as species mass fraction, temperature, and/or progress variable.

Flamelet

In Simcenter STAR-CCM+, the chemistry is calculated using detailed chemical mechanisms in simple 0D or 1D laminar flamelet geometries. The results are then tabulated and interpolated in a 3D simulation of a turbulent flame.

Flamelet Models	Description	Applications
Flamelet Generated Manifold	Mainly for premixed or partially-premixed flames where the flamelet assumption is valid.	• Gas Turbines • Furnaces • Burners
Steady Laminar Flamelet	Mainly for non-premixed combustion where the flamelet assumption is valid.	• Furnaces • Burners
Chemical Equilibrium	When only the temperature is of interest, or there is no chemical mechanism available.	• Fires • Coal Combustors

The following flame propogation models are also available:

- Turbulent Flame Closure
- Coherent Flame Model

See, Flamelet.

Reacting Species Transport

Simcenter STAR-CCM+ solves transport equations for all species and applies a separate mechanism for predicting the chemistry. Possible mechanisms range from simple one or two step reactions to those that require complex chemistry.

Reacting Species Transport Models	Description	Applications
Complex Chemistry	For capturing transient phenomena and slowly forming species in gaseous combustion.	• CI ICE • Gas Turbines • Multifuel Combustion
Eddy Break-Up	For quick flame positioning in gaseous combustion.	• Gas Turbines • Furnaces • Burners
Thickened Flame Model	For premixed or partially premixed flames in Large Eddy Simulations (LES), when flamelet models cannot be used.	• Gas Turbines • Explosions
Eddy Contact Micromixing	For liquid-liquid chemistry, where the chemistry is fast compared to mixing.	Liquid-Liquid Reactors
Polymerization	For polymerization reactions.	Polymerization Reactors

See, Reacting Species Transport.

Other Reacting Flow Models

You can also use other types of reacting flow models alongside the Flamelet, and Reacting Species Transport models:

- **Emissions**: Simcenter STAR-CCM+ provides specific emissions models that you can use with the specific reacting flow models to simulate slowly forming pollutant species, such as Soot, NOx Thermal, NOx Prompt, and NOx Fuel.

  See, Emissions.
- **Surface Chemistry**: Surface chemistry describes the interaction between fluid molecules and a solid surface material. You can model surface chemistry independently or as an additional option alongside other categories of reaction models.

  See, Surface Chemistry.
- **Reacting Channels**: The Reacting Channels model is designed to simulate chemical processes that occur within long narrow tubes.

  See, Reacting Channels.
- **Interphase**: By using combustion models in combination with relevant multiphase models, you can simulate reacting solid particles or fluid droplets.

  See, Modeling Multiphase Flow.
- **Reactor Network**: Once the flame position for a steady-state simulation is calculated using a simple and fast combustion model (a flamelet model or EBU), the Reactor Network model calculates the detailed chemistry within a network of reactors that contain clusters of contiguous cells with similar

compositions. Avoids the computational cost of solving detailed chemistry for each cell in the computational domain.

See: Reactor Network.

Optional Reaction Models	Description	Applications
Emissions	For NOx and soot prediction.	• Gas Turbines • Furnaces • Burners
Particle Reactions (see Interphase)	For combustion of solid particles	• Coal Combustion • Biomass Combustion • Gasification
Surface Chemistry	For catalyses and surface deposition or etching.	• Aftertreatment • CVD
Reacting Channel	For fast calculation (1D) of chemical reactions in long channels.	• Steam Reforming • Ethylene Cracking
Interphase Reactions	For phase-changing reactions.	• Gas Oil Cracking • Fluidized Bed
Reactor Network	To rapidly simulate detailed chemistry in steady combustors.	• Gas Turbines • Steady Combustors

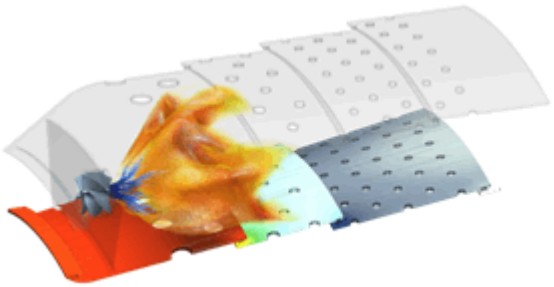
Contents:

Reacting Flow Applications

It is possible to model many different types of reacting flow applications using combinations of the reacting flow models that are provided in Simcenter STAR-CCM+.

The reacting flow general workflow describes how to begin modeling all types of reacting flow applications in Simcenter STAR-CCM+. See Reacting Flow General Workflow. Each specific type of reacting flow application follows an additional workflow, which you choose based on the specific application. A selection of common reacting flow applications and guidelines for selecting a suitable workflow are described in the following sections.

Gas Turbines



You can use either of the following workflows:

- **Reacting Species Transport**

  Best for gas turbines at part load.

  Use any of the following models:

  - Complex Chemistry (computationally expensive, so use only when necessary)
    - when there is a mixture of multiple fuels
    - to simulate flame ignition, quenching, or extinction
    - to simulate slowly forming pollutants
    - to simulate off-design load points
  - Eddy Break-Up (EBU)

    Use if the reactions are predominantly limited by turbulence and the mechanism is small (one or two steps), otherwise, use Complex Chemisty.
  - Thickened Flame Model (TFM)

    Useful for transient LES simulations. This model thickens flames artificially—which can help to reach a converged solution when the other flamelet models cannot.

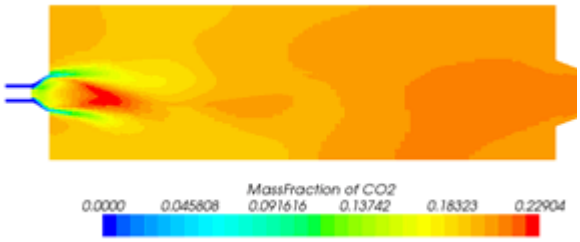
  See Reacting Species Transport.
- **Flamelet**

  Best for gas turbines at full load or in which statistically-steady turbulent combustion occurs.

  Use the Flamelet Generated Manifold (FGM) model.

  See Flamelet.

Coal Combustion



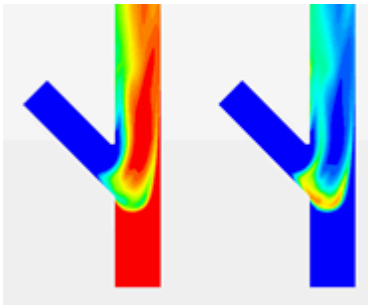
You can use one of the following workflows:

- **Interphase**
  Best for modeling interactions between the solid coal particles and the background gas, such as in coal furnaces. You can select either of the following models:
  - Coal Combustion
    Best for simulating coal furnaces. You can also model NOx emissions that are designed specifically for coal fuel.
  - Particle Reaction
    - Particle Combustion: to simulate particle combustion or char oxidation.
    - Particle Devolatilization: to simulate particle devolatilization, gasification, or sublimation.
- **Reacting Species Transport**
  You can simulate multi-fuel combustion with the complex chemistry model.
  See Reacting Species Transport.
- **Flamelet**
  You can use the chemical equilibrium flamelet model for simulating simple coal combustion or fires.
  See Flamelet.

Additionally, if required, you can model Emissions alongside the Flamelet or Reacting Species Transport workflows. The Interphase workflow provides the option to model specific NOx emissions.

Fluid Catalytic Cracking

Example application: gasoline production.



You can use one of the following workflows:

- **Interphase**
  Best for modeling interactions between the liquid droplets and the background gas.
- **Reacting Species Transport**

You can simulate multi-fuel combustion with the Complex Chemistry model.

See Reacting Species Transport.

Polymerization

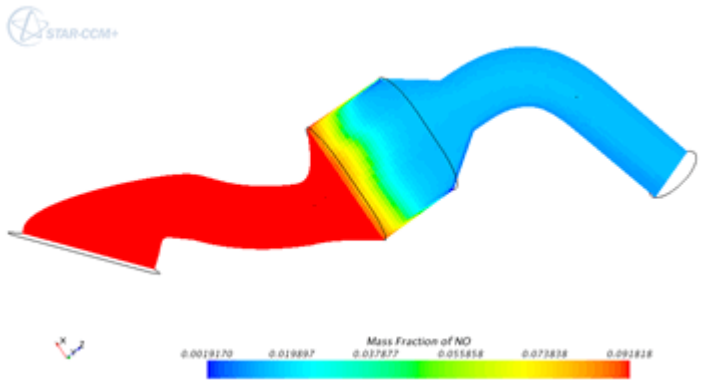
The Polymerization model allows you to simulate all relevant processes, including initiation, propagation, transfer, branching, scission, and termination.

You can use one of the following workflows:

- **Polymerization**
  To simulate polymerization within a multi-component liquid (non-multiphase).
- **Interphase Workflow: Multiphase**
  To simulate multiphase polymerization—for example, in a fluidized bed reactor or a stirred tank reactor—use the Polymerization model within a multi-component liquid phase of the Multiphase model.

See Polymerization.

Catalytic Convertors

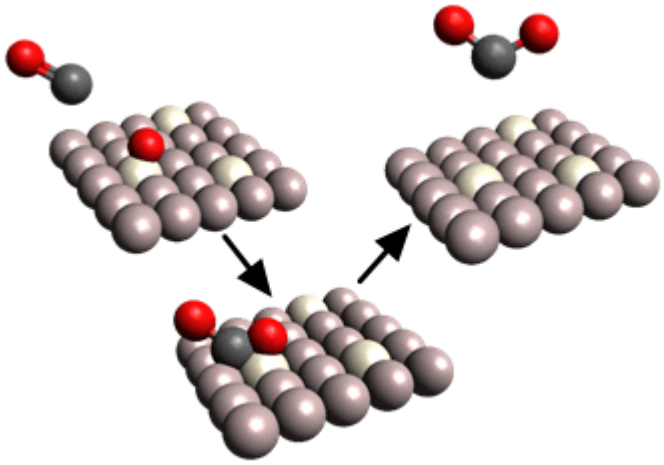


Use the Reacting Species Transport workflow—which allows you to model transport of all species, with the additional Surface Chemistry and Emissions workflows.

See Reacting Species Transport, Surface Chemistry, Emissions.

You can specify the reacting surfaces as walls within solid regions or surfaces in porous regions.

Reacting surfaces



Use the Reacting Species Transport workflow—which allows you to model the transport of all species, with the additional Surface Chemistry workflow.

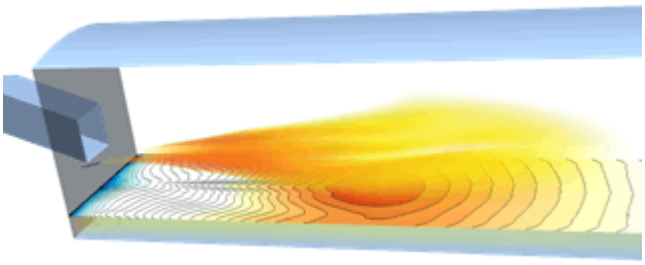
See Reacting Species Transport, Surface Chemistry.

If you want to monitor emissions, you can also use the Emissions workflow alongside the Reacting Species Transport workflow.

See Emissions.

The reacting surfaces can be walls within solid regions, or surfaces in porous regions.

Glass Furnaces



You can use one of the following workflows:

- **Intraphase**

  You can use the Multiphase Volume of Fluid (VOF) model for simulating a reacting phase (which uses a Flamelet model or Reacting Species Transport model) within a flow of several immiscible fluid phases.

  See Intraphase.
- **Reacting Species Transport**
  - Eddy Break-Up

    Use if the reactions are predominantly limited by turbulence and the mechanism is small (one or two steps).
  - Complex Chemisty

Use with a Chemkin formatted mechanism.

See Reacting Species Transport.

- **Flamelet**

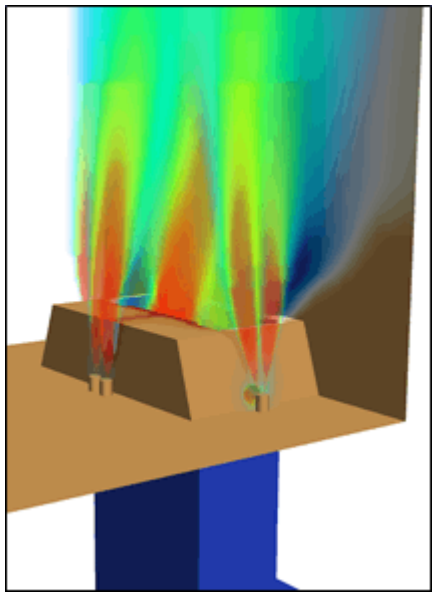
  You can use the Steady Laminar Flamelet model for steady state opposed flow diffusion flames with tabulated detailed kinetics.

  See Flamelet.

If you want to monitor the emission levels of particular species, you can additionally use the Emissions workflow.

See Emissions.

Furnaces and Burners



You can use one of the following workflows:

- **Flamelet** (use with tabulated detailed kinetics)
  - Steady Laminar Flamelet

    for steady state opposed flow diffusion flames.
  - Flamelet Generated Manifold

    Suitable for all premixed or partially premixed flames where the flamelet assumption is valid (there are infinitely fast chemical reactions). Use if you want to capture ignition, extinction, or quenching.

  See Flamelet.
- **Reacting Species Transport** (Use if none of the flamelet models are suitable)
  - Complex Chemistry

    Use with a Chemkin formatted mechanism, for transient calculations, ignition, and extinction.
  - Eddy Break-Up

    Use with one or two simple reactions that you define in the GUI.

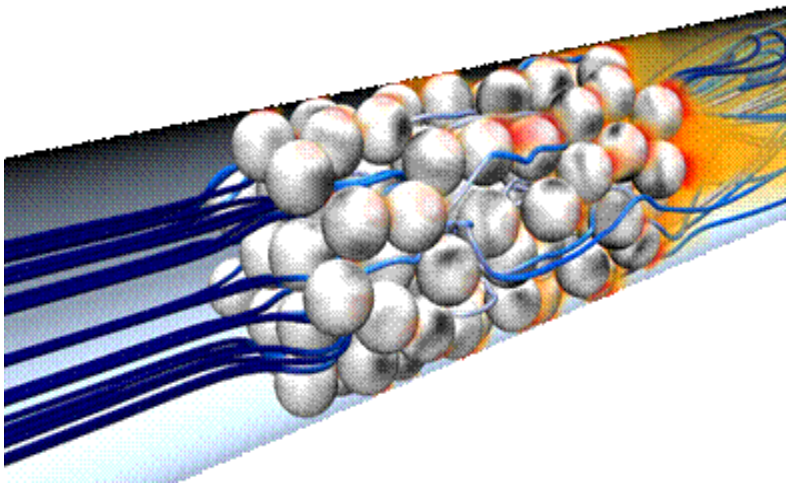
  See Reacting Species Transport.

If you want to monitor the emission levels of particular species, you can additionally use the Emissions workflow.

See Emissions.

Reacting Channels

Example application: Methane reformation.

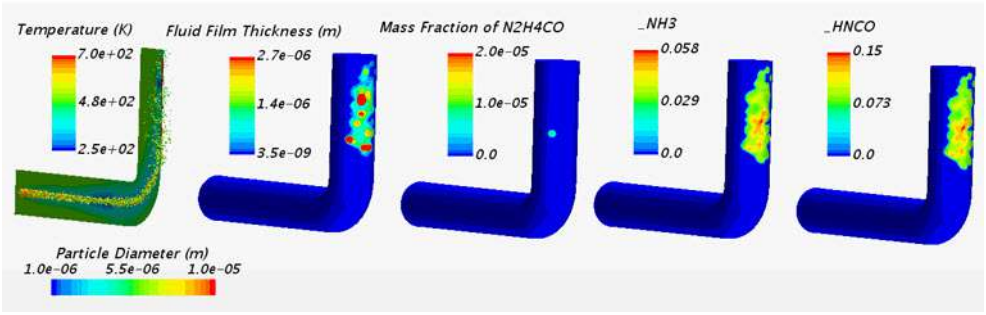


Use the Reacting Channels workflow which describes how to set up the reacting channels and surrounding firebox volume.

See Reacting Channels.

Fluid Film Reactions

Example application: trickle-bed reactors or selective catalytic reduction (SCR) reactions in urea film.



You can simulate reactions within a fluid film (intraphase) using the Reacting Species Transport workflow with the optional model, Fluid Film. You use the Multi-Component Gas model for the background fluid region, and interface the gas with a fluid film shell region.

See Reacting Species Transport.

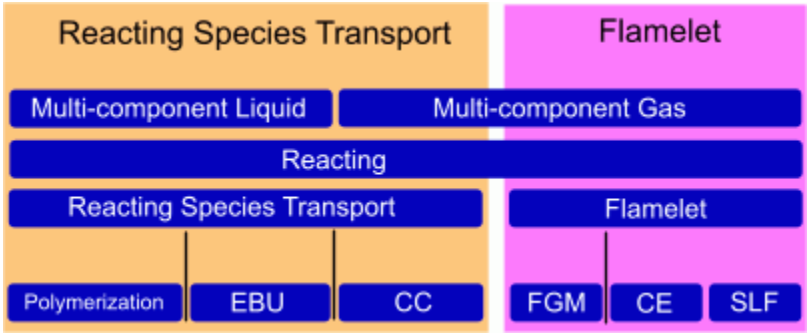
Reacting Flow General Workflow

Simcenter STAR-CCM+ supports several types of combustion analysis, each with their own workflow. Use this section to help identify the choice of models that are appropriate for the type of analyses you intend.

Import or create geometry parts that represent the volume in which the reacting flow occurs. You can use Simcenter STAR-CCM+ in serial or parallel mode.

Before selecting physics models and setting up physics parameters, it is important to have appropriate geometry and a suitably refined mesh in Simcenter STAR-CCM+. The detailed workflow that you follow depends on the physics of the application that you intend to simulate. Simcenter STAR-CCM+ provides a wide range of physics models that you can use in different combinations to suit different types of reacting flow processes. Follow the advice that is given in the introductory pages of the Reacting Flow section to help you determine which specific detailed workflow to use in addition to this workflow.

The following diagram provides an overview of the initial physics models that are required in the two most common detailed reacting flow workflows.

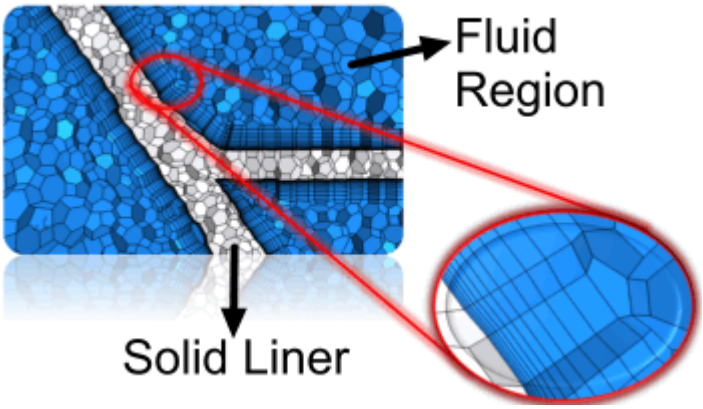


1. Generate a quality mesh to represent the reacting flow volume.

   A polyhedral mesh is suitable for modeling most combustion applications as polyhedral cells generally have a low skewness and can calculate a more accurate face flux than tetrahedral cells. Polyhedral cells also provide a smooth volumetric growth, which is important for capturing complex geometry effectively.

   It is important to consider refining the mesh by increasing the resolution in significant areas or volumes of the geometry. For example:

   - Refine mesh on and around fuel jets.
   - Create a higher resolution mesh in narrow volumes.
   - Refine mesh on impellers and baffles.
   - In simple geometries, where mixing occurs, use volumetric refinement.
   - In complex geometries, where mixing occurs, use solution based refinement.
   - When modeling combustion with conjugate heat transfer, create a conformal mesh at the interface. It is also necessary to capture the boundary layers by using the Prism Layer mesher to create orthogonal prismatic cells next to the walls.



2. Decide which detailed workflow is most suitable for the application that you are modeling.
   It is useful to consider how and where the reactions are happening in the application that you are simulating, as these details help to elicit the most appropriate workflow.

Consider the type of reacting flow models that are available to use within the specific detailed workflow that you have decided to follow. When you proceed to the specific detailed workflow, it is useful to have an idea about which models you intend to use.

3. Before following the steps within one of the specific detailed workflows, for the physics continuum that represents the reacting flow volume, start to select appropriate general physics models:

Group Box	Model
Material	◦ For Flamelet workflows, select **Multi-Component Gas**. ◦ For Reacting Species Transport workflows, select **Multi-Component Gas** or **Multi-Component Liquid**. ◦ For Reacting Channels workflows, you select the type of material that best represents the fluid domain that surrounds the reacting channels (not the material within the reacting channels). ▪ **Multi-Component Gas** ▪ **Multi-Component Liquid** ▪ **Liquid** ▪ **Gas** ◦ For Lagrangian Multiphase, interphase workflows, select the material type that surrounds the reacting particles—not the material of the reacting particles: ▪ **Multi-Component Gas** ▪ **Multi-Component Liquid** ▪ **Liquid** ▪ **Gas** ◦ For Eulerian Multiphase, interphase or intraphase workflows, select **Multiphase**. ◦ For Fluid Film, interphase workflows, select **Multi-Component Gas**. ◦ For Polymerization workflows in which polymerization occurs within: ▪ a multi-component liquid (non-multiphase), select **Multi-Component Liquid**. ▪ a multi-component liquid phase in a multiphase polymerization setup (such as in a fluidized bed reactor or stirred tank reactor), select **Multiphase**. ◦ For Surface Chemistry workflows, select **Multi-Component Gas** or **Multi-Component Liquid**.
Space	◦ **Axisymmetric** ◦ **Three Dimensional** (required for Adaptive Mesh Refinement) ◦ **Two Dimensional**
Time	◦ **Implicit Unsteady** (required for Lagrangian Multiphase Interphase workflows). ◦ **PISO Unsteady** (Segregated Flow Only) ◦ **Steady** (required for Reacting Channels and Reactor Network workflows) When any Unsteady model is selected with a Flamelet reacting flow model, the Ideal Gas is compressible, and when Steady is selected, the Ideal Gas is incompressible.

Group Box	Model
Optional Models	If required, select **Adaptive Mesh** to improve the volume mesh's ability to resolve the internal flame structure by refining or coarsening cells based on adaptive mesh criteria as they query the flow solution. See Adaptive Mesh Refinement.
Reaction Regime (for Multi-Component Gas or Multi-Component Liquid)	◦ For the Flamelet and Reacting Species Transport (including Polymerization) workflows, select **Reacting**. ◦ For Fluid Film, interphase workflows, if reactions occur in the neighbouring gas phase, select **Reacting**, otherwise select **Non-Reacting**. ◦ For the Reacting Channels workflow, if reactions occur in the fluid that surrounds the reacting channels, select **Reacting**, otherwise, select **Non-Reacting**. ◦ For the Lagrangian Multiphase, interphase workflow or the Multiphase Volume of Fluid (VOF) intraphase workflow, select **Non-Reacting**. The reactions are defined in the phase. ◦ For the Surface Chemistry workflow: ▪ If the fluid mixture is only undergoing surface reactions and there are no other reactions, select **Non-Reacting**. ▪ If reactions are occurring within the volume of the fluid mixture in addition to the surface reactions, select **Reacting**.
Multiphase Model (for Multiphase)	For Eulerian Multiphase, interphase or intraphase workflows, select one of: ◦ **Eulerian Multiphase** (EMP) ◦ **Mixture Multiphase** (MMP) ◦ **Volume of Fluid** (VOF). Required when using a flamelet model for intraphase reactions.

4. Proceed to the specific reacting flow workflow that you have decided to follow—keeping in mind any specific models that you think are appropriate for the application that you are simulating.
   a) In addition to the reacting flow physics models that you select in the specific reacting flow workflow, as necessary, also select the following general physics models:

Group Box	Model
Flow	Either: ▪ **Coupled Flow** ▪ **Segregated Flow** (recommended when using the NOx Emission model) Depending on the selection, further models are selected automatically.

Group Box	Model
Equation of State	One of: ▪ **Constant Density** ▪ **Polynomial Density** ▪ **User Defined EOS**
Viscous Regime	One of: ▪ **Inviscid** (not for Fluid Film Interphase Workflows) ▪ **Laminar** ▪ **Turbulent** (required for Flamelet reactions) Depending on the selection, further models are required.

b) In combustion simulations that use the **Coupled Flow** model, also select the **Coupled Energy** model and set *Enthalpy Formulation* to **On**.

See Coupled Energy Properties.

- Reacting Species Transport Workflow (also for intraphase reactions)
- Polymerization Workflow (for polymerization in a non-multiphase multi-component liquid)
- Flamelet Workflow (also for intraphase reactions with VOF Multiphase)
- Interphase Reactions Workflow: Lagrangian Multiphase
- Interphase Reactions Workflow: Multiphase (for multiphase polymerization)
- Interphase Reactions Workflow: Fluid Film
- Surface Chemistry Workflow
- Reacting Channels Workflow
- Reactor Network Workflow

After completing the steps in the specific reacting flow workflow, complete the set-up as follows:

5. For the continuum, define any necessary parameters for the **Reference Values** and **Initial Conditions**.
6. If the **Adaptive Mesh** model is selected, specify the adaptive mesh refinement criteria.
   a) Right-click the **[physics continuum]** > **Models** > **Adaptive Mesh** > **Adaptive Mesh Criteria** node and select **New** > **Mesh Adaption for Reacting Flows**.
   b) Expand the **Adaptive Mesh Criteria** > **Mesh Adaption for Reacting Flows** node and set the following:

Node	Action
Mesh Adaption for Reacting Flows	Set the *Maximum Refinement Level*. See Max Refinement Level.

Node	Action
└ **Variables**	Set the *Variables* property to the variable(s) that Simcenter STAR-CCM+ uses as adaption criteria. For example, when using the FGM model, the mesh can be adapted automatically as the solution proceeds, based on the mixture fraction and progress variable. This is useful to refine the cells in the flame. See Variables.
└ **[variable]**	Set a scalar range `[low, high]` for the error indicator limit. Cells are refined if the error indicator (based on the secondary gradient) is calculated to be greater than the `high` limit, or coarsened if less than the `low` limit. See Mesh Adaption for Reacting Flows.

See Mesh Adaption for Reacting Flows.

7. Define any necessary Physics Conditions and Values for the Region and Boundaries.

   For example:

   - For a wall boundary, you can define any flux at the boundary using the boundary physics condition, **Wall Combustion Scalar Option**.
   - For regions in which reacting flows are affected by a momentum source such as a fan, you can define the momentum source using the region physics condition, **Momentum Source Option**.
   - If you are modeling the Fuel NOx for a purely gaseous fuel, it is important to specify values for the inlet composition which include the intermediate species, HCN and/or NH3.

   Note: It is possible to specify several combustion model constants as parameters. See Global Parameters.

8. Specify the required Solver settings and Stopping Criteria.

   a) Select the **Stopping Criteria** > **Maximum Steps** node and set the *Maximum Steps*.

   If you are unsure of what value to set, maintain the default. If the solution converges before the maximum number of steps, you can stop it manually and note the number of steps to use the next time you run the simulation. If the solution has not converged, you can increase the maximum number of steps and continue running the simulation.

   b) Expand the Solvers node and adjust any solver parameters that are necessary. If you are unsure, maintain the default values.

   When using the Adaptive Mesh model, freeze the Adaptive Mesh solver until you obtain a converged solution on the coarse mesh—then activate the Adaptive Mesh solver.

   Note: Make sure that the Under-Relaxation Factor property for the energy and species solvers are both set to the same values.

9. Set up any Reports, Monitors, Plots, and Scenes that are required for Post-Processing.

   For example:

- To determine if a reacting flow simulation solution is converging, you can generate a heat balance plot from a report.
  a. Right-click the **Reports** node and select **New Report** > **Heat Transfer**.
  b. Select the Heat Transfer 1 node and set Parts to all of the inlet and outlet boundaries for the reacting flow region.
  c. Right-click the **Reports** > **Heat Transfer 1** node and select **Create Monitor and Plot from Report**.
  d. Open the **Plots** > **Heat Transfer 1 Monitor Plot**.
  When you run the simulation and the plot settles at a value that is close to zero, this shows that the heat at the inlet and outlet boundaries is reconciled and the solution has converged.
- To plot a specific field function within the reacting flow region, or at a boundary, you can generate an XY Plot. For example, you can monitor the temperature on the surface of reacting channels, the mass fraction of CO emissions at an outlet, or the progress variable within a reacting flow region. For more information, see Plotting Results.
  a. Right-click the **Plots** node and select **New Plot** > **XY Plot**
  b. Expand the **Plots** > **XY Plot 1** node and set at least the following parameters:

Node	Property	Setting
XY Plot 1	*Parts*	Select the region or boundary on which you want to monitor the chosen field function.
└ **Y Types**		
Y Type 1 > **Scalar Function**	*Field Function*	Select a field function that you want to monitor.

- You can visualize physics values on or within the reacting flow geometry using scalar scenes and vector scenes. For Example, you can visualize the flame area density within a scalar scene, or the velocity of the reacting flow within a vector scene. For more information, see Scenes.

10. Save the simulation.
11. Run the simulation.
    Simcenter STAR-CCM+ provides the Acoustic Modal Analysis post-processing model which uses an n-tau model to model the effect of the unsteady heat release rate on the acoustic pressure. The Acoustic Modal Analysis model allows you to simulate acoustic mode shapes, frequencies, and linear growth rates. You perform acoustic modal analysis from a previously converged solution. For further details see: Acoustic Modal Analysis.

Troubleshooting

Initialising an Unsteady Calculation Through a Steady Calculation

Steady calculations converge best with the incompressible option activated, while unsteady calculations converge best with the incompressible option deactivated. When initialising an unsteady calculation through a steady calculation, the following workflow is advised:

1. Converge the steady calculation with the incompressible option activated (default option when the Steady model is used with a Flamelet model).

2. Deactivate the incompressible option and re-converge.
3. Switch to using the Unsteady model—keep the incompressible option deactivated.

Warning messages in the output window indicate that there are issues with the setup. To resolve the issues, follow the advice given below then re-run the simulation.

Temperature Out Of Bound

When the temperature is out of bounds, a message similar to the following is displayed: `Temperature limited to [maximum/minimum] value [n] times on model-part "[part]"`

Under **Reference Values**, edit the value for Minimum Allowable Temperature or Maximum Allowable Temperature.

Heat Loss Ratio Out Of Bound

When the heat loss ratio (HLR) is out of bounds, a message similar to the following is displayed: `Heat loss ratio limited to [maximum/minimum] value [n] times on model-part "[part]"`. If this message only appears at the start of a computation, or only occasionally throughout the computation, take no action.

- When HLR hits the lower limit (-1), the heat gain in the domain is more than is specified in the combustion table. Increase the combustion table heat gain range by increasing the temperature of the oxidizer in the stream.
- When HLR hits the upper limit (1), too much heat loss is occurring from the domain. Within the combustion table, expand the **Table Generator** > **Parameters** > **Numerical Settings** node and lower the value that is set for the Reference Temperature.

Reacting Flow General Reference

Some reference material is common to different sub-sections within the reacting flow material.

Contents:

Reacting Model Reference

You select the Reacting model for physics continua in which reactions occur in the bulk of the fluid.

Reacting Model Reference

Theory	See Reacting Flow.		
Provided By	**[physics continuum]** > **Models** > *Reaction Regime*		
Example Node Path	**Continua** > **Physics 1** > **Models** > **Reacting**		
Requires	*Material*: **Multi-Component Gas** or **Multi-Component Liquid**		
Activates	Physics Models	*Reacting Flow Models*	
	Model Controls (child nodes)	**Reactions**	Contains details of the reactions in the chemical mechanism. You can define these reactions manually, or they appear upon importing a chemical mechanism. See Importing Species and Reactions or Defining Chemical Reactions Manually.
		└ **[Reaction]**	
		└ **Reactants**	
		└ **Products**	
		└ Properties	
		Reacting System Properties	

[Reaction] > Properties

The Properties node contains further sub-nodes, Complex Reaction Properties, and Reaction Coefficient. When Third Bodies is activated under Arrhenius Coefficients, a Third Body Efficiencies sub node is also available. If pressure-dependent reactions are defined in the imported chemical mechanism, another node also appears,

named after the specific method that is used to specify the pressure-dependent parameters—either, Lindemann Fall-Off Formulation, Troe Fall-Off Formulation, or SRI Fall-Off Formulation. The values for Lindemann, Troe, or SRI, are set automatically from the imported chemical mechanism. However, if necessary, it is possible to set these values manually.

Complex Reaction Properties

Pressure Dependent

Allows you to specify that this reaction uses a pressure-dependent Lindemann mechanism. When activated, the Lindemann Fall-Off Formulation node appears.

Reaction Coefficient

The Arrhenius reaction parameters are used to calculate chemical reaction rates from finite-rate kinetics.

Method	**Corresponding Sub-Nodes**
Arrhenius Coefficients	**Pre-exponent** Defines the pre-exponential factor, A, in Eqn. (3431).

Arrhenius Coefficients: Properties

Temperature Exponent, Beta

Sets the temperature exponent, β, for this reaction in Eqn. (3431).

Activation Energy, Ea

Sets the activation energy, E_a, for this reaction in Eqn. (3431).

Reversible

When activated, the reaction is specified as reversible. In a reversible reaction, you specify the forward rate coefficients and select how the backward rate is calculated using the **Properties** > **Reverse Reaction Coefficient** node. When reversible reactions are read from a Chemkin mechanism, this property is activated and the reaction properties are set automatically. If you define a reversible reaction, make sure that you specify values for the enthalpy, entropy, and specific heat for each component of the mixture. For the specific heat, you choose either the thermodynamic polynomial or polynomial in T option.

Third Bodies

By default, each species in the mixture is assumed to contribute with equal efficiency as a third body. Hence all species are given a third body efficiency of unity. If one or more species contribute more or less as a third body, you can activate this property and then specify the efficiency coefficient of that species under the Third Body Efficiencies node. If the imported mechanism contains details of third body efficiencies, this property becomes activated and the values are imported automatically.

The Arrhenius Coefficients node also provides the **Pre-exponent** sub-node that defines the pre-exponential factor, A, in Eqn. (3431).

Reverse Reaction Coefficient

Available when *Reversible* is activated under the **Reaction Coefficient** > **Arrhenius Coefficients** node.

Method	**Corresponding Sub-Nodes**
Reverse Coefficient By Equilibrium Constant	**Reverse Coefficient By Equilibrium Constant** Uses the Equilibrium Constant to calculate the backward reaction rate coefficient. This calculation requires that enthalpy, entropy, and specific heat are defined in the reaction definition.
Arrhenius Coefficients For Reverse Reaction	**Arrhenius Coefficients For Reverse Reaction** *Temperature Exponent, Beta* Sets the temperature exponent, β, for the backward reaction in Eqn. (3431). *Activation Energy, Ea* Sets the activation energy, E_a, for the backward reaction in Eqn. (3431). **Arrhenius Coefficients For Reverse Reaction > Pre-exponent** Defines the pre-exponential factor, A, for the backward reaction in Eqn. (3431).

Third Body Efficiencies

If third body efficiencies are imported as part of the chemical mechanism, details of the third body species and their efficiency coefficients are displayed under this node. If necessary, you can define third body efficiencies manually by right-clicking this node and selecting the option, **Add Third Body Coefficient** > **[species (continuum)]**. Each species that you include appears as a sub-node for which you can specify the third body efficiency coefficient, α_{ij}, in Eqn. (3438).

Lindemann Fall-Off Formulation

Specifies values for the Arrhenius rate parameters for the high-pressure limits (A_∞, β_∞, and E_∞ in Eqn. (3444)) and low-pressure limits (A_0, β_0, and E_0 in Eqn. (3443)), to account for the pressure-dependence of the rate constants, A_j, β_j, and E_j, respectively, in Eqn. (3431). Terminology within the reaction mechanism determines if the values represent high or low pressure limits.

Troe Fall-Off Formulation

Specifies values for α, $T***$, $T*$, and also optionally $T**$, in Eqn. (3446), which are used to calculate F_{cent}. F_{cent} is then used to calculate the blending factor, F, in Eqn. (3445).

SRI Fall-Off Formulation

Specifies values for a, b, c, and also optionally d and e, in Eqn. (3447), which are used to calculate the blending factor, F, in Eqn. (3445).

Reacting System Properties

Species Reaction Source Jacobian

When using user-coded reaction rates, it is strongly recommended to use the Numerical option for the Jacobian calculation. However, if you require the additional computational speed of an analytical Jacobian, Simcenter STAR-CCM+ does allow the option of a user-code analytical Jacobian.

Method	**Corresponding Sub-Nodes**
`Analytical` An analytical Jacobian is used in the CVODE solver.	**Analytical** • When the *Species Reaction Sources* method is set to `Internal`, Simcenter STAR-CCM+ calculates the Jacobian analytically. • When the *Species Reaction Sources* method is set to `User-Defined`, you specify a user function that defines the analytical Jacobian. See Working With User Functions.
`Numerical Jacobian` The Jacobian is calculated numerically.	**Numerical**

A Jacobian is a square matrix of derivatives of the reaction rate with respect to the species specific mole fractions (mass fraction divided by molecular weight), and temperature. See Eqn. (3491) and Eqn. (3492).

Species Reaction Sources

Method	**Corresponding Sub-Nodes**
Internal The Simcenter STAR-CCM+ CVODE solver provides the reaction rate source terms for reacting species.	None.

Method	**Corresponding Sub-Nodes**

User-Defined
Provides the **User-Defined Species Sources Specification** node which allows you to specify whether you are modifying the internally calculated reaction rate source terms, defining entirely new reaction rate source terms, or modifying the rates of single reactions.
	User-Defined
	Allows you to specify a previously imported user function that defines the species reaction rate source terms. See Working With User Functions.
	Field Functions
	Specifies the scalar field function to be used in corresponding user function for modifying the calculated reaction rates or defining reaction rate source terms.
	The following text is an example of how to access field functions in the user code:
	`struct UserAccessibleData *udata = (struct UserAccessibleData *)data;`
	`if (udata->_fieldFunctionsData._nFF > 1) { double ff0 = udata->_fieldFunctionsData._ffVal[0]; double ff1 = udata->_fieldFunctionsData._ffVal[1]; ... }`
	If you are using clustering in your simulation, these field functions will appear automatically under the **Clustering** > **Components** node.

User-Defined Reactions Density

Available when the User Defined EOS (Equation of State) model is selected with the Complex Chemistry model, and the density of the multi-component gas is specified as a field function.

User Function

Specifies the density of the multi-component gas as user code, for the calculation of the species source terms.

The output of your code must be identical to the field function you created for the density of the multi-component gas.

User-Defined Reactions Density Jacobian

Available when the User Defined EOS (Equation of State) model is selected with the Complex Chemistry model, and the density of the multi-component gas is specified as a field function.

User Function

Specifies the Jacobian of the density of the multi-component gas as user code, for species source term calculations.

The user code for the density Jacobian must return $\frac{d\rho}{dt}$ and $\frac{d\rho}{dz_i}$. $z_i = \frac{Y_i}{W_i}$ is the specific mole fraction where Y_i is the mass fraction and W_i is the molecular weight of the i'th species.

The following text is an example of user-coded functions that return the density and density derivatives for an ideal gas:

```
#include "UserAccessibleData.h"

void rho(double *rho, double T,  unsigned int nSpe, double *z, void *data)
{
  double const Ru = 8314.4621;
  struct UserAccessibleData *udata = (struct UserAccessibleData *)data
  double Rgas = 0.0;
  for( unsigned int i=0; i<nSpe; i++)
  {
    Rgas += z[i];
  }

  Rgas *= Ru;
  *rho = udata->_pressure / ( Rgas * T);
}

void rhoJac(double *drhodT, double *drhodzi, double *rho, double T,  unsigned
int nSpe, double *z, void *data)
{
  struct UserAccessibleData *udata = (struct UserAccessibleData *)data;

  double Rgas = 0.0;
  double const Ru = 8314.4621;
  for( unsigned int i=0; i<nSpe; i++)
  {
    Rgas += z[i];

  }

  Rgas *= Ru;
  *rho = udata->_pressure / ( Rgas * T );

  *drhodT = -*rho/T;
  *drhodzi = -*rho/Rgas * Ru;
}

#include "uclib.h"

void uclib()
{
  ucfunc(rho, "UserDensityForChemistry", "rho");
  ucfunc(rhoJac, "UserDensityJacobianForChemistry", "rhoJac");
}
```

User-Defined Species Sources Specification

Available when the Species Reaction Sources method is set to User-Defined.

Method	**Corresponding Sub-Nodes**
Calculate Species Sources	**Calculate Species Sources** Specifies that entirely new reaction rate source terms are to be defined with a previously imported user function. In this case, the internal reaction rate sources are not calculated. Displays the following property: *Internal Reaction Energy Source* When activated, the source term of the ODE energy equation is calculated internally, assuming a constant pressure reactor. See Eqn. (3488). When deactivated, the ODE energy source term must be calculated and stored in the (N+1)'th element of the reaction rate $\dot{\omega}$ vector.
Modify Internal Species Sources	**Modify Internal Species Sources** Specifies that the existing reaction rate source terms are to be modified with a previously imported user function —typically by multiplying the existing values with a constant.
Modify Internal Reaction Rates	**Modify Internal Reaction Rates** Specifies that existing rates of individual reactions are to be modified. Forward and reverse reaction rates are provided. Internal reaction rates can be modified with a previously imported user function.

You use the **Species Reaction Sources** > **User-Defined** node to select the appropriate user function. For more information on how to create user functions, see Working With User Functions.

Contents:

User-Defined Reaction Rate Source Terms

You can either modify the internally calculated reaction rate source terms, individual reaction rates, or define entirely new reaction rate source terms.

There are three kinds of user-coded reaction rate functions.

- **Custom Reaction Source Terms**
  Simcenter STAR-CCM+ does not initialize the source array passed in the argument to the function. Below, this user function is referred to as `wdotCalculate()`, although any name can be given in the user

code. Custom reaction source terms are appropriate when computing reaction species sources that are not simply a multiple of the internal Arrhenius rate sources.

- **Modified Reaction Source Terms**

  Simcenter STAR-CCM+ initially evaluates the internal Arrhenius species sources, and copies this to the source array passed in the function argument list. In the example below, this user function is referred to as `wdotModify()`, although any name can be given in the user code. Modified Reaction Source Terms are appropriate when modifying the internal Arrhenius species sources by a factor, which is typically a constant.

- **Modified Internal Rates of Individual Reactions**

  Simcenter STAR-CCM+ initially evaluates the internal forward and backward reaction rates from Eqn. (3429) / Eqn. (3460), and copies the result to the source array that is passed in the function argument list. Below, this user function is referred to as `reactionRateModify()` although any name can be given in the user code. Modified reaction rates are appropriate for modifying the internally calculated reaction rates for all the reactions in the chemical mechanism.

  Note: For non-reversible reactions, the internally calculated reverse reaction rate is 0.

The function signature for user-defined reaction rate source terms, for both *wdotModify()* and *wdotCalculate()*, is:

```
 void wdotModify(double *omega, double T, unsigned int nSpe, double *zi, void
*data)
```

The function signature for modifying rates of individual reactions *reactionRateModify()* is:

```
void reactionRateModify(double *reacRateForward, double *reacRateBackward,
double T, unsigned int nSpe, double *zi, void *data)
```

where,

	Reactions in the Gas Phase	Surface Reactions
`nSpe` (type unsigned int)	The number of species in the mixture.	`nSpe = nGas + nSite + nBulk` (where `nGas`, `nSite`, and `nBulk` are the number of gas phase species, surface site species, and bulk species respectively).
`zi`	A pointer to a vector (type double, size `nSpe`) of specific mole fractions = mass fractions of the i'th species divided by the molecular weight of the i'th species (units of molecular weight are kg/kmol).	A pointer to a vector (type double, size `nSpe`) of gas phase specific mole fractions, surface site fractions, bulk activities, and cell temperature.

	Reactions in the Gas Phase	Surface Reactions
`omega` The default units are kmol/kg-s.	A pointer to the output vector (type double, size `nSpe`) of the species source terms, which are the rate of change of specific mole fractions (mass fractions of the i'th species divided by molecular weight of the i'th species).	A pointer to the output vector (type double, size `nSpe`) of the source terms of gas phase species specific mole fractions, surface site fractions, and bulk activities. In the case of porous chemistry, omega also has (as the last element) a cell enthalpy source term (J/kg-s).
`reacRateForward`	A pointer to an array (type double, size `nReactions`) of all reaction rates in forward direction. The default units are kmol/kg-s.	A pointer to an array (type double, size `nReactions`) of all surface reaction rates in forward direction. The default units are mol/cm^2-s.
`reacRateBackward`	A pointer to an array (type double, size `nReactions`) of all reaction rates in backward direction. The default units are kmol/kg-s.	A pointer to an array (type double, size `nReactions`) of all surface reaction rates in backward direction. The default units are mol/cm^2-s.
`T` (type double)	Temperature (K)	Wall temperature (K)
`data`	A pointer to the `UserAccessibleData struct` that is defined in UserAccessibleData.	

UserAccessibleData

The `UserAccessibleData` allows for the transfer of data from Simcenter STAR-CCM+ to user code. To enable user coding, the following text is copied to a file and saved as `UserAccessibleData.h`. Then, user-accessible data are made available to the file that contains the user coding by using an include statement.

Species and reaction names are passed as part of the `UserAccessibleData` structure. The values in `UserAccessibleData` have SI units.

```
#ifndef _UserAccessibleData_h
#define _UserAccessibleData_h

struct UserAccessibleData {
   double _pressure; // absolute pressure (Pa)
   double _dt; // time step size (s)
   double _volume; // (m^3)
   double _volumeFraction; // liquid volume fraction of VOF model
   double _turbLen; // (m)
   double _turbTime; // (s)
   double _totalTime; // for unsteady simulations, current total time (s)

   struct FluidFilmData {
     double _fluidFilmThick; // (m)
     double _shellArea; // (m^2)
   } _fluidFilmData;
```

```
  struct SurfaceChemistryData {
    double _area; // (m^2)
    unsigned int _nGas;
    unsigned int _nBulk;
    unsigned int _nSite;
    unsigned int _isPorousRegion;
    unsigned int _nSiteMaterials;
    unsigned int _nBulkMaterials;
    unsigned int *_nSitePerMaterial;
    unsigned int *_nBulkPerMaterial;
  } _surfaceChemistryData;

  struct ReactingChannelData {
    double _massFlow; // (kg/s)
    double _velocity; // (m/s)
  } _reactingChannelData;

  struct ReactionData {
    unsigned int _nReactions;

    unsigned int *_nGasReactants;
    unsigned int *_nGasProducts;
    unsigned int *_nSiteReactants;
    unsigned int *_nSiteProducts;
    unsigned int *_nBulkReactants;
    unsigned int *_nBulkProducts;

    double **_gasStoichiometryReactants;
    double **_bulkStoichiometryReactants;
    double **_siteStoichiometryReactants;
    double **_bulkReactantRateExponents;
    double **_siteReactantRateExponents;
    double **_gasReactantRateExponents;
    unsigned int **_gasReactantSpeciesIndex;
    unsigned int **_siteReactantSpeciesIndex;
    unsigned int **_bulkReactantSpeciesIndex;

    double **_gasStoichiometryProducts;
    double **_bulkStoichiometryProducts;
    double **_siteStoichiometryProducts;
    double **_bulkProductRateExponents;
    double **_siteProductRateExponents;
    double **_gasProductRateExponents;
    unsigned int **_gasProductSpeciesIndex;
    unsigned int **_siteProductSpeciesIndex;
    unsigned int **_bulkProductSpeciesIndex;
  } _reactionData;

  struct ReactionPropertyDataGeneral {
    double *_lnA; // depends on reaction order (cm, mol, s, K)
    double *_b;
    double *_E; // Ea/Ru (universal gas constant) (K)
    double *_lnA_REV; // depends on reaction order (cm, mol, s, K)
    double *_b_REV;
    double *_E_REV;  // Ea/Ru (universal gas constant) (K)
    unsigned int *_isReversible;
    unsigned int *_isREVreaction;
    char **_reactionName;
  } _reactionPropertyDataGeneral;

  struct ReactionPropertyDataFluid {
    double *_lnA_low; // depends on reaction order (cm, mol, s, K)
    double *_b_low;
    double *_E_low; // Ea/Ru (universal gas constant) (K)
```

```
    unsigned int *_hasPlog;
    unsigned int *_hasThirdBody;
    unsigned int *_hasCabm;
    unsigned int *_isBathGasReaction;
    unsigned int *_PressDepType; // 0 - no, 1-general, 2-Troe, 3-sri
    int *_bathGasMaterialIndex;
    unsigned int *_ThirdBodyCoeffSize;
    unsigned int *_PlogSize;
    unsigned int *_TroeSRISize;

    unsigned int **_ThirdBodyIndex;
    double **_ThirdBodyCoeff;
    double **_TroeSRICoeffs;
    double **_PlogCoeffs;

    unsigned int *_useElectronTemp;
    unsigned int *_isExciRxn;
    double *_exciValue; // (J)
  } _reactionPropertyDataFluid;

  struct ReactionPropertyDataSurface {
    double *_bohmCoefficient;
    unsigned int *_isReactionBohm;
    double *_stickyCoefficient;
    unsigned int *_isReactionSticky;
    unsigned int *_isMotzWiseOff;
    unsigned int *_isReactionLangmuir;
    unsigned int *_reactionCoverageFactorsSize;

    unsigned int **_coverageFactorIndex;
    double **_coverageFactorEta;
    double **_coverageFactorMu;
    double **_coverageFactorEaR;
    double **_langmuirCoeffs;
  } _reactionPropertyDataSurface;

  struct FluidPhaseProperties {
    unsigned int _nGas;
    double *_molecularWeight; // (kg/kmol)
    double *_Tmin; // (K)
    double *_Tmid;  // (K)
    double *_Tmax; // (K)
    unsigned int *_cpHiSicoeffsSize;
    unsigned int *_cpHiSiTrangeSize;
    double **_cpHiSicoeffs; // nasa polynomial coefficients
    double **_cpHiSiTrange; // (K)
    char **_speciesName;
  } _fluidPhaseProperties;

  struct SurfaceMaterialProperties {
    double *_siteMolecularWeight; // (kg/kmol)
    double *_siteOccupancies;
    double *_siteDensity; // (kmol/m^2)
    unsigned int *_isOpenSite;
    double *_TminSite; // (K)
    double *_TmidSite; // (K)
    double *_TmaxSite; // (K)
    unsigned int*_cpHiSicoeffsSiteSize;
    unsigned int*_cpHiSiTrangeSiteSize;
    double **_cpHiSicoeffsSite; // nasa polynomial coefficients
    double **_cpHiSiTrangeSite; // (K)
    double *_bulkMolecularWeight; // (kg/kmol)
    double *_bulkDensity; // (kg/m^3)
    double *_TminBulk; // (K)
```

```
     double *_TmidBulk; // (K)
     double *_TmaxBulk; // (K)
     unsigned int*_cpHiSicoeffsBulkSize;
     unsigned int*_cpHiSiTrangeBulkSize;
     double **_cpHiSicoeffsBulk; // nasa polynomial coefficients
     double **_cpHiSiTrangeBulk; // (K)
     char **_siteSpeciesName;
     char **_bulkSpeciesName;
   } _surfaceMaterialProperties;

   struct ElectronTemperature {
     double _electronTemp;
   } _electronTemperature;

   struct FieldFunctionsData {
     unsigned int _nFF;
     double *_ffVal;
     char **_ffName;
   } _fieldFunctionsData;
};

#endif
```

Note: For backward compatibility, `UserAccessibleData` saved in previous releases still work in the current release of Simcenter STAR-CCM+.

Modifying Reaction Source Terms

The following text is an example of a user-coded reaction rate function which modifies the internal Arrhenius species sources by multiplying them by a constant factor proportional to the pressure in each cell.

```
#include "UserAccessibleData.h"

    void wdotModify(double *omega, double T, unsigned int nSpe, double *zi,
void *data)
    {
            // modify the internal Arrhenius reaction rate to be p / pref
            struct UserAccessibleData *udata = (struct UserAccessibleData
*)data;
         double const factor = udata->_pressure / 101325.;

            for( unsigned int i=0; i<nSpe +1; i++ )
                omega[i] *= factor;
    }

    void wdotJacModify(double *jac, double T, unsigned int nSpe, double *zi,
void *data)
    {
         // modify the internal Arrhenius reaction rate to be p / pref
         struct UserAccessibleData *udata = (struct UserAccessibleData *)data;
            double const factor = data->_pressure / 101325.;

         for( unsigned int i=0; i<(nSpe+1)*(nSpe+1); i++ )
                jac[i] *= factor;
    }

    void uclib()
    {

     ucfunc(wdotModify, "ReactionRate", "wdot");
```

```
     ucfunc(wdotJacModify, "ReactionRate", "wdotJac");
    }
```

Modifying Internal Rates of Individual Reactions

The following text is an example of a user-coded reaction rate function for modifying the rates of all individual reactions by multiplying them by a constant factor in each cell.

```
 #include "UserAccessibleData.h"

    void reactionRateModify(double *reacRateForward, double *reacRateBackward,
double T, unsigned int nSpe, double *zi, void *data)
{
      struct UserAccessibleData *udata = (struct UserAccessibleData *)data;
      unsigned int nReactions = udata->_reactionData._nReactions;
      int i;

          for (i = 0; i < nReactions; ++i)
  {
          reacRateForward[i] *= 2.0;
          reacRateBackward[i] *= 2.0;
  }

}
/*
     Register user-code functions
*/
    void uclib()
{
       ucfunc(reactionRateModify, "IndividualReactionRate", "reacRateModify");



}
```

Creating Custom Reaction Source Terms

When using user-coded reaction rates, it is strongly recommended to use the (default) Numerical option for Species Reaction Source Jacobian (under the **Reacting** > **Reacting System Properties** node). See Reacting System Properties. The functions `wdotJacCalculate()` and `wdotJacModify()` must be provided, with the following signature:

```
 void wdotJacModify(double *jac, double T, unsigned int nSpe, double *zi, void
*data)
```

The double array Jacobian, of size $(\texttt{nSpe}+1)^2$, is the Jacobian of the vector of the species source terms plus the temperature source term. The species source terms are the rate of change of specific mole fractions.

Ignitors

You can control the ignition of some combustion simulations in Simcenter STAR-CCM+ using ignitors.

When combustion models are selected that allow you to control ignition, a **Continuum** > **Ignitors** node appears. The **Ignitors** node allows you to select a specific type of ignitor according to the combustion physics models that are selected.

Spark ignition models are only available for unsteady simulations and grow a spark from a small kernel until it is sufficiently large enough for the combustion model to take over the flame propagation. For other ignitors, the mesh cells which are contained within the ignitor parts have their properties changed as specified by the ignitor when it is on. For more information about spark ignition models, see Spark Ignition Models Reference.

- **EBU Ignitor (EBU)**: When the EBU Ignitor is on, for the cells which are contained within the EBU ignitor parts, it forces reaction rates to be mixing limited without using products.
- **Fixed Temperature Ignitor (FT)**: When the Fixed Temperature Ignitor is on, the temperature that chemical reactions are evaluated at is set to the constant temperature defined in the **Ignitors** node. Reaction rates typically increase with temperature, so when the fuel and the oxidizer are present, cells evaluated at the fixed ignitor temperature burn reactants to products. Since only the chemical rates are accelerated in the ignitor zone, overall energy is conserved and the cell temperatures tend to the burnt (chemical equilibrium) temperature.
- **Flame Area Density Ignitor (FAD)**: When the Flame Area Density ignitor is on, it sets the method by which the model determines the final Flame Area Density (FAD) that the ignitor applies to its cells. When it is off, this ignitor does not affect the values of flame area density.
- **Progress Variable Ignitor (PV)**: When the Progress Variable Ignitor is on, it sets the value of the cells that are contained within the ignitor parts to that of the Ignitor Variable Value property that is set for the ignitor. When it is off, this ignitor does not affect the values of the progress variable.
- **Subgrid Spark Ignitor (SS)**: The Subgrid Spark Ignitor is available when either the Complex Chemistry model or Flamelet Generated Manifold model are selected along with the Spark Ignition physics model and any Unsteady model.

  See Subgrid Spark Ignition Models Reference.
- **ISSIM Spark Ignitor (ISSIM)**: The ISSIM Spark Ignitor is available when the Complex Chemistry model is selected along with the Spark Ignition physics model and any Unsteady model. This model is also available with Simcenter STAR-CCM+ In-cylinder when modeling internal combustion engines.

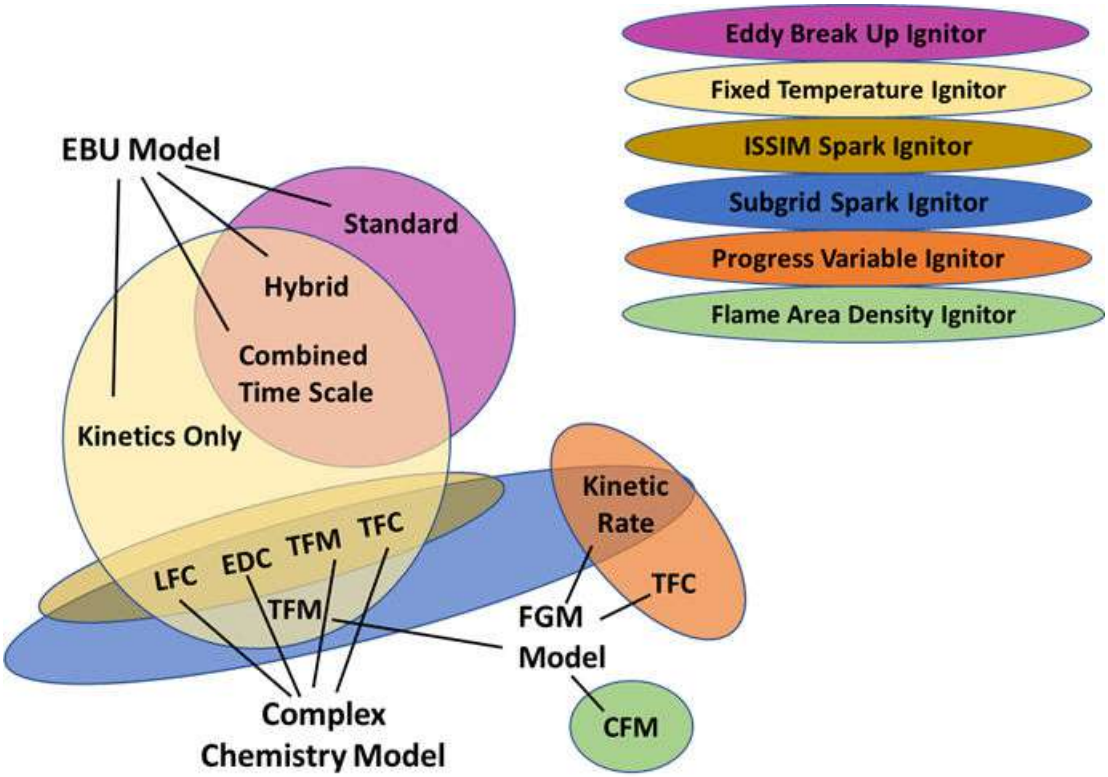
  See ISSIM Spark Ignition Model Reference.
- **FI Spark Ignitor**: The FI Spark Ignitor is only available with Simcenter STAR-CCM+ In-cylinder when modeling internal combustion engines.

  See FI Spark Ignition Model Reference.

Model		EBU	FT	FAD	PV	SS	ISSIM
Eddy Break-Up	Standard EBU	**Yes**	No	No	No	No	No
	Hybrid	**Yes**	**Yes**	No	No	No	No
	Combined Time-Scale	**Yes**	**Yes**	No	No	No	No
	Kinetics Only	No	**Yes**	No	No	No	No

Model		EBU	FT	FAD	PV	SS	ISSIM
Complex Chemistry	Laminar Flame Concept (LFC)	No	**Yes**	No	No	**Yes***	**Yes***
	Eddy Dissipation Concept (EDC)	No	**Yes**	No	No	**Yes***	**Yes***
	Thickened Flame Model (TFM)	No	**Yes**	No	No	**Yes***	**Yes***
	Turbulent Flame Speed Closure (TFC)	No	**Yes**	No	No	**Yes***	**Yes***
Flamelet Generated Manifold	FGM Kinetic Rate	No	No	No	**Yes**	**Yes***	No
	Coherent Flame Model (CFM)	No	No	**Yes**	No	No	No
	Turbulent Flame Speed Closure (TFC)	No	No	No	**Yes**	No	No
	Thickened Flame Model (TFM)	No	**Yes**	No	No	**Yes***	No

* When the Unsteady model is also used.



Ignitor Properties Lookup

Property	EBU Ignitor	Fixed Temperature Ignitor	Flame Area Density ignitor	Progress Variable Ignitor	All Spark Ignitors
Activator	✓	✓	✓	✓	See Spark Ignition Models Reference.
Ignitor Set Method			✓	✓	
Ignitor Variable Value			✓	✓	
Shapes	✓	✓	✓	✓	
Temperature	✓	✓			

Properties

Parts

Allows you to select the geometry parts that represent the ignitor.

Ignitor Variable Value

A floating point value for the progress variable.

Ignitor Set Method

Sets the method to determine the value of flame area density (FAD) in each cell.

Maximum of Cell FAD or Ignitor Constant

Uses the greater of the cell FAD that is obtained from the transport equation and the ignitor constant that is set with the Ignitor Variable Value property.

Ignitor Constant

Overrides the cell value of FAD using the Ignitor Variable Value. This option is helpful when you know the exact FAD value for one cell.

Activator

Selects between options that define when the ignitor is active (on).

- **Always**: Indicates that the Ignitor is always on.
- **Pulse**: Applies the ignition condition for the duration of a pulse that you specify using the properties of the **Pulse** child node:
  - *Ignitor Enabled Trigger*: For steady-state simulations, iterations are specified, and for unsteady simulations, physical time (s) is specified.
  - *Ignitor Starting Iteration/Time* : Iteration or time after which the ignitor is activated.
  - *Ignitor Ending Iteration/Time* : Iteration or time after which the ignitor is de-activated.

Reaction Mechanism Formats

Reaction data, thermodynamic properties, and transport properties are imported in the standard format.

- All species in gas phase and/or surface data files must have unique names.
- Lines in an input file that start with an exclamation mark (!) are regarded as comments.

Gas Chemistry Reaction Files

The gas phase data files state the chemical elements and species that are included in the mechanism. The elements and species are followed by a list of possible reactions that the species can participate in, and the corresponding variables, A, n (β in Eqn. (3431)), and E_a, that are used by the Arrhenius law Eqn. (3431) to calculate the rate constant (k in Eqn. (3423)) for each reaction.

```
ELEMENTS
  C  H  O  N AR
END
SPECIES
H                 O                 OH                HO2               H2O2
CH                HCO               CH2-P             CH2-S             CH2O
CH3               CH3O              CH2OH             CH3O2             CH4
CH3OH             CH3O2H            C2H               C2O               HCCO
C2H2              CH2CO             C2H3              CH2CHO            CH3CO
C                 CO                CO2               H2                H2O
O2                AR                N2
END
REACTIONS
!-------------------------------------------------------------------------------
!Reaction                                          A            n          Ea
!-------------------------------------------------------------------------------
H+O2=O+OH                                          2.000E+14    0.00   1.679E+04
O+H2=H+OH                                          5.100E+04    2.67   6.282E+03
OH+H2=H+H2O                                        1.000E+08    1.60   3.296E+03
OH+OH=O+H2O                                        1.500E+09    1.14   1.003E+02
H+HO2=OH+OH                                        1.500E+14    0.00   1.003E+03
H+HO2=H2+O2                                        2.500E+13    0.00   6.927E+02
H+HO2=O+H2O                                        3.000E+13    0.00   1.720E+03
O+HO2=OH+O2                                        1.800E+13    0.00  -4.060E+02
...                                                ...          ...    ...
END
```

When third-body reactions are specified in a mechanism, the reaction is written with an additional species M as a reactant, a product, or both. Auxiliary information regarding enhanced third-body efficiencies of certain species is given on the line below the reaction. The names of the third-body species are followed by their enhancement factors.

```
O+CO+M<=>CO2+M              1.800E+10    0.00   8600.00
H2/2.00/ O2/6.00/ H2O/6.00/ CO/1.50/ CO2/3.50/ AR/0.50/
```

Gas / Surface Thermodynamic Properties Files

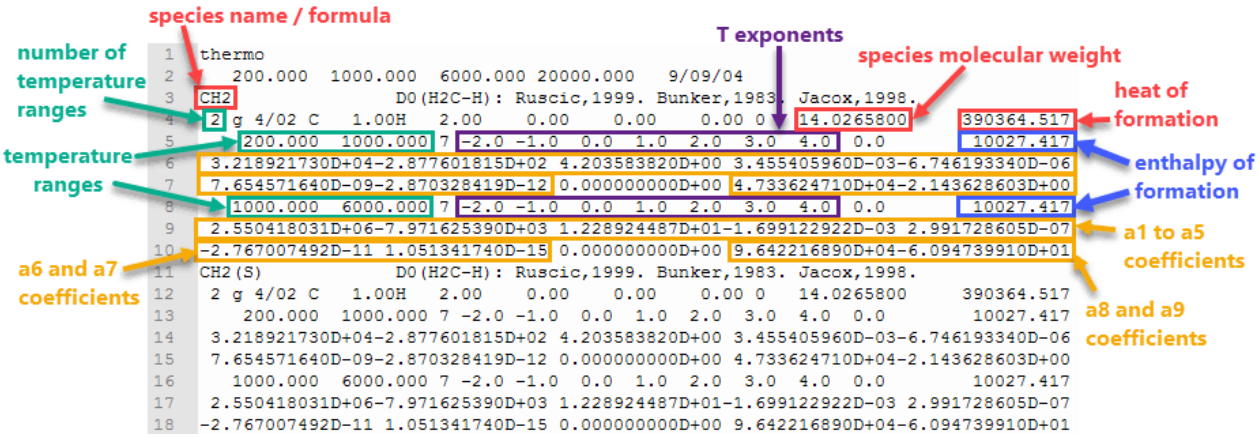
Thermodynamic properties are given in state function data files for either seven-coefficient or nine-coefficient NASA polynomial form for each species:

Seven-coefficient NASA polynomial format

- Line 1: The name of the species, the elemental composition of the species, three temperatures which define the temperature ranges over which the polynomial fits to thermodynamic data are valid. For example, the three temperatures (K) in the example below show the low temperature fit (298.000), the high temperature fit (5000.000), and the common temperature between these fits (1000.00).
- Line 2-4: Fourteen polynomial coefficients are provided (seven coefficients, a_1 through a_7, for two consecutive temperature ranges).

```
H                       H   1    0    0    0    298.000  5000.000 1000.00      1
 0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00    2
 0.25471620D+05-0.46011760D+00 0.25000000D+01 0.00000000D+00 0.00000000D+00    3
 0.00000000D+00 0.00000000D+00 0.25471620D+05-0.46011760D+00                   4
O                       O   1    0    0    0    298.000  5000.000 1000.00      1
 0.25420590D+01-0.27550610D-04-0.31028030D-08 0.45510670D-11-0.43680510D-15    2
 0.29230800D+05 0.49203080D+01 0.29464280D+01-0.16381665D-02 0.24210310D-05    3
-0.16028431D-08 0.38906960D-12 0.29147640D+05 0.29639950D+01                   4
OH                      H   1O   1    0    0    298.000  5000.000 1000.00      1
 0.28827300D+01 0.10139743D-02-0.22768770D-06 0.21746830D-10-0.51263050D-15    2
 0.38868880D+04 0.55957120D+01 0.36372660D+01 0.18509100D-03-0.16761646D-05    3
 0.23872020D-08-0.84314420D-12 0.36067810D+04 0.13588605D+01                   4
HO2                     H   1O   2    0    0    298.000  5000.000 1000.00      1
 0.40721910D+01 0.21312960D-02-0.53081450D-06 0.61122690D-10-0.28411640D-14    2
-0.15797270D+03 0.34760290D+01 0.29799630D+01 0.49966970D-02-0.37909970D-05    3
 0.23541920D-08-0.80890240D-12 0.17622730D+03 0.92227240D+01                   4
```

Nine-coefficient NASA polynomial format



For more information, see Using Thermodynamic Polynomial Data.

Gas Transport Properties Files

Gas phase transport properties are given (optionally) by a molecular data file which provides seven variables for each species in the mechanism:

- chemical name
- indicator for the structure of the species (0 = atom, 1 = linear molecule, 2 = non-linear molecule)
- two parameters describing the shape of the Lennard-Jones potential well:
  - well depth divided by Boltzmann's constant [K]
  - collision diameter [Å]—the (finite) distance at which the inter-particle potential is zero. (If you adjust this value, make sure that it realistically represents values given in literature for the specific material.)
- the bond dipole moment [Debye]
- the polarizability [Å3]
- the rotational collision number (ZROT) at 298 K

Since the molecular data is species-specific, you can use any file which contains data for all species in the gas or solid state phase. Molecular data files are not tied to a specific kinetic scheme.

```
H                 0 0.145D+03 0.205D+01 0.000D+00 0.000D+00 0.000D+00
O                 0 0.800D+02 0.275D+01 0.000D+00 0.000D+00 0.000D+00
OH                1 0.800D+02 0.275D+01 0.000D+00 0.000D+00 0.000D+00
HO2               2 0.107D+03 0.346D+01 0.000D+00 0.000D+00 0.100D+01
H2O2              2 0.107D+03 0.346D+01 0.000D+00 0.000D+00 0.380D+01
CH                1 0.800D+02 0.275D+01 0.000D+00 0.000D+00 0.000D+00
HCO               2 0.498D+03 0.359D+01 0.000D+00 0.000D+00 0.000D+00
...               . ...       ...       ...       ...       ...
```

Surface Chemistry Reaction Files

Surface data files contain relevant solid state data and look much the same as gas phase data files. In addition it contains data for the material of the surface, the surface sites, and the site density.

```
MATERIAL Pt1A1
SITE/PLATINUM    SDEN/3.28E-008/
  PT(S) O(S) NO2(S) NO(S)
END
REACTIONS
!-------------------------------------------------------------------------------
!Reaction                    A          n        Ea
!-------------------------------------------------------------------------------
O2+2PT(S)=2O(S)             4.900E+18    0.00   3.040E+01
   Rev                      3.100E+22    0.00   2.094E+02
NO+PT(S)=>NO(S)             6.300E+12    0.00  -2.350E+01
NO(S)=>NO+PT(S)             1.060E+16    0.00   1.155E+02
NO2+PT(S)=>NO2(S)           6.710E+12    0.00   0.210E+00
NO(S)+O(S)=NO2(S)+PT(S)     3.300E+20    0.00   1.273E+02
...                         ...           ...    ...
END
```

Keywords

All Input Files

The following keywords are accepted in all types of input files.

BULK

Precedes lines with surface bulk species in the mechanism. You can specify this keyword immediately before a custom name for the bulk data.

ELEMENTS / ELEMENT / ELEM

Precedes lines with elements of the species in the mechanism.

END

Required on the line below the data which follows each of the above keywords.

MATERIAL

Precedes the name of the material that the subsequent surface data corresponds to. You can state more than one material, where each material is followed by material-specific surface data.

REACTIONS / REAC

Precedes lines with reaction data for all reactions in the mechanism.

- To set the unit of E_a in the mechanism, follow this keyword with one of:
  - CAL/MOLE
  - KCAL/MOLE
  - JOULES/MOLE
  - KELVINS
  - EVOLTS
- To set the unit of A in the mechanism, follow this keyword with one of:
  - MOLES
  - MOLECULES

Units for E_a and A can be set on the same line. If no unit is specified, data is assumed to be given in cal/mole.

If you specify the unit of A in the mechanism as MOLECULES, then upon importing the mechanism, the pre-exponential factors are converted to the moles unit system by the equation:

$$A_j\big(MOLES\big) = A_j\big(MOLECULES\big) \times {N_A}^{n-1} \tag{285}$$

where:

- A_j is the pre-exponential factor of the jth reaction
- N_A is the Avogadro number
- n is the sum of reactant stoichiometric coefficients, also referred to as the reactant order.

SDEN

Standard-state density for the site in units of moles/cm².

SITE

Precedes lines with surface species in the mechanism. SITE must be followed by the SDEN keyword.

You can specify this keyword immediately before a custom name for the site data.

SPECIES / SPEC

Precedes lines with species in the mechanism.

THERMO ALL

Same as THERMO but shows that all state functions data of the mechanism is found after the keyword and not in additional sections of the mechanism.

THERMO / THERM

Precedes lines with state function data in the mechanism.

Gas Input Files

The following keywords are only accepted in gas phase data input files.

DUPLICATE / DUP

If a reaction path can have multiple sets of reaction coefficients, follow each set by a line with this keyword.

FORD

In order to alter the forward rate of a specific reaction, you use this keyword on the line below the specific reaction, followed by a species name and reaction order. Specifying a reaction order in this way replaces existing reaction orders or adds new species and reaction orders to the reaction rate calculation.

HIGH

Placed on the line below a pressure-dependent, chemically activated bimolecular reaction, followed by reaction coefficients for the high-pressure limit: A_∞, β_∞, and E_∞ in Eqn. (3444).

LOW

Placed on the line below a pressure dependent fall-off reaction, followed by reaction coefficients for the low-pressure limit: A_0, β_0, and E_0 in Eqn. (3443).

PLOG

Given after a reaction, this keyword is followed (within forward slashes) by its corresponding pressure ranges, in units of bar, with pre-exponential factors, temperature exponents, and activation energies in Eqn. (3450).

REV

For one-way reactions, you can specify this keyword on the line below a reaction followed by reaction data for the reverse reaction.

RORD

In order to alter the reverse (backwards) rate of a specific reaction, you use this keyword on the line below the specific reaction, followed by a species name and reaction order. Specifying a reaction order in this way replaces existing reaction orders or adds new species and reaction orders to the reaction rate calculation.

SRI

For SRI pressure dependent reactions, this keyword is placed on a separate line after the keywords LOW and HIGH. This keyword is followed by five parameters: a, b, c, d, and e in Eqn. (3447).

TROE

For Troe pressure dependent reactions, this keyword is placed on a separate line after the keywords LOW and HIGH. This keyword is followed by four parameters: α, $T*$, $T**$, and $T***$ in Eqn. (3446).

Surface Input Files

The following keywords are only accepted in surface data input files.

COV

This keyword followed by a species and three coverage parameters, $\eta_{i,j}$, $\mu_{i,j}$, and $\varepsilon_{i,j}$, modifies the forward reaction rate constant according to Eqn. (3465).

DUPLICATE / DUP

If a reaction path can have multiple sets of reaction coefficients, precede each set by a line with this keyword.

FORD

In order to alter the forward rate of a specific reaction, you use this keyword on the line below the specific reaction, followed by a species name and reaction order. Specifying a reaction order in this way replaces existing reaction orders or adds new species and reaction orders to the reaction rate calculation.

REV

For one-way reactions, you can specify this keyword on the line below a reaction followed by reaction data for the reverse reaction.

RORD

In order to alter the reverse (backwards) rate of a specific reaction, you use this keyword on the line below the specific reaction, followed by a species name and reaction order. Specifying a reaction order in this way replaces existing reaction orders or adds new species and reaction orders to the reaction rate calculation.

STICK

To use sticking coefficients instead of reaction coefficients, provide this keyword without parameters on the line below a reaction. Replace the reaction variables (A, β, and E_a in Eqn. (3431)) of the preceding reaction by sticking coefficients: a_i, b_i and c_i in Eqn. (3466).

Mesh Adaption for Reacting Flows Reference

When the Adaptive Mesh model is selected alongside a combustion model, the Mesh Adaption for Reacting Flows option is available as an adaptive mesh criterion.

The Adaptive Mesh model refines and coarsens cells in flame zones based on the secondary gradient of selected combustion variables, such as species mass fraction, or mixture fraction and progress variable.

Mesh Adaption for Reacting Flows Reference

Example Node Path	**Continua** > **Physics 1** > **Models** > **Adaptive Mesh** > **Adaptive Mesh Criteria** > **Mesh Adaption for Reacting Flows**
Requires	*Space*: **Three Dimensional** *Time*: any *Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: any (except ICE models).
Properties	See Mesh Adaption for Reacting Flows Properties.

Activates	Model Controls (child nodes)	Variables.
	Field Functions	Error Indicator of [variable].

Mesh Adaption for Reacting Flows Properties

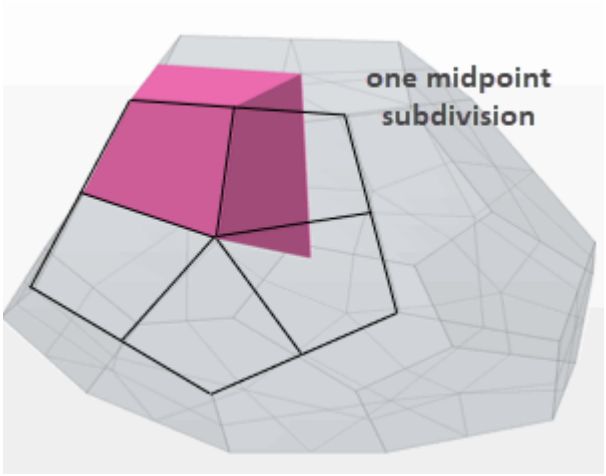
Max Refinement Level

Sets the maximum limit on the number of times a cell can be refined in a simulation.

One refinement level for a cell means one step of midpoint subdivision. The resulting number of child cells are equal to the vertices of the parent cell.

For trimmed cells, one refinement level means 8 subdivided child cells from one parent cell as shown in the image below:

For poly cells, the midpoint subdivision results in as many child cells as there are vertices in the parent cell, that is, typically 12-15 child cells. One example is shown in the image below:



The refinement level increases or decreases only by one level in each adaption—mesh adaption is a successive procedure.

Variables

Variables

The following table shows which variables are available with which combustion models.

Variables	**Complex Chemistry / EBU models**	**FGM model**	**SLF / Chemical Equilibrium**	**Any other combustion model**
Mixture Fraction 0		✓*	✓*	
Progress Variable		✓*		
Temperature	✓	✓	✓	✓*
[species] H2O and OH (if present) are selected by default. Other species are also available.	✓*			

* default variables

Error Indicator Limits

The error indicator limits are available to set for each variable as a scalar range `[low, high]`. The Adaptive Mesh model calculates the error indicator (EI) as the output of the secondary gradient of the selected *Variables* and uses the error indicator limits to determine if cells are marked for refinement as follows:

- If EI > `high`, cells are marked for refinement.
- If EI < `low`, cells are marked for coarsening (cannot be coarser than the starting mesh).
- If `low` <= EI <= `high` , cells are kept unchanged.

Default `[low, high]` values are suitable for most cases. Otherwise, follow these guidelines:

Requirement	**Action**
Adapt fewer cells.	Increase the `high` limit, and optionally also increase the `low` limit.
Adapt more cells.	Lower the `high` limit, and optionally also lower the `low` limit.

If several adaptive mesh criteria are active at the same time, their relative influence on the adaptive mesh refinement is prioritized as follows:

- Refine and Coarsen → Refine
- Refine and Keep → Refine
- Keep and Coarsen → Keep

By this approach a finer mesh takes precedence over a coarse mesh.

Field Functions

Error Indicator of [variable]

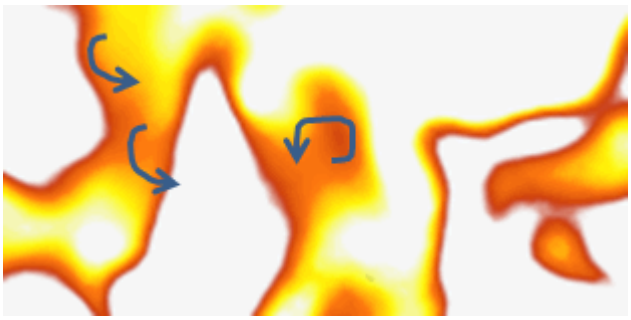
EI, a normalized second gradient, is used to determine if the adaptive mesh model refines or coarsens cells based on `[low, high]` values that are specified for each selected variable.

For more information on Adaptive Meshing, see Adaptive Mesh Refinement.

Reacting Species Transport

When using Reacting Species Transport models, Simcenter STAR-CCM+ solves transport equations for the mass fractions of all species that are involved in the chemical reactions. These species mass fractions are passed to a separate chemistry solver that returns the amount of product.

In the following diagram, the dark area shows a thick reaction front (where the reactions occur). Since some reactions happen slower than turbulent mixing, the turbulent mixing causes some slowly-reacting intermediate species to escape this thick reaction front and continue mixing further downstream.



The Reacting Species Transport models include:

- Complex Chemistry: for simulating reacting flow using detailed mechanisms within a turbulent flame in which kinetic phenomena are significant.
- Eddy Break-Up (EBU): for simulating reacting flow with a simple (one or two step) mechanism, where kinetic phenomena are not significant.
- Eddy Contact Micromixing
- Thickened Flame Model (TFM)
- Polymerization

Use the Reacting Species Transport workflow for simulating reacting flow within a multi-component liquid or within a gas-phase turbulent flame.

Complex Chemistry

The Complex Chemistry model employs a stiff solver to integrate the chemistry over a time-step, and uses techniques, such as Clustering, Dynamic Mechanism Reduction, In-Situ Adaptive Tabulation (ISAT), and Acceleration Factor Control to mitigate this expense. Since the Complex Chemistry model uses a detailed mechanism, you can model kinetic phenomena—such as flame ignition, slowly forming pollutants, flame quenching, and extinction. Complex chemistry mechanisms are usually imported in Chemkin format.

This model offers the most general approach in modeling finite-rate kinetics. Use this model if other models do not capture the finite-rate effects that drive the process.

The Complex Chemistry model has submodels for simulating turbulence-chemistry interactions—the Laminar Flame Concept (LFC), the Eddy Dissipation Concept (EDC), and the Turbulent Flame Speed Closure (TFC) model.

The LFC and EDC turbulence-chemistry interaction models are informal Thickened Flame Models (TFMs) since the local turbulent diffusivity acts similarly to the TFM, to thicken the flame and increase the flame propagation speed over the laminar value. However, when using the LFC model or EDC model, the turbulent

flame speed is very sensitive to the mesh size—although it is possible to control this speed by changing the diffusivity (using the turbulent Schmidt number), it is generally impractical. Instead, the TFC model is available for modeling premixed and partially-premixed flame fronts where the propagation speed of the flame is explicitly specified.

- Laminar Flame Concept: Evaluates the instantaneous reaction rate at the mean temperature, pressure, and species mass fraction—which, for steady-state, corresponds to integrating the chemistry with respect to the residence time in a cell. The LFC model is appropriate for premixed, partially premixed, and unsteady flames.
- Eddy Dissipation Concept: Integrates chemistry for a time-scale close to the Kolmogorov (smallest eddy) time-scale in a cell. The EDC model is appropriate for steady-state diffusion flames, which gives a lower reaction rate than with the LFC model.
- Turbulent Flame Speed Closure: Identifies premixed flame fronts and propagates these fronts at the specified turbulent flame speed. The TFC model is appropriate for modeling turbulent flames with premixed and partially-premixed flame fronts.

These models account for turbulent-chemistry interaction through the enhanced diffusivity of the turbulence model. You can adjust the flame position by changing the turbulent Schmidt number.

Eddy Break-Up Model

The Eddy-Break-Up model assumes that reactions are limited by the rate that turbulence can mix the reactants and heat into the flame zone. The EBU model limits kinetic reaction rates by the large-scale turbulent mixing rate. Since kinetic rates are replaced by a single turbulent mixing rate, use only small mechanisms with one or two steps. The EBU model is a flame position model and is not intended for modeling kinetically dominated phenomena such as ignition and pollutants.

If kinetic data exist, you can choose between the combined time scale model and hybrid model. These models account for finite-rate kinetic effects—required for premixed flames where turbulence would otherwise ignite the mixture before the flame holder. However, for diffusion flames that are purely turbulence-controlled, the standard EBU model is adequate and efficient.

Eddy Contact Micromixing Model

The Eddy Contact Micromixing Model is a combustion model for liquids. In liquids, where species diffusivities are typically small and molecular mixing time-scales are long, the Eddy Contact Micromixing model accounts for diminished molecular diffusivity in the turbulent mixing rate by reducing the reaction rate. The Eddy Contact Micromixing model is a variant of the EBU model.

Thickened Flame Model

Premixed laminar flames are typically very thin relative to the mesh size. Since the flame speed is determined by diffusion and reaction inside the flame, accurate flame speed prediction requires sufficient resolution of the internal flame structure. One approach to overcome this stringent resolution requirement for Large Eddy Simulations is to use the TFM model, where the premixed flame front is artificially thickened by increasing the local diffusivity, so that the flame can be resolved on the mesh.

Polymerization Model

The Polymerization model is a dedicated model for simulating liquid polymerization processes—either in a multi-component liquid, or as a multi-component liquid phase in a Eulerian multiphase simulation. It tracks the polymer size distribution for live and dead polymers.

Polymerization is the process of creating long-chain molecules by chemically combining large numbers of small monomer molecules. This process starts by mixing monomer and initiator molecules in a solvent. The process of polymerization is comprised of several chemical reactions, such as initiation, propagation, chain transfer, chain branching, scission, and termination, that involve radicals of different chain lengths.

The polymerization model in Simcenter STAR-CCM+ simulates free-radical polymerization and uses Method of Moments to describe the size distribution of the polymers.

Reacting Species Transport Model Ignitors

When the Complex Chemistry, EBU, or TFM models are selected, a **Continuum** > **Ignitors** node appears which allows you to control ignition.

The Complex Chemistry, EBU, or TFM models allow you to create a Fixed Temperature Ignitor. When active, a Fixed Temperature Ignitor applies a constant temperature for the cells that are contained within the ignitor parts.

In addition to the Fixed Temperature Ignitor, the EBU model also provides the EBU Ignitor. When the EBU Ignitor is on, for the cells which are contained within the EBU ignitor parts, the ignitor forces reaction rates to be mixing limited without using products.

The type of ignitor that is available for the EBU model depends upon the setting that you select for the EBU Reaction Control property.

EBU Reaction Control Property Setting	EBU Ignitor available?	Fixed Temperature Ignitor available?
Standard EBU	Yes	No
Hybrid	Yes	Yes
Combined Time-Scale	Yes	Yes
Kinetics Only	No	Yes

For more details, see the specific combustion model reference page.

Contents:

Chemistry Acceleration

You can use Clustering, ISAT, or Dynamic Mechanism Reduction methods to speed up Complex Chemistry calculations.

The following are chemistry acceleration options:

- Clustering
- In Situ Adaptive Tabulation (ISAT)
- Dynamic Mechanism Reduction

The Relax to Chemical Equilibrium model is not an acceleration option, however, you can use it to provide a quick approximate solution for detailed chemistry computations. See Relax to Chemical Equilibrium.

Clustering

The clustering method groups cells with similar thermal and chemical states before integrating the averaged state for the group. The reaction mapping is then interpolated back to the cells assuming the net reaction rate of all cells in the cluster is the same as the cluster average.

Clustering usually provides a substantial speed-up as the number of clusters is less than the number of cells in the simulation. Since the number of clusters increases much slower than the number of cells, clustering performance improves with mesh size.

The clustering algorithm uses a uniform N-dimensional grid, where N is the number of clustering variables. The cells in the simulation are then binned into each clustering grid. By default, Simcenter STAR-CCM+ uses three clustering variables for unsteady simulations, namely equivalence ratio, temperature, and mass fraction of OH. For steady-state simulations, the log of the chemical time scale is used as an additional clustering variable.

Simcenter STAR-CCM+ provides other user-selectable clustering variables, including other species mass fractions, mixture fraction, pressure, enthalpy, and entropy.

The default clustering variables of equivalence ratio and temperature represent the underlying trajectory of mixing followed by reaction. These default clustering variables are suitable for most hydrocarbon combustors. However, there are cases where careful selection of additional clustering variables can improve accuracy. For example, for slowly forming NO formation behind a premixed flame front, where the equivalence ratio and temperature are nearly uniform, you can add the NO species mass fraction to the clustering variables list. For supersonic combustion with shock-waves, you can include the pressure variable since the pressure changes substantially through the domain.

You can view the clusters that Simcenter STAR-CCM+ generates by visualizing the Clustering Index. Each cluster has its own unique index, with the maximum value representing the total number of clusters. A Clustering Index of zero represents cells that are excluded from the reaction, such as cells with temperatures that are below the Minimum Temperature that is required for reactions. The Clustering Equivalence Ratio and Clustering Mixture Fraction are also available for post-processing.

In Situ Adaptive Tabulation (ISAT)

In Situ Adaptive Tabulation (ISAT) is a tabulation method in which computationally expensive functions are tabulated and then interpolated at run time. In this case, the stiff chemistry ODEs (ordinary differential equations) are tabulated. If there are many thermo-chemical states that are similar in time and/or space, ISAT can reduce simulation times. ISAT can substantially speed up complex chemistry simulations for steady state problems (including unsteady LES of steady combustion) in which the tabulated chemistry mappings are regularly retrieved and mechanisms have less than 40 species. However, it is not recommended to use the ISAT method for complex chemistry internal combustion engine (ICE) simulations due to the fluctuations in chemical states such as pressure.

Dr. Stephen B. Pope developed the ISAT method [784].

The ISAT tables are created at a constant pressure and time-step. If the pressure or time-step in the domain varies (as occurs in steady simulations), the ISAT solver bins the pressure and time-step values into appropriate ranges automatically, creating one table per bin.

The ISAT method approximates the solution of the ODE for a given initial condition through:

- The thermodynamic variable (sensible enthalpy)
- The composition variable (specific molar number)
- The absolute pressure and time-step (depending on the type of simulation)

You can use ISAT to retrieve approximate values for multi-dimensional functions that are expensive to compute. In reacting simulations, you can use ISAT to store and retrieve approximate reaction mapping solutions from a system of coupled ODEs. During the chemistry step, the ISAT solver computes the reaction mapping in a particular cell. ISAT searches the table for an existing point with which to approximate the reaction mapping within the specified error tolerance. If ISAT finds such a point, then the new reaction mapping is not calculated with the CVODE solver, but rather interpolated based on the stored reaction mapping in the table. Otherwise, if ISAT cannot find a suitable point in the table, the CVODE solver is called, and a reaction mapping for this point is calculated. This newly calculated point is stored in the table. The size of the table therefore grows as the simulation progresses. See Complex Chemistry.

Dynamic Mechanism Reduction

When using the Complex Chemistry model, you can choose to allow the CVODE solver in Simcenter STAR-CCM+ to solve for a reduced number of species that are taken from the full chemical mechanism that is imported. The mechanism is reduced dynamically—in every cell at every time-step or iteration. Solving for fewer species reduces computational time, however, accuracy is also reduced. Dynamic Mechanism Reduction is based on the Directed Relation Graph (DRG) algorithm [773] where species that do not change any other species substantially over the each time-step or iteration are eliminated from the mechanism. See Dynamic Mechanism Reduction.

You provide the inputs for the DRG algorithm—a tolerance and a small set of target species, which are retained in the mechanism. If the species, NO, is present in a mechanism, it is automatically included in the target species.

Reacting Species Transport Workflow

Use this workflow for simulating multi-component liquid reactions or gas-phase turbulent flames which involve kinetic phenomena such as flame ignition, slowly forming pollutants, flame quenching, and extinction.

The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow.

Note: If you are modeling Reacting Channels, follow the Reacting Channels Workflow—even when using a reacting species transport model. See Reacting Channels Workflow.

1. For the physics continuum or phase that represents the reacting flow, select the following models—in addition to the models that are previously selected, with **Auto-Select recommended models** activated:

Group Box	Model
Reacting Flow Models	**Reacting Species Transport**

Group Box	Model
Reacting Species Models	◦ For multi-component gas turbulent flames with a large mechanism: **Complex Chemistry** ◦ For multi-component liquid-liquid reactions limited by finite-rate kinetics: **Complex Chemistry** ◦ For multi-component liquid or gas reactions with a simple mechanism: **Eddy Break-Up** ◦ For multi-component liquid or gas reactions which are slow: **Eddy Break-Up** with the *Kinetics Only* property activated. ◦ For multi-component liquid reactions with a simple mechanism in which the chemical reactions are fast (molecular mixing time-scales are long): **Eddy Contact Micromixing**
Turbulence Chemistry Interactions (for Complex Chemistry)	◦ For turbulent flames with premixed or partially-premixed flame fronts: **Turbulent Flame Speed Closure** ◦ For steady-state diffusion flames: **Eddy Dissipation Concept** ◦ For premixed, partially-premixed, and unsteady flames, or slow reactions: **Laminar Flame Concept**

2. Select any Optional models.

   For example:

   - **NOx Emission** or **Soot Emissions**—to model the formation of these pollutants.
   - **Fluid Film**—to model intraphase or interphase reactions such as in trickle-bed reactors, or selective catalytic reduction (SCR) reactions in urea film. See Modeling Fluid Film.
   - The **Radiation** model is useful for modeling applications in which radiative heat transfer is important, as is the case for most combustion systems. The soot emission models influence the **Participating Media Radiation (DOM)** and **Gray Thermal Radiation** models by contributing to the absorption coefficient of the continuous phase (the absorption coefficient describing both absorption and emission).
   - **VOF**—Useful for modeling multi-phase reacting flow applications where two phases co-exist with a distinct interface, such as glass furnaces.
   - **Gravity**—Use when gravity forces significantly influence the solution, for example in fire simulations.

3. If using Emissions models or Surface Chemistry, follow the specific workflow before continuing with the following steps.
   See Emissions Workflow, or Surface Chemistry Workflow.

4. Define the parameters of the Reacting Species physics/phase model:

   Note: It is possible to specify several combustion model constants as parameters. See Global Parameters.

   - For the Complex Chemistry model, define the properties of the Complex Chemistry model and its sub-nodes.
     a. Select the **Models** > **Complex Chemistry** node and set the required Properties.
        The CVODE solver calculates reaction rates and solves complex chemistry problems in Simcenter STAR-CCM+.

b. Select the **Complex Chemistry** > **Chemistry Acceleration** node and, if required, activate the necessary acceleration options:
   - *Clustering* (activated by default)
   - *Dynamic Mechanism Reduction*
   - *ISAT* (not compatible with Dynamic Mechanism Reduction and not advised with Clustering)

   Then define the acceleration option Properties, see Chemistry Acceleration Properties.

c. To relax species to their equilibrium compositions over a set time-scale, select the **Complex Chemistry** > **Approximation Options** node and activate *Relax to Chemical Equilibrium*. Select the **Approximation Options** > **Relax to Chemical Equilibrium** node and set the Properties.

For more information, see Complex Chemistry Model Reference.

- For the Eddy Break-Up (EBU) or Eddy Contact Micromixing (ECM) model, define the EBU or ECM properties.
  - The EBU property, *Reaction Control*, is set to **Hybrid** by default—which is appropriate for most simulations. Hybrid specifies the reaction rate as the smaller of the two rates that are predicted by turbulent mixing and finite-rate chemical kinetics. However, if the rate is determined solely by the turbulent mixing scale, select **Standard EBU** instead.

  See Eddy Break-Up Model Reference or Eddy Contact Micromixing Model Reference.

5. Import or create the mechanism which represents the reacting flow reactions.
   - For Complex Chemistry, import the complex chemistry definition using the **Models** > **Complex Chemistry** node. It is possible to create the mechanism using the **Models** > **Reacting** > **Reactions** node—however, this approach is impractical, as most Complex Chemistry definitions are too large. You can find chemical mechanisms that are developed by academia on university websites worldwide.
   - For EBU or ECM, create or import reactions using the **Models** > **Reacting** > **Reactions** node.

   See Importing Species and Reactions.
6. Specify the properties of the turbulence-chemistry interactions models.
   - When using the Turbulent Flame Speed Closure (TFC) model, set the turbulent flame speed method (see Turbulent Flame Speed) and define the properties of the TFC model.

     The TFC model simulates thin flames which can cause rapid density changes associated with larger normal stresses. Normal stresses are by default neglected in turbulence kinetic energy, which causes unphysically high levels of turbulence which results in fuel-consumption rates that are too fast. Therefore, it is also recommended to activate the *Normal Stress Term* property for the turbulence model (see Normal Stress Term).
   - When using the Eddy Dissipation Concept model, or the Laminar Flame Concept model, you can adjust the flame position by changing the **Multi-Component Gas** > **Material Properties** > **Turbulent Schmidt Number**.
7. Set the parameters of any other **[continuum]** > **Models** or **[phase]** > **Models**, as required.
8. Return to the Reacting Flow General Workflow.

Polymerization Workflow

Polymerization processes involve various chemical reactions during which monomer molecules combine to form polymer chains. These processes require the reacting species transport physics model in Simcenter STAR-CCM+.

The steps in this workflow are intended to follow on from the Reacting Flow General Workflow (or, where applicable, from Interphase Workflow: Multiphase).

1. For the physics continuum (or Eulerian phase) that represents the reacting flow, select the following models—in addition to the models that are previously selected, with **Auto-select recommended models** activated:

Group Box	Model
Enabled Models	**Reacting Species Transport** (selected automatically when following the Reacting Flow General Workflow)
Reacting Species Models	**Polymerization**

2. Select any Optional models that are also required.

The process of polymerization is comprised of several sub-reactions which include free radical polymer reactions. Free radicals are small, charged molecules that react with monomers and create charged monomers. The charged monomers then combine with other monomers and form a polymer chain. Throughout the polymerization process, free radical polymer reactions consume and create free radicals at different rates. In Simcenter STAR-CCM+, you can specify which free radical polymer reactions occur and define the rates.

3. Set the free-radical polymer reaction properties.
   a) Expand the **[Continuum]** > **Models** > **Polymerization** > **Free-Radical Polymer Reactions** node.
   b) To define the reaction rate for a free-radical polymer reaction, select the required free-radical polymer reaction sub-node and set the **Method** that you require as a scalar profile.
   c) Define the *Unit System* property appropriate to the reaction.
   d) If you do not wish to specify the reaction rate for any of the free-radical polymer reactions, select the relevant sub-node and:
      - Set the **Method** property for the sub-node to **Constant**.
      - Set *Value* to 0.0.

The **Polymer Scalars** and **Polymer Moments** sub-nodes allow you to specify User Rate and User Rate Jacobian source terms directly to the Polymer Scalar and Polymer Moment equations.

4. If you intend to specify User Rate or User Rate Jacobian source terms:
   a) Select the **Polymerization** node and activate the property, *User Rates*.
      The **Polymer Scalars** and **Polymer Moments** sub-nodes become populated.
   b) Set the **User Rate** and / or **User Rate Jacobian** values for the **Polymer Scalars** and **Polymer Moments** as required.
5. Set the remaining Polymerization model Properties as required.
   See: Polymerization Model Reference.
6. Specify the Liquid Components and Material Properties of the Multi-Component Liquid.

a) Right-click the **[Continuum]** > **Models** > **Multi-Component Liquid** > **Liquid Components** node and select one of the following options:

- Import Species.

  In the dialog that appears, **Browse** to and select the file which contains the monomer species that you are importing.
- Select Mixture Components.

  Browse the Standard Materials Database that appears and select the liquid components that represent the monomers. Click **Apply** then **Close**.

For more information, see Managing Mixture Components.

b) Expand the **Multi-Component Liquid** > **Liquid Components** node and define the material properties as required.

For more information, see Setting Material Properties Methods.

7. Set the parameters of any other **[Continuum]** > **Models**, as required.
8. For the continuum, define any necessary parameters for the **Reference Values** and **Initial Conditons**.

   Set the Initial Condition concentrations for the **Polymer Initiator**, **Polymer Monomer**, **Polymer Radical**, **Polymer Solvent**, and**Polymer Modifier** scalars.
9. Define any necessary Physics Conditions and Values for the Region and Boundaries.

   For the Inlet boundaries, expand the **Physics Values** node and set concentrations for the **Polymer Initiator**, **Polymer Monomer**, **Polymer Radical**, **Polymer Solvent**, and**Polymer Modifier** using scalar array profiles.
10. If necessary, set up Injectors. For example, if any of the polymerization reaction components are injected into the domain.

    See: Working With Injectors.
11. Return to the Reacting Flow General Workflow.

Reacting Species Transport Reference

This section provides reference material, including properties, sub-nodes, field functions, and other model-specific settings, for all of the reacting species transport models.

Contents:

Complex Chemistry Model Reference

The Complex Chemistry model requires gas-phase or liquid-phase chemical mechanisms which typically contain tens or hundreds of species, with hundreds or thousands of reactions. Since different species evolve at different rates, the kinetics are termed stiff, and integrating the reaction step is computationally expensive.

Theory	See Complex Chemistry	
Provided By	**[physics continuum]** > **Models** > *[Combustion Models]*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Complex Chemistry**	
Requires	*Material*: **Multi-Component Gas** or **Multi-Component Liquid** *Reaction Regime*: **Reacting** *Reactive Flow*: **Reacting Species Transport**	
Properties	Key properties are: **Source Enabled Trigger**, **Begin**. See Complex Chemistry Properties.	
Specific Right-Click Actions	See Right-Click Actions.	
Activates	Physics Models	*Turbulence Chemistry Interactions* See Turbulence-Chemistry Interactions Model Reference.
	Model Controls (child nodes)	Approximation Options, Chemistry Acceleration , CVODE, Acceleration Factor Control.
	Region Settings	Active Reactions
	Report Options	Chemistry Acceleration Factor, Complex Chemistry Quantity Parallel Max, Complex Chemistry Quantity Parallel Min, Complex Chemistry Quantity Parallel Sum. See Reports.
	Other Continuum Nodes	The **Ignitors** node provides the right-click option to create a **Fixed Temperature Ignitor**, **ISSIM Spark Plug**, or a **Subgrid Spark Ignitor**. See Ignitors.
	Field Functions	Chemistry Heat Release Rate, Chemistry Time Step, Clustering Equivalence Ratio, Clustering Index, Clustering Mixture Fraction, Number of DMR Retained Species. See Field Functions.

Complex Chemistry Model Properties

Source Enabled Trigger

Controls whether Simcenter STAR-CCM+ starts calculating the chemistry at the time-step, iteration, or physical time that you specify in the *Begin* property, or whether this model never contributes any sources.

Begin

Specifies the iteration, time-step, or physical time after which the reactions are activated. Before this iteration, time-step, or physical time, reactions are deactivated. Specifying a physical time [degCA] allows you to activate chemistry sources just before spark ignition. When specifying it as an expression which

varies during the simulation, reactions are only active when the current iteration, time-step, or physical time is higher than the value provided by the expression.

Minimum Temperature For Reactions

Below this temperature, chemical reactions are deactivated.

Reaction Rate Multiplier

Tuning parameter that multiplies every reaction rate r_k in Eqn. (3424) by this value. You can use this parameter to adjust the rate of chemical reactions which determine kinetic phenomena such as ignition delay times and premixed flame speeds.

Dynamic Load Balancing

When activated, dynamic load-balancing is turned on for complex chemistry calculations.

Right-Click Actions

Import Chemistry Definition (Chemkin format)

Activates an *Import Chemkin Files* dialog that allows you to import a chemical mechanism file, thermodynamic properties file, and optionally a transport properties file.

If you are using the Surface Chemistry model, the *Import Chemkin Files* dialog also allows you to import surface chemical mechanism files and surface thermodynamic properties files—you can select more than one of each.

Upon importing a chemistry definition, the reactions for the definition appear as sub-nodes of the Chemistry Definition node.

Delete Chemistry Definition

Removes the reactions, and optionally the species, that are used for the chemistry definition. Upon deletion, in the *Output* window, Simcenter STAR-CCM+ notifies from which regions, boundaries, or interfaces, the reactions are removed.

Delete Species?	
Activated	All species and related properties from the mechanism are deleted.
Deactivated	All species and their related properties are maintained and are not overwritten when importing another Chemkin mechanism (any additional species are added—none are removed).

Region Settings

Applies to all regions:

Active Reactions Option

Activates or deactivates chemical reactions in this region.

Complex Chemistry Reports

Chemistry Acceleration Factor

When the **Acceleration Factor Control** property, *Automatic Control*, is activated, the chemistry acceleration plot shows the varying level of acceleration—between 0.0 (full ω_i source term linearization—which is slow to run) and 1.0 (no ω_i source term linearization—which is faster to run, but less stable).

The following Complex Chemistry reports take a particular value and perform a global operation (maximum, minimum or sum) over all of the processors. For a serial run, all three types of reports report the same value. Several of the Complex Chemistry Variable options only produce reports with values when ISAT is used. If ISAT is not available, these reports have a zero value.

Complex Chemistry Quantity Parallel Max

Complex Chemistry Quantity Parallel Min

Complex Chemistry Quantity Parallel Sum

Complex Chemistry Reports Properties

The maximum, minimum or sum reports have the following properties available:

Units

The units that are used for specifying the quantity.

Complex Chemistry Variable

Allows you to choose the type of Complex Chemistry Variable to plot.

- **None**
- **CPU Time**: The time that the CPU takes for complex chemistry calculations with the ODE solver.
- **Elapsed Time**: The time that has elapsed during complex chemistry calculations with the ODE solver.
- **Adds**: The number of points that have been added to the table. (ISAT only).
- **Grows**: The number of points in the table that have increased their region of accuracy. (ISAT only).
- **Retrieves**: The number of points that are retrieved from the ISAT table; these retrieves avoid expensive direct ODE solver calculations (ISAT only).
- **Direct Evaluations**: The number of points that are calculated by calling the ODE solver. (ISAT only).
- **Table Size**: The ISAT table size.
- **Queries**: The total number of queries given to ISAT.
- **Direct ODE Queries**: The number of queries that result in direct ODE solver calculations. Low values in this report reflect a good setup of ISAT parameters.

Variable Accumulation Type

Format of displayed value for those Complex Chemistry Variables that report a value of time.

- **Cumulative**:
  The time taken for the complex chemistry solver calculations in all iterations.
- **Per Iteration** : The time taken for the complex chemistry solver calculation for each iteration.

Field Functions

Chemistry Heat Release Rate

The chemistry heat release shows the amount of heat that is released due to complex chemistry reactions. This value is $\dot{h}$ in Eqn. (3432).

Chemistry Time Step

For steady state simulations, the chemistry time step is the total time that is spent integrating the chemistry in the cell.

Clustering Equivalence Ratio

The clustering equivalence ratio is defined by Eqn. (3498).

Clustering Index

Clustering index is an integer value showing the cluster that the cell belongs to. Values of zero represent cells which are not chemically active, such as cells with a temperature below the Minimum Temperature for Reactions.

Clustering Mixture Fraction

The clustering mixture fraction is defined as the atomic mass fraction that originates from the fuel stream. Since the fuel is assumed to be hydrocarbons, the clustering mixture fraction is the mass fraction of C and H in the cell.

Number of DMR Retained Species

Available when the chemistry acceleration property, *Dynamic Mechanism Reduction*, is activated. Displays the actual number of species from the full chemical mechanism that the CVODE solver retains and solves for.

Approximation Options Properties

The Approximations Options node is available when using the Complex Chemistry model.

Approximation Options Properties

Relax to Chemical Equilibrium

When activated, an **Approximation Options** > **Relax to Chemical Equilibrium** node appears.

The *Relax to Chemical Equilibrium* (RTCE) option relaxes the species composition in each cell to the local equilibrium composition.

Use the RTCE option when a chemical kinetic mechanism is not available, or for a fast solution with a few major species where only the flame position is required.

You are advised to use this option if NH_3 is the only fuel.

Relax to Chemical Equilibrium

When the **Complex Chemistry** > **Approximation Options** property *Relax to Chemical Equilibrium* (RTCE) is activated, the species field is relaxed to its chemical equilibrium compositions over a set turbulent time-scale τ_{char}.

- When using the Relax to Chemical Equilibrium option with the Complex Chemistry model—but without the Turbulent Flame Speed Closure model—τ_{char} is determined by considering the timescales for the flow and chemistry as in Eqn. (3482).
- When using the Relax to Chemical Equilibrium option with the Complex Chemistry model and the Turbulent Flame Speed Closure model, τ_{char} is determined by the Kolmogorov timescale—which you can scale using a timescale constant as in Eqn. (3483).

Since no chemical kinetics are calculated, the RTCE option is an approximation that is usually used as an initial condition for finite-rate chemistry simulations. The RTCE method cannot predict ignition or slowly forming pollutants such as NOx.

The chemistry time scale is computed based on the specified fuel species.

See Complex Chemistry.

Relax to Chemical Equilibrium Properties

Timescale Constant

c_t in Eqn. (3483) which allows you to control the relaxation time of the reaction behind the flame front by scaling the Kolmogorov timescale τ_k.

The following properties are unavailable when using the Turbulent Flame Speed Closure (TFC) model:

Flow Time Constant

Scales the flow timescale τ_{flow} that is used to calculate τ_{char} in Eqn. (3482).

Chemistry Time Constant

Scales the chemical timescale τ_{chem} of the fuel in Eqn. (3482).

Include Chemistry Time

Only available when reactions are specified.

When activated, the chemical timescales of the selected *Fuel Components* are considered alongside the turbulent flow timescale to determine the characteristic time scale.

Including the chemical timescales can prevent auto-ignition ahead of the flame front.

Fuel Components

The fuel component species that are considered when determining the chemistry time step when *Include Chemistry Time* is activated.

Chemistry Acceleration Properties

The **Complex Chemistry** > **Chemistry Acceleration** node allows you to speed up complex chemistry calculations using In-Situ Adaptive Tabulation (ISAT), Clustering, or Dynamic Mechanism Reduction.

Chemistry Acceleration

When the In Situ Adaptive Tabulation and the Clustering properties are activated at the same time, accuracy can be reduced. Therefore, if In Situ Adaptive Tabulation is activated, deactivate Clustering. ISAT is not available when using Dynamic Mechanism Reduction.

In Situ Adaptive Tabulation

When this option is activated, a **Chemistry Acceleration** > **In Situ Adaptive Tabulation** node appears in which you can specify the ISAT tables.

Clustering

When this option is activated, a **Chemistry Acceleration** > **Clustering** node appears in which you can specify the clustering components.

Dynamic Mechanism Reduction

When this option is activated, a **Chemistry Acceleration** > **Dynamic Mechanism Reduction** node appears in which you can specify the parameters for reducing the number of species in the mechanism that are solved for by the CVODE solver.

In Situ Adaptive Tabulation

Tabulates computationally expensive functions and then interpolates these at run time. You can use ISAT to retrieve approximate values for multi-dimensional functions that are expensive to compute. See In Situ Adaptive Tabulation.

Absolute Tolerance

Absolute tolerance for the ISAT approximation.

Table Size (MB)

Maximum size for the ISAT table.

Sensitivity Absolute Tolerance

The absolute tolerance of the CVODE solver which computes the sensitivity matrix that is used in the ISAT approximation.

Sensitivity Relative Tolerance

The relative tolerance of the CVODE solver which computes the sensitivity matrix that is used in the ISAT approximation.

In Situ Adaptive Tabulation Context Menu

Clear ISAT Table

Clears all of the internal ISAT tables and statistics (such as: adds, retrieves, and grows).

Clustering

Components

The available clustering components are listed below—default clustering components are marked with an asterisk*. For unsteady simulations, the chemistry time-step is the flow time-step—which is constant and therefore unavailable for clustering.

- **[available species]**
- **Chemistry Time Step***

- **Entropy**
- **Equivalence Ratio***
- **OH*** (when present)
- **Mixture Fraction**
- **Pressure**
- **Progress Enthalpy**
- **Static Enthalpy**
- **Temperature***
- **TFC Reaction Rate***
- **TFC Unburnt Progress Variable** (this is the Unburnt Unnormalized Progress Variable)
- **[User Component n]**
- **X Co-ordinate**
- **Y Co-ordinate**
- **Z Co-ordinate**

[Clustering Component] Properties

Tolerance

Allows you to specify the tolerance of the component for clustering.

Tolerance Type

There are two ways to specify the clustering table resolution for any clustering variable:

- **Relative**: The clustering bin size is calculated as the maximum of that variable in the computational domain minus the minimum, which is then multiplied by the Relative Tolerance, ε_{rel} in Eqn. (3496).
- **Absolute**: The clustering bin size is the Absolute Tolerance, ε_{abs} in Eqn. (3497).

Dynamic Mechanism Reduction

If the complex chemistry approximation option, *Relax to Chemical Equilibrium*, is activated, the dynamic mechanism reduction option is unavailable.

Error Tolerance

The lower the number, the closer the solution is to that of the full chemical mechanism—less species are removed from the mechanism. Higher values exclude a greater number of species from the solution, which is therefore less accurate.

Imposed Target Species

Species that you select from the full chemical mechanism that are target species for the Directed Relation Graph (DRG) algorithm Eqn. (3499). These species are always included in the reduced chemical mechanism.

If the species, NO, is present in a mechanism, it is automatically included in the target species.

Minimum Number of Target Species

The minimum number of target species (including the imposed target species). If this value is greater than the number of *Imposed Target Species*, the remaining target species are taken to be those with the fastest reaction rates.

CVODE Properties

The Complex Chemistry model uses the CVODE ODE solver.

Absolute Tolerance

Specifies the absolute error tolerance for each ODE step in the CVODE ODE solver. The solver makes sure that the error is less than the relative tolerance multiplied by the quantity that is being integrated, plus the absolute tolerance.

Relative Tolerance

Specifies the relative error tolerance for each ODE step in the CVODE ODE solver. The solver makes sure that the error is less than the relative tolerance multiplied by the quantity that is being integrated, plus the absolute tolerance.

Error Codes

If you receive an error code when using the CVODE solver and building a combustion table, you can find the meaning of the error code value in Appendix B.2, *CVODE main solver module*, here: https://computation.llnl.gov/sites/default/files/public/cv_guide.pdf

Acceleration Factor Control Properties

You can specify a fixed acceleration factor, or allow Simcenter STAR-CCM+ to set it automatically.

The acceleration factor specifies the level of linearization that is applied to the stiff complex chemistry reaction source terms ω_i for the i'th species in Eqn. (3478). When the acceleration factor is low, a high level of source term linearization occurs and the solution converges slowly. Increasing the acceleration factor decreases the linearization and speeds up the solution. However, when the acceleration factor is too high, the solution can diverge.

The **Acceleration Factor Control** node only appears under the **Complex Chemistry** model when using the **Steady** model.

Automatic Control

When activated, Simcenter STAR-CCM+ dynamically adjusts the acceleration factor that is used as the solution proceeds. When deactivated, you specify a fixed *Acceleration Factor*.

Simcenter STAR-CCM+ monitors the behaviour of a small proportion of the most recent reacting species residuals as it adjusts the acceleration factor. At any given time, whichever reacting species residuals have the largest values are monitored—these may change during iterations. As the solution proceeds, Simcenter STAR-CCM+ compares a *Residual Sample Size* of consecutive residual values from each of the selected residuals to their respective least squares approximation to see what proportion of values fit the line. Based on these comparisons, Simcenter STAR-CCM+ increases, decreases, or maintains the acceleration factor—starting from a specified *Initial Acceleration Factor*.

Acceleration Factor

Available when *Automatic Control* is deactivated.

Set a value between 0.0 (full ω_i source term linearization—which is slow to run) and 1.0 (no ω_i source term linearization—which is faster to run, but less stable). A value of 0.5 is appropriate for the majority of simulations—however, if residuals diverge, lower this value.

Turbulence-Chemistry Interactions Model Reference

Turbulence-chemistry interactions require additional modeling, as well as RANS or LES modeling, to allow chemical reactions in thin reaction zones to be solved.

Turbulence-Chemistry Interactions Reference

Model Names and Abbreviations	**Eddy Dissipation Concept**		**EDC**
	Laminar Flame Concept		**LFC**
	Thickened Flame Model		**TFM**
	Turbulent Flame Speed Closure See Turbulent Flame Speed Closure (Complex Chemistry) Model Reference		**TFC**
Theory	See Complex Chemistry.		
Provided By	**[physics continuum]** > **Models** > *Turbulence Chemistry Interactions*		
Example Node Path	**Continua** > **Physics 1** > **Models** > **Eddy Dissipation Concept**		
Requires	*Material*: **Multi-Component Gas** or **Multi-Component Liquid** *Reaction Regime*: **Reacting** *Reactive Flow*: **Reacting Species Transport** *Reacting Species Models*: **Complex Chemistry**		
Properties	none		
Activates	Model Controls (child nodes)	EDC only: • EDC Fine Structure Time Factor • EDC Fine Structure Length Factor When modeling Steady simulations, the **Eddy Dissipation Concept** > **Acceleration Factor** or **Laminar Flame Concept** > **Acceleration Factor** node appears. See Acceleration Factor Properties.	
	Field Functions	EDC Fine Structure Length Fraction, EDC Fine Structure Time, EDC Mean Reaction Rate Ratio. (There are no LFC-related field-functions). See Field Functions.	

EDC Fine Structure Time Factor

Allows you to specify the fine structure (flamelet) time factor, C_t in Eqn. (1181) as a scalar profile.

EDC Fine Structure Length Factor

Allows you to specify the fine structure (flamelet) length factor, C_l in Eqn. (3479) as a scalar profile.

Acceleration Factor Properties

Acceleration Factor

Setting a value of 1.0 indicates that the species source term is fully explicit which results in unstable, but fast, convergence. When a value of 0.0 is set, the species source term is taken as fully implicit which results in stable, but slow, convergence. In practice, you set a value between 0.0 and 1.0 which provides the best convergence when using default Under Relaxation Factor values.

Turbulence-Chemistry Interactions Field Functions

Complex Chemistry with EDC

The following field functions are made available when using the Complex Chemistry and Eddy Dissipation Concept (EDC) models:

EDC Fine Structure Length Fraction

$C_l\left(\frac{\upsilon T}{L^2}\right)^{0.25}$ in Eqn. (3479).

EDC Fine Structure Time

The fine structure (flamelet) region residence time, τ in Eqn. (3480).

EDC Mean Reaction Rate Ratio

The ratio f that is calculated by Eqn. (3479) which is used to modify the chemical reaction source term in Eqn. (3478).

Turbulent Flame Speed Closure (Complex Chemistry) Model Reference

The Turbulent Flame Speed Closure (Complex Chemistry) model is a turbulence-chemistry interactions model which you can use with the Complex Chemistry model.

Turbulent Flame Speed Closure (Complex Chemistry) Model Reference

Theory	See Turbulent Flame Speed Closure.
Provided By	**[physics continuum]** > **Models** > *Turbulence Chemistry Interactions*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Turbulent Flame Speed Closure (TFC)**
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport** *Reacting Species Transport Models*: **Complex Chemistry**
Properties	Key properties are: *Flame Speed Scaling Factor*, *Heat Release Rate Activation Threshold*, and *Flame Curvature Effect*. See Turbulent Flame Speed Closure (Complex Chemistry) Model Properties.

Activates	Model Controls (child nodes)	Laminar Flame Speed and Turbulent Flame Speed
	Field Functions	**Laminar Flame Speed**, **TFC Activity Indicator**, **Turbulent Flame Speed**, **Unburnt Thermal Diffusivity**, and **Wall Direction**. See Field Functions.

Turbulent Flame Speed Closure (Complex Chemistry) Model Properties

Flame Speed Scaling Factor

A multiplier of the turbulent flame speed which allows you to increase the turbulent flame speed.

Heat Release Rate Activation Threshold

Only available when the **Complex Chemistry** > **Approximation Options** property *Relax to Chemical Equilibrium* is deactivated. Increasing this value (up to 1) selects fewer cells for flame propagation, which leads to more robust behaviour, however, flame positioning may become less accurate.

Flame Curvature Effect

Adds the contribution of the flame curvature to the turbulent flame speed. Usually this contribution is minor and tends to decrease the turbulent flame speed.

Enable Model before Start of Spark Time

Allows the TFC model to be activated before spark time.

The default is **Off**, meaning that only the underlying Complex Chemistry model (Laminar Flame Closure LFC) operates up to spark time.

Field Functions

Laminar Flame Speed

s_l, defined by either Metghalchi Eqn. (3506) or Gulder Eqn. (3510).

TFC Activity Indicator

The volume in which the Turbulent Flame Speed Closure (TFC) model alters the chemical and diffusion terms to propagate the premixed flame front at the specified turbulent flame speed.

TFC Reaction Rate

The TFC reaction rate that is used in clustering is the target source from the TFC model for Y_c, that is $\dot{\omega}_{Y_c}^{\mathrm{tfc}}$ in Eqn. (3501).

Turbulent Flame Speed

s_t, defined by either Zimont Eqn. (3511) or Peters Eqn. (3516).

Unburnt Heat Release Rate

The heat that is released due to kinetic activity in the unburnt gases. This field function allows you to visualize areas in which the unburnt heat release rates are high—which indicates that knock is more likely to occur.

Unburnt Thermal Diffusivity

α_u in Eqn. (3511).

Wall Direction

In addition to the above field functions, the following field functions are also available only when the *Temporary Storage Retained* property is activated for the **Segregated Species** solver.

Equivalence Ratio

Equivalence ratio Φ in Eqn. (3509).

Exhaust Gas Recirculation Mass Fraction

Mass fraction of product (burnt) species Y_{EGR} in Eqn. (3518).

Progress Variable

c, in Eqn. (3601).

Species Correction Factor

$\mathbf{n_f}$ calculated by Eqn. (3503).

Thermal Diffusion Flux Energy Source

D in Eqn. (3500).

Unburnt Temperature

The conditional temperature in the unburnt gases. Allows you to construct the flame speed.

Laminar Flame Speed

Method	Corresponding Method Node
Gulder Laminar Flame Speed	Uses the Gülder laminar flame speed correlation Eqn. (3645). Activates the **Gulder Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Metghalchi Laminar Flame Speed	Uses the Metghalchi laminar flame speed correlation Eqn. (3639). Activates the **Metghalchi Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Precomputed LFS Table	Uses values taken from the Laminar Flame Speed Table that is specified under the **Table Generators** > **LFS Table Generator** node.

	Activates the **Precomputed LFS Table** node which allows you to select the Laminar Flame Speed Table defined in LFS Table Generator.
User Defined Laminar Flame Speed	Allows you to specify the unstrained laminar flame speed. **Laminar Flame Speed** > **User Defined Laminar Flame Speed** > **Laminar Flame Speed Profile**

Flame Speed Multiplier

Available for all Laminar Flame Speed (LFS) methods.

Allows you to multiply the LFS with a scale factor. The flame speed multiplier is applied to S_l obtained from any of the LFS methods in Turbulent Flame Speed Closure.

Increasing the multiplier will increase the LFS and therefore the Turbulent Flame Speed. The recommended value ranges from 0.5 to 2. The default of 1 indicates that no multiplier is applied.

Turbulent Flame Speed

Method

Method	Corresponding Child Node
Peters Turbulent Flame Speed Selects the Peters method Eqn. (3516) for calculating the turbulent flame speed source term.	**Peters Turbulent Flame Speed** Properties: *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Select a setting from `0` (fully extinguished) to `1` (no effect). *Constant, A1* Coefficient A_1, from Eqn. (3517). *Constant, A4* Coefficient A_4, from Eqn. (3517). *Constant, B1* Coefficient B_1, from Eqn. (3517). *Constant, B3* Coefficient B_3, from Eqn. (3517). *Ewald's Corrector Constant* c_{ew}, from Eqn. (3517) Sub-nodes: **Unburnt Thermal Diffusivity** You can define the unburnt thermal diffusivity D_u using the **Power Law** Eqn. (3552), or as a **User-Defined Unburnt Thermal Diffusivity** profile.

Method	Corresponding Child Node
User Defined Turbulent Flame Speed Selects the User-Defined method for calculating the turbulent flame speed source term.	**User Defined Turbulent Flame Speed** Properties: *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Select a setting from `0` (fully extinguished) to `1` (no effect). Sub-nodes: **Turbulent Flame Speed Profile** Scalar profile value.

Method	Corresponding Child Node
Zimont Turbulent Flame Speed Selects the Zimont method Eqn. (3511) for calculating the turbulent flame speed source term.	**Zimont Turbulent Flame Speed** Properties: *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Specify a setting from `0` (fully extinguished) to `1` (no effect). *Flame Stretch Effect* When activated, uses the flame stretch factor G Eqn. (3512), which takes the flame stretch effect into account by representing the probability of unquenched flamelets. Activates the **Flame Stretch Effect** node. Sub-nodes: **Unburnt Thermal Diffusivity** You can define the unburnt thermal diffusivity using the **Power Law** or as a **User-Defined Unburnt Thermal Diffusivity** profile. **Flame Stretch Effect** *Constant, ustr* Coefficient μ_{str} from Eqn. (3513). *Critical Strain Rate Control* Select either the **Chemical Time Scale Method**with which you can set the constant B in Eqn. (3515), or **User Defined Profile**

Eddy Break-Up Model Reference

Eddy Break-Up (EBU) combustion models solve individual transport equations for mean species concentrations on the computational grid.

The reaction rates that are used in the transport equations are calculated as functions of the mean species concentrations, turbulence characteristics and, depending on the specific model that is used, temperature. A mean enthalpy equation is solved in addition to the species transport equations. The mean temperature and density are then calculated knowing the mean enthalpy and species concentrations.

Four variants are available for this model, selectable from the *Reaction Control* property in the *Properties* window.

Eddy Break-Up Combustion Models

Theory	See Eddy Break-Up	
Provided By	**[physics continuum]** > **Models** > *[Non-Premixed] Combustion Models*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Eddy Break-Up**	
Requires	*Material*: either **Multi-Component Gas** or **Multi-Component Liquid** *Reaction Regime*: **Reacting** *Reactive Flow*: **Reacting Species Transport**	
Properties	Key properties are: **Reaction Control**, **Store Reaction Rates**, **Begin**, **Source Enabled Trigger**, and **Source Term Limiting**. See EBU properties.	
Specific Right-Click Actions	See Right-Click Actions.	
Activates	Model Controls (child nodes)	Reactions. See Reactions.
	Region Settings	Active Regions Option. See Region Settings.
	Monitors	**FuelMassFr**: Fuel Mass Fraction.
	Other Continuum Nodes	The **Ignitors** node provides the right-click option to create a **Fixed Temperature Ignitor**. See Ignitors.
	Field Functions	Chemistry Heat Release Rate, Residence Time. See EBU Field Functions

EBU Model Properties

Reaction Control

Selects the variant of EBU combustion model. Apart from the Kinetics Only variant, these models are not compatible with the Spalart-Allmaras and Spalart-Allmaras-DES turbulence models.

- **Standard EBU**
  Selects Standard EBU—assumes that the reaction rate is dictated solely by the turbulent mixing time scale.
- **Hybrid**
  Selects Hybrid—reaction rate is the minimum of the rate predicted by turbulent mixing and the rate predicted by finite-rate chemical kinetics.
- **Combined Time Scale**
  Selects Combined Time Scale—reaction rate is given by the sum of the rates predicted by turbulent mixing and by chemical kinetics.
- **Kinetics Only**

Selects Kinetics Only—assumes that the reaction rate is dictated by finite-rate chemical kinetics. This option is very similar to the Complex Chemistry option, however, without the stiff solver for solving several stiff reactions simultaneously. Therefore, it is suggested that you use the Complex Chemistry model instead of EBU with Kinetics Only.

Store Reaction Rates

Activates the capability to post-process reaction rates, forward and backward (where applicable).

- **Activated**
  Stores reaction rates during the simulation run and makes them available among scalar field functions.
  After the simulation run, each reaction rate is available in the scalar field function list under the item Reaction Rate Forward or Reaction Rate Backward.
  If you set the *Reaction Control* property of the EBU model to Standard EBU, you can only visualize forward reaction rates.
- **Deactivated**
  Does not store reaction rates (default).

Begin

Specifies the iteration or time-step after which the reactions are activated. During previous iterations or time-steps, reactions are deactivated. This feature is useful when modeling significant flow as you can deactivate reactions until a flow solution is found.

Source Term Limiting

For the EBU combustion model (particularly with the **Kinetics Only** option), the specified reaction rate can be large enough to drive the reactant concentration below zero. To keep all reactant concentrations in a physically correct range, activate this limit on the final reaction rate that is applied to the species transport equation.

For most applications, leave this option deactivated. Use it only when a reasonable convergence cannot be obtained and the species concentrations clearly show unphysical values.

- **Activated**
  Limits the final reaction rate that is applied to the species transport equation Eqn. (3528). Provides the field function, Residence Time (chemistry time step).
- **Deactivated**
  Does not limit the final reaction rate (default).

Right-Click Actions

Import Chemistry Definition (Chemkin format)

Activates a standard Open dialog that allows you to import a chemical mechanism file, thermodynamic data file, and optionally, a transport properties file.

Delete Chemistry Definition

Removes the reactions—and optionally, the species—that are used for the chemistry definition.

Reactions

Right-Click Actions

New Reaction

Creates a **Reaction [n]** sub-node.

See Reaction [n] Reference.

[reaction]

The defined reaction *Type* can only be **Eddy Break-Up**.

Reactants

Defines the reactant components of the Eddy Break-Up reaction.

Products

Defines the product components of the the Eddy Break-Up reaction.

Properties > Eddy Break-Up Coefficient

Available with the **Standard EBU**, **Hybrid**, and **Combined Time Scale** EBU combustion models.

Defines the reaction rate method for the Eddy Break-Up reaction.

Use Products for the Rate

When activated, it uses products Eqn. (3521) for computing the reaction rate.

EBU Rate Cofficient, A

Specifies the coefficient A_{ebu} in Eqn. (3520) for EBU reaction rate.

EBU Rate Cofficient, B

Specifies the coefficient B_{ebu} in Eqn. (3521) for EBU reaction rate.

Properties > Reaction Coefficient

Available with the **Hybrid**, **Combined Time Scale**, and **Kinetics Only** EBU combustion models.

Defines the reaction rate method for EBU reaction. Following are the methods that can be applied:

Method	Corresponding Method Node/Sub-Node
`Arrhenius Coefficients` The Arrhenius reaction parameters are used to calculate chemical reaction rates from finite-rate kinetics.	**Arrhenius Coefficients** **Pre-exponent** Defines the pre-exponential factor, A, in Eqn. (3431).

Method	Corresponding Method Node/Sub-Node
`User Reaction Coefficient` The user reaction coefficient allows you to specify custom reaction coefficients.	**User Reaction Coefficient** Specifies the custom reaction coefficients. After combining with species concentration contributions, the units for the corresponding reaction rates are Quantity/Length^3-Time. See Eqn. (3430).

Region Settings

Applies any region:

Active Reactions Option

Activates or deactivates chemical reactions in this region.

EBU Field Functions

Chemistry Heat Release Rate

The chemistry heat release rate is $\dot{h}$ in Eqn. (3432).

Residence Time

For steady state simulations, represents the time duration, t_r in Eqn. (3528), over which the chemistry is calculated (transient/unsteady simulations use the time step as the duration for calculating the chemistry). This field function is available when the property, *Source Term Limiting*, is activated.

Restoring the Premixed Eddy Break Up Model

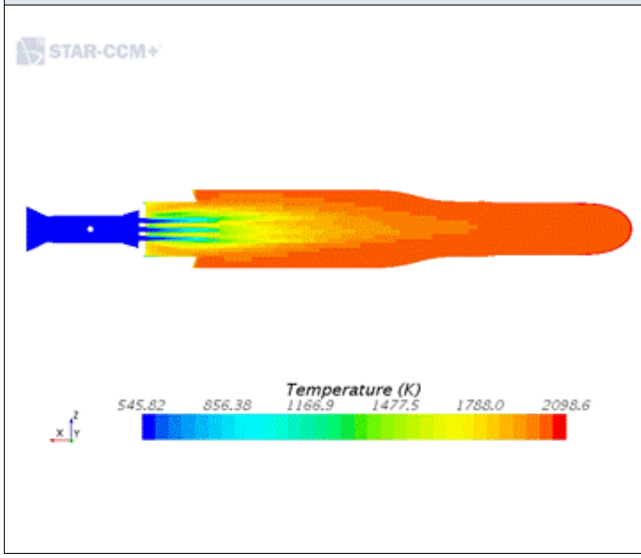
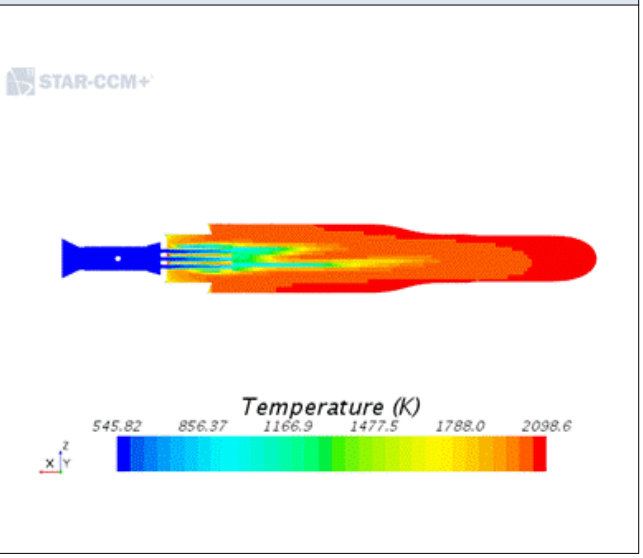
The Premixed Eddy Break-Up model in Simcenter STAR-CCM+ v.11.04 behaves as a Partially Premixed version. You can restore the Premixed model settings as described in this section.

As part of a plan to improve and simplify the procedure for selecting combustion models, the Premixed version of the Eddy Break Up model is discontinued in Simcenter STAR-CCM+ v.11.04.

The new Eddy Break Up Model is an improvement on the deprecated Premixed Eddy Break Up Model—the new Eddy Break Up model:

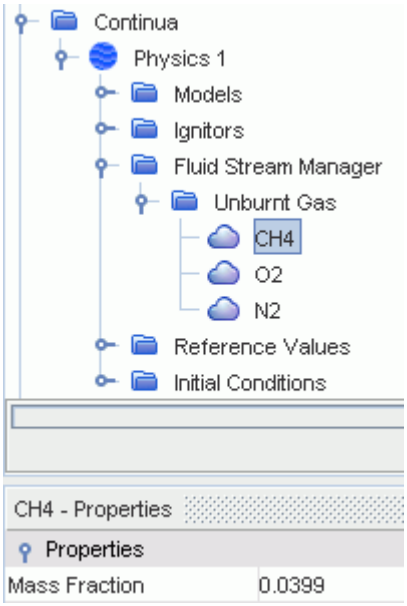
- Supports multiple reactions as well as hybrid and kinetics-based schemes. Therefore, you can perform calculations more accurately and over wider operation ranges.
- Accounts for oxidizer and product concentrations when calculating the source term.
- Allows you to switch between fully premixed and partially premixed calculations.

When loading a simulation in Simcenter STAR-CCM+ v.11.04 or later that was saved in a version of Simcenter STAR-CCM+ before v11.04, the Premixed Eddy Break Up model behaves as a Partially-Premixed Eddy Break Up model. Several settings are defined differently and must be set up again. The following images show a comparison of the temperatures on the cross section of a flame holder.

PEBU 11.02	PEBU 11.04 (Partially Pre-Mixed)
	

Simcenter STAR-CCM+ v.11.04 provides the EBU model as an option for Premixed Combustion. However, this model is the same as that provided for Partially-Premixed combustion. Further steps are required to restore the premixed behaviour that was available in Simcenter STAR-CCM+ v.11.02 and earlier. These steps are as follows:

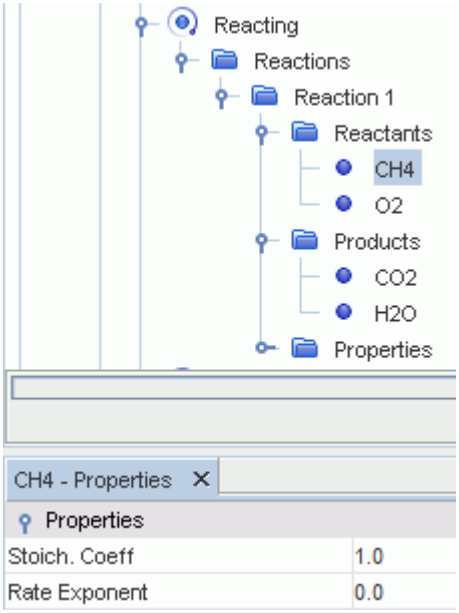
In Simcenter STAR-CCM+ v11.02, the reactants and corresponding mass fractions are defined under the **[Continuum]** > **Fluid Stream Manager** node.



1. In Simcenter STAR-CCM+ v11.02, you use the Fluid Stream Manager to set the species composition of a fuel and an oxidizer. In Simcenter STAR-CCM+ v11.04, you define the reaction framework as follows:
   a) Define the reactants and products for the reaction under the **Models** > **Reacting** > **Reactions** node. Make sure that you create one reaction between a fuel and an oxidizer and specify the products of the complete combustion.

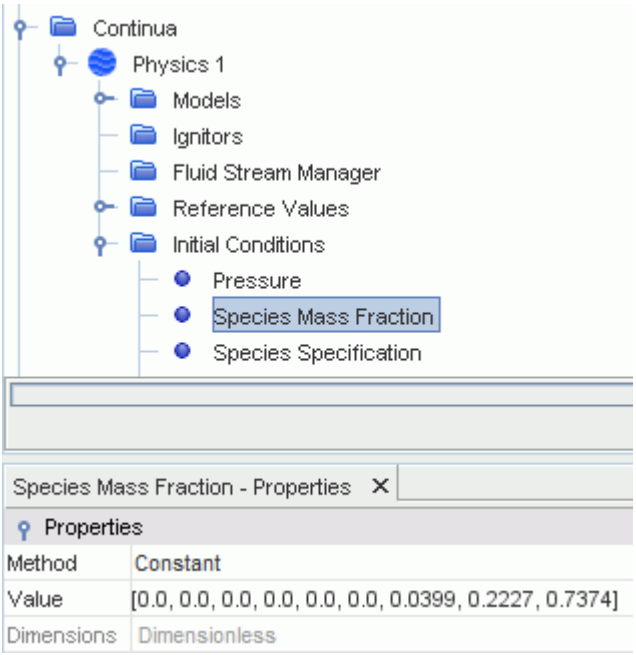
      See Defining Chemical Reactions Manually.

b) Specify stoichiometric coefficients for each component to represent a balanced complete combustion reaction.

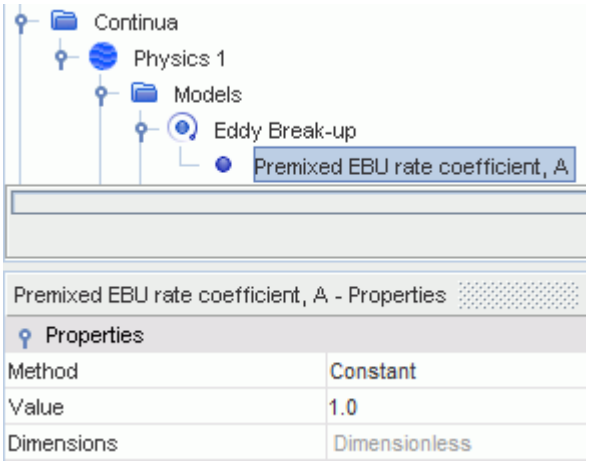


c) To specify the mass fractions of each component, select the **[Continuum]** > **Initial Conditions** > **Species Mass Fraction** node.

d) For the *Value* property, specify the mass fractions of each species in the composition of the initial mixture.



In Simcenter STAR-CCM+ v11.02, the Eddy Break-Up Coefficients are defined under the **Models** > **Eddy Break-Up** > **Premixed EBU rate coefficient, A** node.



In Simcenter STAR-CCM+ v11.04 or later, the Eddy Break-Up Coefficients are defined in the general reactions framework.

2. Select the **Models** > **Eddy Break-Up** node and set *Reaction Control* to **Standard EBU**.
3. Define the EBU rate coefficient A to suit Simcenter STAR-CCM+ v11.04 or later—this value is different from the value that is set for the Premixed EBU rate coefficient A in Simcenter STAR-CCM+ v11.02.
   a) Expand the **Models** > **Reacting** > **Reactions** > **[Reaction]** > **Properties** node.
   b) Select the **Properties** > **EBU Coefficients** > **EBU Rate Coefficient, A** node and specify the *Value*.
4. To restore the Ignitor:
   a) Right-click the **[Continuum]** > **Ignitors** node and select **New** > **EBU Ignitor**.
   b) Select the **EBUIgnitor 1** node and specify the properties as they are set in Simcenter STAR-CCM+ v11.02.
   c) If the **EBUIgnitor 1** node *Activator* is set to **Pulse**, select the **Pulse** sub-node and specify the necessary properties.
5. For all inlet and outlet boundaries within each physics continuum, select the **[Boundary]** > **Physics Values** > **Species Mass Fraction** node and specify the mass fractions of each species with the same values as are specified in the initial conditions.

Eddy Contact Micromixing Model Reference

This physics model allows you to model turbulent molecular-scale mixing and reaction of multi-component liquids, dominated by viscous-convective and viscous-diffusive processes.

The Eddy Contact Micromixing model [775] is numerically efficient, reasonably accurate, and easy to use for multiple reactions. It can be used for both steady and unsteady cases. This model is only available with the multicomponent liquid model, and requires turbulence modeling. It works with all turbulent models that are available for the EBU hybrid model.

Eddy Contact Micromixing Model Reference

Theory	See Eddy Contact Micromixing.
Provided By	**[physics continuum]** > **Models** > *Reacting Species Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Eddy Contact Micromixing**

Requires	*Material*: **Multi-Component Liquid** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport**	
Properties	Key properties are: Source Enabled Trigger, Begin, and Store Reaction Rates. See Eddy Contact Micromixing Properties.	
Activates	Model Controls (child nodes)	Reactions. See Reactions.
	Materials	Specify the liquid materials under the Multi-Component Liquid model.

Eddy Contact Micromixing Properties

Begin

Specifies the iteration or time-step after which the reactions are activated. During previous iterations or time-steps, reactions are deactivated. This feature is useful when modeling significant flow as you can deactivate reactions until a flow solution is found.

Store Reaction Rates

Provides the capability to post-process reaction rates, forward and backward (where applicable).

- **Activated** Stores reaction rates during the simulation run and makes them available among scalar functions.
- **Deactivated** Does not store reaction rates (default).

Reactions

Right-Click Actions

New Reaction

Creates a **Reaction [n]** sub-node.

See Reaction [n] Reference.

[reaction]

The defined reaction *Type* can only be **Eddy Contact**.

Reactants

Defines the reactant components of the Eddy Contact Micromixing reaction.

Products

Defines the product components of the Eddy Contact Micromixing reaction.

Properties > Micromixing Timescale

Allows you to select the method for calculating the micromixing timescale.

Select Method	Corresponding Method Node/Sub-Node
`Classical Scalar Dissipation` Selects the Classical Scalar Mixing method (considers the high-Schmidt number effect for liquids) [776].	**Dissipation Coefficient** The mixing coefficient A, in Eqn. (3554).
`Kolmogorov` Selects the Kolmogorov Method (corresponds to Engulfment type of mixing). See Source Term Definition.	**Mixing Coefficient** The mixing coefficient A, inEqn. (3553).
`No Micromixing (Kinetics Only)` Selects the assumption that the reaction rate is dictated solely by finite-rate chemical kinetics.	None.
`User Micromixing` Selects the User Defined method, allowing you to work with a user-defined field function.	**User Micromixing TimeScale** Specifies the user defined micromixing timescale.

Properties > Reaction Coefficient

Defines the reaction rate method for Eddy Contact Micromixing reaction. Following are the methods that can be applied:

Method	Corresponding Method Node/Sub-Node
`Arrhenius Coefficients` The Arrhenius reaction parameters are used to calculate chemical reaction rates from finite-rate kinetics.	**Arrhenius Coefficients** **Pre-exponent** Defines the pre-exponential factor, A, in Eqn. (3431).
`User Reaction Coefficient` The user reaction coefficient allows you to specify custom reaction coefficients.	**User Reaction Coefficient** Specifies the custom reaction coefficients. After combining with species concentration contributions, the units for the corresponding reaction rates are Quantity/ Length^3-Time. See Eqn. (3430).

Thickened Flame Model Reference

The propagation speed of premixed flame fronts depends on the rate that heat and species diffuse into the flame as well as the subsequent chemical reaction rate. To capture the correct propagation speed with a specified diffusion model and a chemical reaction model, the internal flame structure must be resolved.

Typical premixed flame thicknesses are about 1mm, which is usually smaller than the mesh size. The Thickened Flame Model (TFM) artificially thickens premixed flame fronts to sufficiently resolve the internal flame on the mesh.

The Thickened Flame Model is available with the Complex Chemistry (CC), Eddy Break Up (EBU), and Flamelet Generated Manifold (FGM) models—however, only with Large Eddy Simulation (LES).

Thickened Flame Model Reference

<table>
<tr><td>Theory</td><td colspan="3">See Thickened Flame.</td></tr>
<tr><td>Provided By</td><td colspan="3">• [physics continuum] > Models > Turbulence Chemistry Interactions (when CC is selected)
• [physics continuum] > Models > Optional Models (when EBU is selected)
• [physics continuum] > Models > Progress Variable Source (when FGM is selected)</td></tr>
<tr><td>Example Node Path</td><td colspan="3">Continua > Physics 1 > Models > Thickened Flame Model</td></tr>
<tr><td rowspan="4">Requires</td><td colspan="3">Material: Multi-Component Gas
Space: Three Dimensional
Time: any Unsteady
Reaction Regime: Reacting
Reacting Flow Models: Flamelet or Reacting Species Transport</td></tr>
<tr><td colspan="2">For Flamelet models:
Flamelet Models: Flamelet Generated Manifold (FGM) (FGM Reaction and Ideal Gas selected automatically)
Progress Variable Source: Thickened Flame Model</td><td>For Reacting Species Transport models:
Reacting Species Models: Complex Chemistry or Eddy Break-up
For Complex Chemistry: Turbulence Chemistry Interactions: Thickened Flame Model
For Eddy Break-up: Optional Models: Thickened Flame Model</td></tr>
<tr><td colspan="3">Although the TFM is selected, continue to select the LES model:</td></tr>
<tr><td colspan="3">Flow: Segregated Flow (Gradients, Segregated Species, and Segregated Fluid Enthalpy selected automatically)
Turbulence: Large Eddy Simulation (WALE Subgrid Scale, Wall Distance, and All y+ Wall Treatment selected automatically)</td></tr>
<tr><td>Properties</td><td colspan="3">Number of Cells in Flame and Maximum Flame Thickening Factor.
See Thickened Flame Model Properties.</td></tr>
<tr><td rowspan="2">Activates</td><td>Model Controls (child nodes)</td><td colspan="2">• Efficiency Factor
• Reaction Zone Sensor
• Laminar Flame Properties</td></tr>
<tr><td>Field Functions</td><td colspan="2">Efficiency Factor, Flame Thickening Factor, Reaction Zone Sensor
See Field Functions.</td></tr>
</table>

Thickened Flame Model Properties

These properties are used for calculating the Flame Thickening Factor.

Number of Cells in Flame

The value N in Eqn. (3531). The default value is 8.

Maximum Flame Thickening Factor

The global maximum flame thickening factor, $F_{\max}$ in Eqn. (3531). The local maximum flame thickening factor $F_{\max}^{\text{loc}}$ is calculated in every cell. If $F_{\max}^{\text{loc}}$ exceeds the specified global maximum, the flame thickening factor is clipped to the specified value. $F_{\max}$ has a default value of 20.

Model Controls

Efficiency Factor

Sets the method by which Simcenter STAR-CCM+ computes the efficiency factor. This factor increases the flame speed in order to correct underestimation of the flame front wrinkling.

Method	Corresponding Method Node
Power Law Evaluates the efficiency factor E according to a Power law expression as given by Eqn. (3539).	**Power Law** • *Constant Alpha*, exponent α, from Eqn. (3539) • *Constant b*, exponent b, from Eqn. (3540) • *Constant Ck*, coefficient C_k, from Eqn. (3541) through Eqn. (3543)
Turbulent Flame Speed Evaluates the efficiency factor based on the ratio of turbulent flame speed to laminar flame speed, as specified in Eqn. (3549). See Turbulent Flame Speed.	**Turbulent Flame Speed** • *Constant Alpha*, the constant multiplier α from Eqn. (3549) • *Turbulent Flame Speed Option* ◦ **Turbulent Flame Speed - Zimont** See Zimont Turbulent Flame Speed. ◦ **Turbulent Flame Speed - Peters** See Peters Turbulent Flame Speed. ◦ **Turbulent Flame Speed - User-Defined** See User Defined Turbulent Flame Speed.
Wrinkling Factor Ratio Evaluates the efficiency factor from the expression in Eqn. (3546).	**Wrinkling Factor Ratio** • *Constant cms*, coefficient c_{ms}

Reaction Zone Sensor

The Thickened Flame Model artificially thickens premixed flame fronts to resolve them on the mesh, by increasing thermal and species diffusivities. Enhanced diffusivities away from the flame front would affect other physics such as mixing, droplet evaporation and wall heat transfer. Hence, thickening is only performed around the flame front, and moves dynamically in time with the flame front. There are several options to calculate this reaction zone sensor.

Method	Corresponding Method Node
Arrhenius Available for the Eddy Break-up model only, as formulated in Eqn. (3534) to Eqn. (3530). Applies to global chemistry schemes.	**Arrhenius** • *Constant Beta*, coefficient β, from Eqn. (3530) • *Constant Gamma*, coefficient Γ, from Eqn. (3535).
Progress Variable Available for the Flamelet Generated Manifold model only.	**Progress Variable** • *Constant Beta*, coefficient β, from Eqn. (3532).
Progress Variable Reaction Rate Available for the Flamelet Generated Manifold model only.	**Progress Variable Reaction Rate** • *Constant Beta*, coefficient β, from Eqn. (3533).
Heat Release Rate Available for the Eddy Break-up model and the Complex Chemistry model only.	**Heat Release Rate** • *Constant Beta*, coefficient β, from Eqn. (3537).
Reaction Rate Available for the Eddy Break-up model and the Complex Chemistry model only.	**Reaction Rate** • *Constant Beta*, coefficient β, from Eqn. (3538).
User-Defined Sets the reaction zone sensor.	**User-Defined** The user scalar profile should be unity inside the flame zone and zero outside.

Laminar Flame Properties

Laminar Flame Speed

Provides options for controlling the laminar flame speed in its properties.

Method	Corresponding Method Node
Flamelet Table Laminar Flame Speed Available when the FGM model is used and the Reactor Type is set to **1D Premixed Freely Propagating**.	Uses the laminar flame speed that is stored in the flamelet table generated by the FGM Table Generator. See FGM Table. Activates the **Flamelet Table Laminar Flame Speed** node.
Gulder Laminar Flame Speed	Uses the Gülder laminar flame speed correlation Eqn. (3645). Activates the **Gulder Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.

Metghalchi Laminar Flame Speed	Uses the Metghalchi laminar flame speed correlation Eqn. (3639). Activates the **Metghalchi Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Universal Laminar Flame Speed Available for the Flamelet Generated Manifold model only.	Simcenter STAR-CCM+ identifies the best laminar flame speed correlation for each individual fuel in a mixture of fuels and then uses the Hirasawa method to calculate the laminar flame speed of the blended mixture of fuels that are specified Eqn. (3637). Hydrocarbons, alcohols, hydrogen and ammonia are considered as fuels. Activates the **Universal Laminar Flame Speed** node.
Precomputed LFS Table Available for the Complex Chemistry model only.	Uses values taken from the Laminar Flame Speed Table that is specified under the **Table Generators** > **LFS Table Generator** node. Activates the **Precomputed LFS Table** node which allows you to select the Laminar Flame Speed Table defined in LFS Table Generator.
User Defined Laminar Flame Speed	Allows you to specify the unstrained laminar flame speed. Activates the **User Defined Laminar Flame Speed** node.

Flame Speed Multiplier

Available for all Laminar Flame Speed (LFS) methods.

Allows you to multiply the LFS with a scale factor. The flame speed multiplier is applied to S_l obtained from any of the LFS methods in Flame Speed Calculations.

Increasing the multiplier will increase the LFS and therefore the Turbulent Flame Speed. The recommended value ranges from 0.5 to 2. The default of 1 indicates that no multiplier is applied.

Laminar Flame Thickness

The **Laminar Flame Thickness** node provides options for controlling the flame thickness.

Method	Corresponding Method Node
Power Law Thermal Diffusivity	**Power Law Thermal Diffusivity** The laminar flame thickness is calculated using Eqn. (3552).
Sutherland Law Thermal Diffusivity	**Sutherland Law Thermal Diffusivity** The laminar flame thickness is calculated using Eqn. (3550).
User Defined Laminar Flame Thickness	**User Defined Laminar Flame Thickness** Sets the laminar flame thickness using its **Laminar Flame Thickness Profile** sub-node. The options for user defined laminar flame thickness include field functions, tables as functions of equivalence ratio, and user code.

Field Functions

Efficiency Factor

The efficiency factor models an increase in the turbulent flame speed due to eddies smaller than the thickened flame, which are lost in the artificial thickening process. See E in Eqn. (3529).

Flame Thickening Factor

The flame is artificially thickened by F to resolve on the mesh. See F in Eqn. (3531).

Reaction Zone Sensor

The zone around the flame front where diffusivities are increased and reaction rates decreased. See Ω in Eqn. (3529).

Polymerizaton Model Reference

Polymerization is the process of creating long-chain molecules by chemically combining large numbers of small monomer molecules. This process starts by mixing monomer and initiator molecules in a solvent.

The process of polymerization is comprised of several chemical reactions, such as initiation, propagation, chain transfer, chain branching, scission, and termination, that involve radicals of different chain lengths.

The Polymerization model in Simcenter STAR-CCM+ simulates free-radical polymerization and uses Method of Moments for size distribution calculations.

Polymerizaton Model Reference

Theory	See Polymerization.
Provided By	**[physics continuum / phase]** > **Models** > *Reacting Species Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Polymerizaton** or **Continua** > **Physics 1** > **Models** > **Multiphase** > **Eulerian Phases** > **[Eulerian Phase]** > **Models** > **Polymerizaton**
Requires	*Material*: **Multi-Component Liquid** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport**
Properties	A key property of this model is *User Rates*. See Polymerizaton Properties.

Activates	Model Controls (child nodes)	The Polymerization model contains three sets of sub-nodes for polymer scalars, polymer moments, and free-radical polymer reactions. See Model Controls.	
	Initial Conditions	Polymer Dead Moment Polymer Initiator Polymer Live Moment Polymer Modifier	Polymer Monomer Polymer Radical Polymer Solvent See Initial Conditions.
	Boundary Inputs	Polymer Dead Moment Polymer Initiator Polymer Live Moment Polymer Modifier	Polymer Monomer Polymer Radical Polymer Solvent See Boundary Settings.
	Solvers	Polymerizaton Solver. See Polymerizaton Solver Properties.	
	Monitors	DeadPolymerMoment0 DeadPolymerMoment1 DeadPolymerMoment2 InitiatorConcentration LivePolymerMoment0	LivePolymerMoment1 LivePolymerMoment2 MonomerConcentration RadicalConcentration
	Field Functions	Initiator Concentration Modifier Concentration Monomer Concentration Polydispersity Index Polymer Mass Average Chain Length Polymer Moment Dead 0 Polymer Moment Dead 1	Polymer Moment Dead 2 Polymer Moment Live 0 Polymer Moment Live 1 Polymer Moment Live 2 Polymer Number Average Chain Length Radical Concentration Solvent Concentration See Field Functions.

Polymerizaton Properties

Secondary Gradients

There are two sources of secondary gradients in Simcenter STAR-CCM+ flow solvers:

- boundary secondary gradients for diffusion
- interior secondary gradients at cell faces

Use this property to control which gradients are included in the solver. **On** gives both gradients while **Off** excludes them. **Interior Only** and **Boundaries Only** select the corresponding gradients.

Convection

Sets the discretization scheme that Simcenter STAR-CCM+ uses for computing the convection flux on a cell face in appropriate transport equations. More information is given in the related topic for the Convection Term:

- **1st-Order**: First-order upwind scheme. This scheme scales the transported quantity by the upstream or downstream mass flowrate depending on flow direction. Only use when a higher-order scheme fails to give convergence, or in order to obtain an initial solution before switching to a higher-order scheme.

- **2nd-Order**: Second-order upwind scheme. This scheme introduces linear interpolation of cell values on either side of the upstream or downstream face. Using this scheme can lead to poorer convergence properties, but gives accuracy as good as or better than the first-order scheme.

User Rates

Allows you to add user sources to Polymer Scalars and Polymer Moment equations, in addition to the built-in sources. Activating this property populates the **Polymer Scalars** and **Polymer Moments** sub-nodes. See User Rates Sub-Nodes.

Model Controls

Free-Radical Polymer Reactions Properties

- *Initiator Efficiency, f*: Allows you to specify the efficiency of the initiator of the chain in Eqn. (3862), Eqn. (3864), and Eqn. (3866).
- *Chain Transfer to Modifier*: Activating this property creates an extra **Free-Radical Polymer Reactions** sub-node that represents a chain transfer to modifier reaction.
- *Chain Transfer to Solvent*: Activating this property creates an extra **Free-Radical Polymer Reactions** sub-node that represents a chain transfer to solvent reaction (Eqn. (3854)).
- *Chain Transfer to Polymer*: Activating this property creates an extra **Free-Radical Polymer Reactions** sub-node that represents a chain transfer to polymer reaction (Eqn. (3856)).
- *Beta Scission*: Activating this property creates an extra **Free-Radical Polymer Reactions** sub-node that represents a Beta Scission reaction (Eqn. (3857) and Eqn. (3858)).
- *Heat of Propagation*: Allows you to specify a value for the heat that is released due to propagation reactions.
- *Heat of Initiation*: Allows you to specify a value for the heat that is released due to initiation reactions.

Free-Radical Polymer Reaction Sub-Nodes

Some of these sub-nodes are available by default while others require activation in the properties of the **Free-Radical Polymer Reactions** node.

- **Initiator Decomposition (I -> 2R')**
- **Radical Chain Initiation (R' + M -> R1)**
- **Propagation (Rn + M -> Rn+1)**
- **Chain Transfer to Monomer (Rn + M -> Pn + R1)**
- **Disproportionation (Rn + Rm -> Pn + Pm)**
- **Combination (Rn + Rm -> Pn+m)**
- **Chain Transfer to Modifier (Rn + X -> Pn + R1)**
- **Chain Transfer to Polymer (Rn + Pm -> Pn + Rm)**
- **Beta Scission (Rn + Pm -> Pm + Rp + Pm-p)**
- **Terminal Double Bond (Rn + Pm -> Rn+m)**

See Reacting Flow Nomenclature.

Free-Radical Polymer Reaction Sub-Node Properties

- *Method*: Allows you to specify the **Method** as a scalar profile.
- *Value*: Specifies the value with a text entry. You can also enter an expression, such as `10 * sin(3.14 * $Time)`, directly. This property is only available when *Method* is set to **Constant**.

- *Scalar Function*: Activates an object selector dialog from which you can choose a field function. This property is only available when **Method** is set to **Field Function**.
- *Unit System*: Allows you to define **Units** that are appropriate to the reaction:
  - **kmol, m, s, K**
  - **mol, cm, s, K**

User Rates Sub-Nodes

When the **User Rates** property is activated, the following sub-nodes of the **Polymer Scalars** and **Polymer Moments** nodes allow you to specify User Rate and User Rate Jacobian source terms directly to the Polymer Scalar and Polymer Moment equations. Each of these sub-nodes functions as a scalar profile.

Polymer Scalars

Initiator, **Modifier**, **Monomer**, **Radical**, and **Solvent**

Polymer Moments

Dead Moment and **Live Moment**

Initial Conditions

Available within each continuum or phase for which the Polymerization model is selected.

Polymer Dead Moment, Polymer Live Moment

Respectively, sets concentrations for dead moment (Eqn. (3867), Eqn. (3869), and Eqn. (3871)) and live moment (Eqn. (3861), Eqn. (3863), and Eqn. (3865)). Scalar array profile values.

Polymer Initiator, Polymer Modifier, Polymer Monomer, Polymer Radical, Polymer Solvent

Respectively, sets concentrations for initiator (Eqn. (3849)), modifier, monomer (Eqn. (3852)), radical (Eqn. (3850)), and solvent (Eqn. (3855)). Scalar profile values.

Boundary Settings

Available for boundaries within regions that are associated with a continuum (or phase within that continuum) which uses the Polymerization model.

Polymer Dead Moment, Polymer Live Moment

Respectively, sets concentrations for dead moment (Eqn. (3867), Eqn. (3869), and Eqn. (3871)) and live moment (Eqn. (3861), Eqn. (3863), and Eqn. (3865)). Scalar array profile values.

Polymer Initiator, Polymer Modifier, Polymer Monomer, Polymer Radical, Polymer Solvent

Respectively, sets concentrations for initiator (Eqn. (3849)), modifier, monomer (Eqn. (3852)), radical (Eqn. (3850)), and solvent (Eqn. (3855)). Scalar profile values.

Flow Boundaries

The following boundary types have all of the above-listed physics values available by default.

- Free Stream
- Mass Flow Inlet

- Pressure Outlet
- Stagnation Inlet
- Velocity Inlet

Wall Boundary

Wall Combustion Scalar Option

Wall Combustion Scalar	**Corresponding Physics Value Nodes**
Zero Flux	None
Specified Value	All of the above-listed physics values

Polymerizaton Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence and do not decrease, reduce the under-relaxation factor for the relevant solvers. The default value is 0.9.

Reconstruction Frozen

When activated, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is deactivated by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When activated, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. Deactivated by default.

Field Functions

When simulating multiphase polymerization, each field function is available for each phase in which the Polymerization model is selected—the field function names are appended with the name of the phase.

Polymer Moments

- **Polymer Moment Dead 0**
- **Polymer Moment Dead 1**
- **Polymer Moment Dead 2**
- **Polymer Moment Live 0**
- **Polymer Moment Live 1**

- **Polymer Moment Live 2**

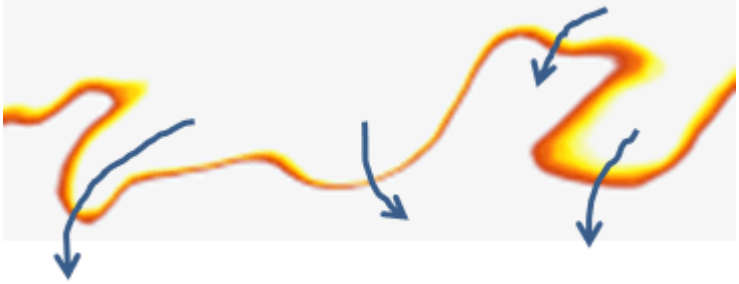
Polymer Scalars

- **Polydispersity Index**
- **Polymer Mass Average Chain Length**
- **Polymer Number Average Chain Length**
- **Initiator Concentration**
- **Modifier Concentration**
- **Monomer Concentration**
- **Radical Concentration**
- **Solvent Concentration**

Flamelet

Flamelet models avoid the computational expense of complex chemistry calculations by pre-calculating the chemistry in gas-phase laminar flames using simple 0D or 1D geometries with detailed chemical mechanisms. A reduced set of variables are used to parameterize and tabulate the species from these simple flames, which are then interpolated in the 3D simulation of turbulent flames in Simcenter STAR-CCM+.

In the following diagram, the dark area shows a thin reaction front in which reactions happen faster than turbulent mixing. Intermediate species do not exist for long enough to be transported out of the reaction front by turbulent mixing.



All Flamelet models in Simcenter STAR-CCM+ use mixture fraction as one parameter. The mixture fraction is defined as the atomic (or elemental) mass fraction that originated from the fuel stream. For combustors with one fuel and one oxidizer stream, if all species diffuse at the same rate—a good assumption for turbulent flows—you can define one unique mixture fraction. Since atomic elements are conserved in chemical reactions, the mixture fraction is conserved and therefore the corresponding transport equation does not have a source term.

Simcenter STAR-CCM+ provides the following Flamelet models:

- Flamelet Generated Manifold (FGM): generally the most accurate flamelet model.
- Steady Laminar Flamelet (SLF): only better than FGM for some highly strained non-premixed flames.
- Chemical Equilibrium: least accurate flamelet model, but is straightforward to use when you do not have a mechanism, or when the combustor is large.

The Chemical Equilibrium and SLF models are best-suited for turbulent diffusion (non-premixed) flames. However, you can apply Flamelet models to partially premixed and even perfectly premixed flames by combining a Flamelet model with a flame position model. See Flame Propagation.

For guidance on which of the combustion models are best for a selection of applications, see Combustion and Other Reacting Flows in Simcenter STAR-CCM+.

A few parameters, such as mixture fraction, reaction progress, scalar dissipation, and enthalpy, are used to parameterize the thermochemical state (species composition and temperature) of the system. Since the number of parameters are small, it is feasible to use presumed Probability Density Functions (PPDF) to account for fluctuations. A Beta function approximates the distribution of mixture fraction as it is a conserved scalar. The Beta function requires a variance, or second moment, which can be solved from a transport equation in RANS and an algebraic expression in LES. The Flamelet models use beta PPDF functions for mixture fraction, and delta functions for the other parameters such as enthalpy and scalar dissipation.

You use Flamelet models for gas-phase flames where the thermo-chemistry occurs near the flamelet manifold. For example, in statistically steady, constant pressure combustors, such as gas-turbines at full power.

Flamelet Generated Manifold Model

The Flamelet Generated Manifold (FGM) model parameterizes flamelet species by mixture fraction and reaction progress variable. To generate the flamelet manifold, the FGM implementation in Simcenter STAR-CCM+ uses 0D ignition reactors or 1D laminar premixed flame reactors. To account for non-adiabatic effects and heat loss or gain, species are also parameterized with enthalpy. The FGM model assumes that the chemical states in turbulent flames are similar to the chemical states in laminar flames. Unlike SLF, no assumption is made about flame structure. You can use the FGM model for modeling:

- High Damkohler-number zones, where reaction zones are thin.
- Low Damkohler-number zones, where reaction zones are diffuse. However, this model does not capture slowly forming pollutants.
- Premixed and partially premixed flames.

To initiate flame ignition, the FGM model provides the **Progress Variable Ignitor**. Access this ignitor by right-clicking the **Continuum** > **Ignitors** node. When active, a Progress Variable Ignitor applies its specified progress variable value to the cells that are contained within the ignitor parts. When inactive, this ignitor does not affect the value of the progress variable.

Chemical Equilibrium Model

The Chemical Equilibrium model parameterizes species by the mixture fraction and enthalpy, or heat loss/gain. The chemistry is assumed to be infinitely fast so that thermo-chemical equilibrium is reached instantaneously. Since chemical equilibrium is a thermodynamic property and independent of the chemical mechanism, the Chemical Equilibrium model is appropriate for modeling:

- fuels for which a chemical mechanism is not available
- combustors where the residence time is large enough that the thermo-chemistry is near chemical equilibrium—for example, in fires

Steady Laminar Flamelet Model

The Steady Laminar Flamelet (SLF) model solves 1D opposed-flow diffusion flames and parameterizes species by mixture fraction and scalar dissipation, which corresponds to the strain (compression) of the opposed flow flame. The SLF model embeds these opposed-flow flames in the CFD turbulent flame brush and assumes that the local turbulent flow field compresses the flamelets. The chemistry is assumed to be fast and therefore responds to the local turbulent strain instantaneously. However, it is not possible to model extinction or ignition with the SLF model.

Since a non-premixed flame is resolved, the SLF model is suitable for modeling steady state diffusion combustion, such as in non-premixed furnaces and burners.

Flamelet Tables

You can create flamelet tables for each of the flamelet models within Simcenter STAR-CCM+.

See Flamelet Tables.

Contents:

Flamelet Reference

Flame Propagation

Simcenter STAR-CCM+ has two types of flame position models which you can use with all flamelet models—the Coherent Flame Model (CFM) and the Turbulent Flame Speed Closure (TFC) model. You can also use the TFC model with the Complex Chemistry model.

Each flamelet model describes how species and temperature is calculated in the flow field—it defines the species and temperature in the flame and after the flame. A flame position model is used to calculate the flame movement in space, for premixed and partially-premixed systems, through calculation of the turbulent flame speed.

You can select one of the following flame position models in Simcenter STAR-CCM+:

- Coherent Flame Model (CFM)
- Turbulent Flame Speed Closure (TFC)

The flamelet flame position models solve for the flame position by transporting a reaction progress variable. Normalized product species are used to define the reaction progress variable—so that it is zero for unburnt reactants and one for burnt products at chemical equilibrium.

Coherent Flame Model (CFM)

The CFM model solves an additional transport equation for the Flame Surface Density, which represents the extent of convolution of the premixed flame. The Flame Surface Density is then used to calculate the source term for the reaction progress variable. The CFM model is designed for simulating flames where the fuel and oxidizer are perfectly mixed before entering the computational domain.

To initiate combustion, the CFM model provides the **Flame Area Density ignitor**, accessible by right-clicking the **Continuum** > **Ignitors** node. While active, the Flame Area Density ignitor applies its specified value to the cells that are contained within the ignitor parts. When inactive, this ignitor does not affect the values of flame area density.

Turbulent Flame Speed Closure (TFC)

The TFC model uses an algebraic expression, called the turbulent flame speed, to calculate the source term for the mean reaction progress variable equation (for Flamelets) or the species (for Complex Chemistry).

To initiate combustion,

- The flamelet TFC model provides the **Progress Variable Ignitor** that you access by right-clicking the **Continuum** > **Ignitors** node. While active, the Progress Variable ignitor applies its specified progress variable to the cells that are contained within the ignitor parts. When inactive, this ignitor does not affect the values of the progress variable.
- The complex chemistry TFC model provides the **Fixed Temperature Ignitor** that you access by right-clicking the **Continuum** > **Ignitors** node. When the Fixed Temperature Ignitor is on, the temperature that chemical reactions are evaluated at is set to the constant temperature defined in the **Ignitors** node.
- For any unsteady TFC setups, you can also use any of the spark models to initiate combustion.

Flamelet Tables

Flamelet library tables are precomputed laminar flames that are parametrized by a few thermodynamic variables. Turbulent fluctuations are included in the tables.

Combustion models can lookup these tables and access data through a vector of independent variables. The tables store data independently of the combustion model which avoids a high computational cost while providing accurate results.

Each thermodynamic state of a given temperature and composition, is parametrized by mixture fraction Z, enthalpy h, and possibly other variables such as scalar dissipation χ and reaction progress variable c.

You can create flamelet tables for each of the flamelet models within Simcenter STAR-CCM+. If you run Simcenter STAR-CCM+ in parallel, the flamelet table is generated in parallel. Each flamelet model table generator allows you to specify the chemistry definition, the composition of fluid streams, and several other parameters. You can choose to save flamelet tables in the .sim file, or in a separate location—which is useful to save disk space when using the same flamelet tables in different .sim files. The **[Table Generator]** > **Parameters** > **[Numerical Settings]** node contains a set of Table Dimensions, each of which provides the option to use adaptive gridding. All flamelet variables that are plotted are given in SI units, which cannot be changed—this is regardless of any preferred unit choice.

Adaptive gridding places table points such that table interpolation is accurate to a tolerance that you specify. Adaptive gridding is useful for resolving flamelet tables where the variables that are stored in the table change non-linearly. Since adaptive tables generally provide more accurate as well as smaller, tables, adaptive gridding is recommended for all table dimensions except the FGM Progress Variable Variance. For FGM Progress Varaible Variance, a single point (delta function PDF) is recommended.

When using adaptive gridding, Simcenter STAR-CCM+ starts to generate the flamelet table using an initial coarse mesh. Simcenter STAR-CCM+ then inserts a new table point midway between these existing points. If the difference between linear interpolation of the two existing points and the newly inserted point is less than the normalized tolerance, the newly inserted point is discarded. If not, the process is repeated until the maximum number of grid points are reached.

For more information about flamelet tables and adaptive gridding, see Flamelet Tables (Theory).

Simcenter STAR-CCM+ allows you to load pre-existing flamelet tables, or create them using one of the following model-specific flamelet table generators:

- Chemical Equilibrium Table Generator
  See Chemical Equilibrium Table Reference.
- SLF Table Generator
  See Steady Laminar Flamelet Table Reference.
- FGM Table Generator
  See FGM Table Reference.

For instructions on how to create a flamelet table, see Creating Flamelet Tables.

Flamelet Workflow

Follow the steps in this workflow to simulate single phase or VOF Multiphase (VOF) intraphase combustion using the flamelet models that are provided in Simcenter STAR-CCM+.

The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow.

1. For the physics continuum or Eulerian VOF phase that represents the reacting flow, select the following models—in addition to the models that are previously selected, with **Auto-Select recommended models** activated:

Group Box	Model
Reacting Flow Models	**Flamelet**
Flamelet Models	◦ For perfectly-premixed and partially-premixed flames, the **Flamelet Generated Manifold (FGM)** model is recommended. ◦ For non-premixed flames, the **Steady Laminar Flamelet** model is recommended. ◦ If no chemical mechanism is available, use the **Chemical Equilibrium** model.
Progress Variable Source (for FGM)	◦ **FGM Kinetic Rate** ◦ **Coherent Flame Model (CFM)**. ◦ **Turbulent Flame Speed Closure (TFC)**.
Flame Type (for Chemical Equilibrium or Steady Laminar Flamelet)	◦ **Non-Premixed Flame** ◦ **Partially-Premixed Flame**
Flame Propagation (required for partially-premixed flames)	◦ **Coherent Flame Model (CFM)**. ◦ **Turbulent Flame Speed Closure (TFC)**.

2. Select any Optional models.

   For example:

   - **NOx Emission** or **Soot Emissions**—to model the formation of these pollutants.
   - **Inert Stream**—allows the simulation to model an inert (chemically inactive) stream in addition to the flamelet fuel and oxidizer streams. This model allows you to define the inert stream species outside of the flamelet table, which avoids unnecessary computation of inactive species in the flamelet generation and tabulation. Useful when simulating exhaust gas recirculation (EGR) in internal combustion engines (ICE), and steam injection in gas-turbines.
   - The **Radiation** model is useful for modeling applications in which radiative heat transfer is important—as is the case for most combustion systems—such as in glass furnaces and in gas turbines. The soot emission models influence the **Participating Media Radiation (DOM)** and **Gray Thermal Radiation** models by contributing to the absorption coefficient of the continuous phase (the absorption coefficient describing both absorption and emission).
   - **Gravity**—if gravity forces significantly influence the solution, such as in fire simulations.

3. When the model selection process is complete, you then define the flamelet table. Choose one of the following options:

Using ASCII files.	You can import the chemistry definition in standard Chemkin format—using ASCII files, and then have Simcenter STAR-CCM+ generate the flamelet tables directly. See Creating Flamelet Tables.
Using a DARS library.	Alternatively, if you have a FGM or SLF library, you can import it into Simcenter STAR-CCM+ and construct the table. See Loading Library Tables.

Note: If required, you can automate the flamelet table generation using the Simulation Operations feature. See Run Flamelet Table Generator.

When the flamelet table generation is complete, you then define any properties that are required for the physics models that you are using.

4. Set the properties of any **[continuum]** > **Models** or **[phase]** > **Models**, and model sub-nodes, as required.

   Note: It is possible to specify several combustion model constants as parameters. See Global Parameters.

   For example, if you are using the CFM or TFC models, make sure that all necessary reaction constants are specified.

   - If you are using the **Flamelet Generated Manifold (FGM)** model, select the **Flamelet Generated Manifold (FGM)** > **Progress Variable Variance** node and set the method for solving the progress variable variance. See: Flamelet Generated Manifold Model Reference.
   - If you are using the **Steady Laminar Flamelet** model, by default, the Steady Laminar Flamelet model selects the **Ideal Gas** model and the **Non-Adiabatic** model—which is necessary even for insignificant heat losses/gains.
   - For the CFM model, set the following properties under the **Coherent Flame Model (CFM)** node.
     - *CFM Constant, Alpha*, α in Eqn. (3628).
     - *CFM Constant, Beta*, β, in Eqn. (3628).
     - *CFM Constant, A*, the flame surface annihilation coefficient, A.
     - *CFM Constant, B*, the flame quenching coefficient by stretch, B.
   - For the TFC model, set the *TFC Rate Coefficient, A* constant, A in Eqn. (3622), under the **Turbulent Flame Speed Closure (TFC)** > **TFC Rate Coefficient, A** node.

5. Return to the Reacting Flow General Workflow.

Contents:

Creating Flamelet Tables

You can import the chemistry definition in standard Chemkin format—using ASCII files and then have Simcenter STAR-CCM+ generate the flamelet tables directly.

You can find the **[flamelet model] Table Generator** node within physics continua (or phases) that use a flamelet model.

To speed up the flamelet table generation, you can generate flamelet tables in Simcenter STAR-CCM+ when using multiple processors in parallel.

1. Import the chemistry definition that is used to create a flamelet table in Simcenter STAR-CCM+.
   a) Right-click the **[physics continuum] / [phase]** > **[flamelet model] Table Generator** > **Chemistry Definition** node and select **Import Complex Chemistry Definition (Chemkin format)**.
   b) Select appropriate files for each of the required fields.
      - *Chemical Mechanism File*: Contains the chemistry of the reactions.
      - *Thermodynamic Properties File*: Contains details of the thermal properties.
      - *Import Transport Properties File*: Activates the import of the Transport Properties File. Importing this file is optional.
      - *Transport Properties File*: If *Import Transport Properties File* is activated, select a file which contains details of the species transport properties. If you select a transport properties file here, under the **Multi-Component Gas** > **Material Properties** node, the **Dynamic Viscosity**, **Thermal Conductivity**, and **Molecular Diffusivity** nodes then contain the option to set the *Method* to **Flamelet Table**. Simcenter STAR-CCM+ calculates the mean molecular dynamic viscosity and thermal conductivity from the flamelet species and temperature, and molecular diffusivity from the unity Lewis number assumption Eqn. (140).

   See Reaction Mechanism Formats.
2. Specify the composition and temperature of the fluid streams for flamelet generation.
   Make sure that the sum of the mass fractions or mole fractions for each stream equals `1.0`.
   a) Select the **[flamelet model] Table Generator** > **Fluid Streams** > **Fuel** node and specify the components of the fuel stream. If the fuel is premixed or partially-premixed with the oxidizer, include the correct proportions of fuel and oxidizer within this stream.
   b) Select the **[flamelet model] Table Generator** > **Fluid Streams** > **Oxidizer** node and specify the components of the oxidizer stream. By default, the composition of the oxidizer stream is set to that of air.

   See Fluid Streams Reference.
3. If you are creating an FGM flamelet table, select the **[flamelet model] Table Generator** > **Reactor Type** node and set one of the following options:
   - **0D Ignition**—is the default.
   - **1D Premixed**—is the most appropriate when modeling premixed combustion.

   See Reactor Type.
4. Specify the table parameters under the **[flamelet model] Table Generator** > **Parameters** node.

Absolute Pressure	Set the table pressure.
Species for Tabulation	By default, the specified fuel and oxidizer species, as well as CO2 and H2O, are selected. However, make sure that you specify any more species that are to be included in the table. For example, you can add CO for monitoring emissions, or OH for monitoring the position of the flame front. When modeling NOx emissions, do not select any NOx species for tabulation.

Emissions	To model NOx and/or soot emissions, activate *Thermal NOx* and/or *Soot Moments*. NOx and/or soot source terms for the transport equation are tabulated during the generation of the table. Coefficients for NOx/soot are included in the final table and are transported as a passive scalar.
Numerical Settings	Default values are suitable in the majority of cases.
Species Weights	The default progress variable species weights are defined for CO and CO2—which is appropriate for the majority of hydrocarbon combustion simulations.
Heat Loss Ratio Range	Specify the range for the heat loss ratio. If heat loss ratio warnings appear, increase the enthalpy space that is covered in the flamelet table—or for better resolution, decrease it. For simulations that involve heat loss only, with no heat gain, you can set the minimum heat loss ratio limit to 0 and the maximum heat loss ratio to 1.0.

See,

- FGM Table Reference: Parameters
- Steady Laminar Flamelet Table Reference: Parameters
- Chemical Equilibrium Table Reference: Parameters

When trying to reach a flamelet table grid independent solution, you can refine the grid resolution—for adaptive gridding tables you can decrease the tolerance, or for fixed tables you can increase the number of data points—then re-converge the solution until it stops changing.

5. If necessary, refine the flamelet table dimensions (grid resolution).
   a) Expand the **[flamelet model] Table Generator** > **[flamelet model] Table** node.
   b) Select each of the dimensions.
   c) Adjust the *Table Dimension* property as required for each dimension node.

   See Table Dimensions Reference.

When the flamelet table is set up, you generate the flamelet table.

6. Right-click the **[flamelet model] Table Generator** > **[flamelet model] Table** node and select **Generate Library and Construct Table**.

   The time taken to generate the table varies depending on the number of dimensions and the level of refinement. The progress is described in the *Output* window.

   Note: If you run out of memory generating or importing large tables in parallel, use an MPI that supports the 3.1 standard, like Open MPI or Intel MPI.

You can create XY Plots to visualize the values that are stored in a flamelet table for each variable. You can use XY plots to make sure that the heat loss ratio covers the full range of temperatures that are required for certain mixture fractions.

7. To visualize values for variables that are stored in the flamelet table:
   a) Right-click the **[flamelet model] Table Generator** > **[flamelet model] Table** > **[flamelet model] XY Plots** node, then select **New Plot** and the **[variable]** to plot.

b) Right-click the **[flamelet model] XY Plots** > **[variable]** node and select **Add New Table View for Plotting**.

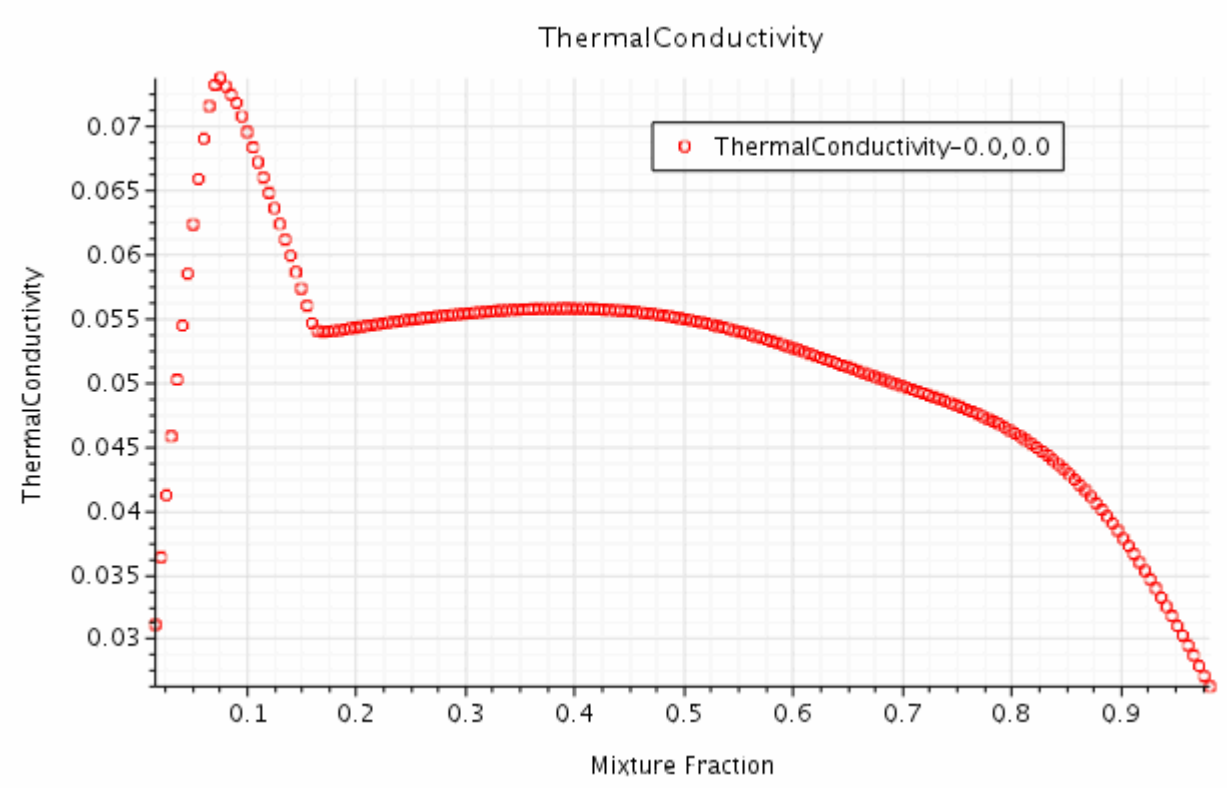
c) In the *Select Points for Plotting* dialog, enter the parameters that are required for the table and click **OK**.

d) To display the XY plot, double-click the **[flamelet model] XY Plots** > **[variable]** node.

See Flamelet Table XY Plots Reference.

If required, you can also change the *X-Axis Variable* property to display different grid resolution variables.

For example, the following XY plot shows the thermal conductivity variable for the mixture fraction grid resolution variable:



Note: Flamelet tables generally contain a large number of tabulated variables, including species and temperature. Cell values of a tabulated variable are not calculated until the variable is displayed in a plot or scene. Hence, when a new plot or scene is created, the variable is displayed as zero and only updated after an iteration.

If required, you can print a summary of the table conditions.

8. To print a summary of the table conditions that were used to generate the table, right-click the **[flamelet model] Table** node and select **Print Table Summary**.

   The *Output* window displays a summary of the table parameters and conditions with which the table was built.

   If a table exists, it is not possible to change a constant value for the table conditions in the GUI. However, table conditions can be changed, without deleting the table first, using global parameters instead of constant values for the conditions. See Global Parameters.

When executing the **Print Table Summary** action for tables that use global parameters, if the conditions differ from those that were specified when the table was built, a warning is displayed in the *Output* window at each iteration. These warnings are not displayed for tables that are imported from Simcenter STAR-CCM+ versions prior to 2410, or from tables that are constructed using DARS libraries.

Loading FGM Library Tables

You can import an FGM library file into Simcenter STAR-CCM+—in which you can then construct the table.

To load a library table:

1. Right-click the **[physics continuum]** > **FGM Table Generator** > **FGM Table** node and select **Import FGM User Library File and Construct Table...**.
2. In the *Open* dialog, select an appropriate `.tbl` file.

Since tables are saved in single precision, *Table Precision*—under the **FGM Table Generator** > **Parameters** node—is switched to `Single` after importing a table.

Flamelet Reference

This section provides reference material, including properties, sub-nodes, field functions, and other model-specific settings, for all of the flamelet models.

Contents:

Chemical Equilibrium Model Reference

The Chemical Equilibrium model assumes local instantaneous chemical equilibrium conditions.

In this model, a few parametric variables such as the mean mixture fraction (and in non-adiabatic cases, the mean enthalpy) are tracked on the grid. The mean species concentrations, temperature, and density are obtained as functions of the mean parametric variables, after an averaging process around a presumed probability distribution (PPDF) that is considered to represent turbulent fluctuations.

Chemical Equilibrium Model Reference

Theory	See Chemical Equilibrium.	
Provided By	**[physics continuum]** > **Models** > *Flamelet Models*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Chemical Equilibrium**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet**	
Properties	Key properties are: Active Species, Dissipation Constant, Number of Streams. See Chemical Equilibrium Model Properties.	
Activates	Physics Models	*Equation of State*: **Ideal Gas** *Energy Option*: **Non-Adiabatic***
	Reference Values	Minimum Allowable Temperature, Maximum Allowable Temperature. See Reference Values.
	Boundary Settings	Wall Combustion Scalar Option
	Region Settings	See Region Settings
	Material Properties	See Materials and Methods
	Other Continuum Nodes	Chemical Equilibrium Table Generator. See Chemical Equilibrium Table Reference.
	Monitors	**MixFrac0**: Mixture Fraction 0 **MixFracVar0**: Mixture Fraction Variance 0
	Solvers	PPDF Combustion See also: CFM Combustion Solver Properties and TFC Combustion Solver Properties
	Field Functions	Chemistry Heat Release Rate Indicator, Mixture Fraction 0, Mixture Fraction Variance 0. See Field Functions.
	Simulation Operations	See Run Flamelet Table Generator.

*The **Non-Adiabatic** model is selected by default when the Chemical Equilibrium model is selected with *Auto-select recommended models* activated. If required, you can deselect **Non-Adiabatic** and select **Adiabatic** instead. Both the **Non-Adiabatic** and **Adiabatic** models provide properties that relate to the Chemical Equilibrium model. See Adiabatic and Non-Adiabatic Model Properties.

Chemical Equilibrium Model Properties

Active Species

Read only. Displays, from the species that are available for post-processing in the flamelet table, a sub-set of species that are accessed, used, or interpolated during the simulation. For example, species that are used in plots, reports, monitors, scenes, or custom field functions. The remaining post-processing species in the flamelet table that are not accessed during the simulation are inactive.

Dissipation Constant

Represents the ratio of velocity and chemical species fluctuations.

Reference Values

Minimum Allowable Temperature

The smallest temperature value that is permitted anywhere in the continuum.

The Energy models (Coupled Energy, Coupled Solid Energy, Segregated Solid Energy, Segregated Fluid Enthalpy, Segregated Fluid Temperature) limit temperature corrections such that the corrected value does not go below this minimum. If this occurs, a message is printed to the *Output* window.

Maximum Allowable Temperature

The largest temperature value that is permitted anywhere in the continuum.

The Energy models (Coupled Energy, Coupled Solid Energy, Segregated Solid Energy, Segregated Fluid Enthalpy, Segregated Fluid Temperature) limit temperature corrections such that the corrected value does not exceed this maximum. If this occurs, a message is printed to the *Output* window.

Boundary Settings

Wall Combustion Scalar

Selects the scalars for the wall combustion calculation.

See Wall Combustion Scalar Option.

Region Settings

Applies to any region:

Flamelet Sources Option

Provides the *Flamelet Sources Term* property which when activated creates the following physics conditions:

- **Mixture Fraction Source Option**
- **Mixture Fraction Variance Source Option**

Mixture Fraction Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None No source term is defined.	None.
Add to Built-In Source Term	**Mass Source** Allows you to define a new source term for the mass fraction that is associated with the mixture fraction. This source term is added to the existing source term in the mixture fraction transport equation. **Mass Source Pressure Derivative** Allows you to define a new source term to represent the derivative of the **Mass Source** with respect to pressure. This source term is added to the existing source term linearization in the mixture fraction transport equation. **Mixture Fraction User Source** Allows you to define a new source term to add to the existing source term in the mixture fraction transport equation. **Mixture Fraction User Source Jacobian** Allows you to define a new source term linearization to add to the existing source term linearization in the mixture fraction transport equation.

User Source Term	**Corresponding Physics Values Nodes**
Replace Built-In Source Term	**Mass Source** Allows you to define a new source term for the mass fraction that is associated with the mixture fraction. This source term replaces the existing source term in the mixture fraction transport equation. **Mass Source Pressure Derivative** Allows you to define a new source term to represent the derivative of the **Mass Source** with respect to pressure. This source term linearization replaces the existing source term linearization in the mixture fraction transport equation. **Mixture Fraction User Source** Allows you to define a new source term to replace the existing source term in the mixture fraction transport equation. **Mixture Fraction User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the mixture fraction transport equation.

Mixture Fraction Variance Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None No source term is defined.	None.

User Source Term	**Corresponding Physics Values Nodes**
Add to Built-In Source Term	**Mixture Fraction Variance User Source** Allows you to add a new source term to add to the existing sources in the mixture fraction variance transport equation. **Mixture Fraction Variance User Source Jacobian** Allows you to add a new source term linearization to add to the existing sources linearization in the mixture fraction variance transport equation.
Replace Built-In Source Term	**Mixture Fraction Variance User Source** Allows you to define a new source term to replace the existing source term in the mixture fraction variance transport equation. **Mixture Fraction Variance User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the mixture fraction variance transport equation.

Materials and Methods

Turbulent Schmidt Number

σ_t in all applicable scalar transport equations, except when the **Adiabatic** or **Non-Adiabatic** model property, *Separate Turbulent Schmidt Number* is activated. If values are specified separately (for **Turbulent Schmidt Number for Mixture Fraction**, or **Turbulent Schmidt Number for Mixture Fraction Variance**), this **Turbulent Schmidt Number** property setting applies to all instances of the turbulent Schmidt number other than those that are specified separately.

Turbulent Schmidt Number for Mixture Fraction

Available when the **Adiabatic** or **Non-Adiabatic** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,Z}$ that is specifically applied to the mixture fraction Z transport equation Eqn. (3560).

Turbulent Schmidt Number for Mixture Fraction Variance

Available when the **Adiabatic** or **Non-Adiabatic** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,Z_{\mathrm{var}}}$ that is specifically applied to the mixture fraction variance Z_{var} transport equation Eqn. (3561).

PPDF Combustion Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

URF for Mixture Fraction

Appears only when the solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the mixture fraction Z in Eqn. (3560).

URF for Mixture Fraction Variance

Appears only when the solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the mixture fraction variance Z_{var} in Eqn. (3561).

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Separate URF Numbers

When activated, the *Under-Relaxation Factor* property for the solver is removed and replaced by separate URF properties for each relevant transport equation. For example, *URF for Mixture Fraction* and *URF for Mixture Fraction Variance*.

Field Functions

Chemistry Heat Release Rate Indicator

The chemistry heat release rate is $\dot{h}$ in Eqn. (3436) for the partially-premixed Chemical Equilibrium model, and is not available for the non-premixed Chemical Equilibrium model.

Mixture Fraction 0

Represents the atomic mass fraction that originated from the fuel stream.

Mixture Fraction Variance 0

Represents the turbulent fluctuations in the fuel mixture fraction values.

Adiabatic and Non-Adiabatic Model Properties

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.
- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.
- **Boundaries Only**: Solves for the boundary secondary gradients only.

Flow Boundary Diffusion

When activated, this property includes the flow-boundary diffusion fluxes (or viscous fluxes for flow models) as given by Eqn. (908). This property is activated by default.

Separate Turbulent Schmidt Number

When activated, allows you to specify a different turbulent Schmidt number for each flamelet transport equation that is applicable—such as the transport equations for unnormalized progress variable y Eqn. (3599), unnormalized progress variable variance y_{var} Eqn. (3603), mixture fraction Z Eqn. (3560), and mixture fraction variance Z_{var} Eqn. (3561).

It is only possible to specify custom turbulent Schmidt numbers for y_{var} and Z_{var} when the relevant flamelet table contains multiple points in the y_{var} and Z_{var} table dimensions—and additionally, if the **Transport Equation** method is used to calculate them.

Contents:

Chemical Equilibrium Table Reference

The Chemical Equilibrium model uses a flamelet table called the Chemical Equilibrium Table.

Chemical Equilibrium Table Generator

Properties

None

Right-Click Actions

`Import Table`...

Loads a previously saved Chemical Equilibrium table.

> **Note:** Since tables are saved in single precision, *Table Precision*—under the **Chemical Equilibrium Table Generator** > **Parameters** node—is switched to `Single` after importing a table.

`Delete Table`

Removes a stored table from memory. The flamelet table must be deleted before making changes to the table settings.

`Stop Calculations`

Stops the calculations during the flamelet library generation.

Child Nodes

The Chemical Equilibrium Table Generator node contains the following sub-nodes:

- Chemistry Definition
- Fluid Streams (see Fluid Streams Reference)
- Parameters
- Chemical Equilibrium Table

Chemistry Definition

The Chemistry Definition describes the species and their thermodynamic properties, from which chemical equilibrium is calculated.

Properties

None

Right-Click Actions

`Import Complex Chemistry Definition (Chemkin format)`

Activates a standard *Open* dialog that imports a library file for the complex chemistry definition in Chemkin™ format.

`Select Mixture Components`

Opens a dialog which allows you to manually select the species from the Material Databases that are available. Use this option if you don't have a Chemkin format mechanism with the species.

`Delete Complex Chemistry Definition`

Removes the library that is used for the chemistry definition.

Parameters

Properties

Table Precision

Specifies the precision—`Single` or `Double`—to which the flamelet table is generated. The default is `Single`.

Child Nodes

Absolute Pressure

Value

The pressure that is used when generating the flamelet table.

Species for Tabulation

Species

Allows you to select which species are stored in the flamelet table. These species are then made available in a simulation, for example, to use for post-processing in contours or reports.

Emissions

Thermal NOx

When activated, the NOx source term coefficients are calculated and tabulated.

Numerical Settings

Minimum Temperature

Specifies the minimum temperature for enthalpy normalization in the flamelet table.

Numerical Settings > Table Dimensions

Allows you to define the dimensions for the flamelet table. See Table Dimensions Reference.

Heat Loss Ratio Range

Specifies the heat loss ratio range. You can increase the enthalpy space that is covered in the Flamelet table in response to heat loss ratio warnings, or decrease it for better resolution. For example, if your simulation involves heat loss only, with no heat gain, you can set the minimum heat loss ratio limit to 0 and the maximum heat loss ratio to 1.0.

You can set either the minimum heat loss ratio limit or the maximum heat loss ratio limit to 0, but you cannot have both set to 0 at the same time.

Minimum Heat Loss Ratio

Sets the minimum heat loss ratio limit.

Maximum Heat Loss Ratio

Sets the maximum heat loss ratio limit. However, if the resulting minimum temperature drops below a physical limit, the temperature is clipped to the table minimum temperature that is specified at the table generation.

Chemical Equilibrium Table

Properties

Save Table in .sim File

When activated, stores the flamelet table in the sim file. When deactivated, the flamelet table is not stored in the .sim file—which is useful to save disk space when using the same flamelet table in different .sim files, or when auto-saving many sim files. If the flamelet table is required for future use, you must export it manually by right-clicking the flamelet table node and selecting Export Table. Then save it separately from the .sim file.

Path for Table Read

Specifies the file path location of the flamelet table file that has been exported from Simcenter STAR-CCM+ and saved previously. Useful to reduce the .sim file size and save disk space when several .sim files use the same flamelet table.

Verbosity

When activated, if selected tolerance criteria are not met in adaptive grid generation steps, Simcenter STAR-CCM+ prints a summary of tolerance warnings to the *Output* window at each step during the table generation.

For example:

```
WARNING: For 'Heat Loss Ratio' the   maximum error of 0.00652988 is
greater than the specified tolerance of 0.0001. To achieve the prescribed
tolerance, delete the table, increase the maximum number of points
(currently 9) and regenerate the table.
```

When deactivated, all of the warning messages about exceeding the defined tolerance for adaptive table dimensions are hidden.

High Mixture Fraction Limit

For mixture fraction values above a certain limit, the mixture can fail to burn because it is too fuel-rich. Simcenter STAR-CCM+ does not perform the chemical equilibrium calculation above this limit, but calculates a composition for a non-reacting state that is based on pure mixing. To impose this non-reacting state, set this property at less than 1.0.

High Limit Window Size

Allows for a gradual change in flow properties from the reacting to the non-reacting state. Specifically, when you set High Mixture Fraction Limit to a value less than 1.0, the transition from the reacting

chemical equilibrium state to the non-reacting pure mixing state can be abrupt as well as discontinuous. The greater the High Limit Window Size (from 0.0 through 1.0), the smoother the transition between the two states.

Right-Click Actions

`Generate Chemical Equilibrium and Construct Table`

Generates Chemical Equilibrium flamelet libraries and constructs flamelet table.

`Print Estimated Maximum Table Size`

Prints the estimated maximum table size (in KB) in the output window. This value also appears as a read-only property of the **Table Dimensions** node.

`Export Table`

Saves a table that is stored in Simcenter STAR-CCM+'s memory to a file with extension `.tbl`.

`Delete Table`

Removes a stored table from memory. The flamelet table must be deleted before making changes to the table settings.

`Stop Calculations`

Stops the calculations during the flamelet library generation.

`Print Table Summary`

The *Output* window displays a summary of the table parameters and conditions with which the table was built. When running the simulation, if the current parameters and conditions differ from those that were specified when the table was built, a warning is displayed in the *Output* window at each iteration.

Parameters and conditions are not displayed for tables that are imported from Simcenter STAR-CCM+ versions prior to 2410, or from tables that are constructed using DARS libraries.

Child Nodes

Final Table Grid Size

Contains sub-nodes for each of the table dimensions. Each table dimensions sub-node displays the read only, *Number of Grid Points*, that are used from the data for that parameter. The values are specified before building the table by defining settings under the **Table Dimensions** node. See Table Dimensions Reference.

Chemical Equilibrium XY Plots

To visualize the chemical equilibrium flamelet table, you can create an XY plot—right-click this node and select New Plot. See Flamelet Table XY Plot Reference.

Steady Laminar Flamelet Model Reference

The Steady Laminar Flamelet model accounts for chemical non-equilibrium and finite-rate chemistry effects in turbulent non-premixed flames.

In this model, a few parametric variables such as the mean mixture fraction (and in non-adiabatic cases, the mean enthalpy) are tracked on the grid. The mean species concentrations, temperature, and density are obtained as functions of the mean parametric variables, after an averaging process around a presumed probability distribution (PPDF) that is considered to represent turbulent fluctuations.

Steady Laminar Flamelet Model Reference

Theory	See Steady Laminar Flamelet.	
Provided By	**[physics continuum]** > **Models** > *Flamelet Models*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Steady Laminar Flamelet**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet**	
Properties	Key properties are: Active Species, Dissipation Constant, Number of Streams. See Steady Laminar Flamelet Model Properties.	
Activates	Physics Models	*Equation of State*: **Ideal Gas** *Energy Option*: **Non-Adiabatic***
	Reference Values	Minimum Allowable Temperature, Maximum Allowable Temperature. See Reference Values.
	Boundary Settings	Wall Combustion Scalar Option
	Region Settings	See Region Settings
	Material Properties	See Materials and Methods
	Other Continuum Nodes	SLF Table Generator. See Steady Laminar Flamelet Table Reference .
	Solvers	PPDF Combustion See also: CFM Combustion Solver Properties or TFC Combustion Solver Properties
	Field Functions	Chemistry Heat Release Rate Indicator, Mixture Fraction 0, Mixture Fraction Variance 0, Scalar Dissipation Rate. See Field Functions.
	Simulation Operations	See Run Flamelet Table Generator.

*The **Non-Adiabatic** model is selected by default when the Steady Laminar Flamelet model is selected with *Auto-select recommended models* activated. If required, you can deselect **Non-Adiabatic** and select **Adiabatic** instead. Both the **Non-Adiabatic** and **Adiabatic** models provide properties that relate to the Steady Laminar Flamelet model. See Adiabatic and Non-Adiabatic Model Properties.

Steady Laminar Flamelet Model Properties

Active Species

Read only. Displays, from the species that are available for post-processing in the flamelet table, a sub-set of species that are accessed, used, or interpolated during the simulation. For example, species that are used in plots, reports, monitors, scenes, or custom field functions. The remaining post-processing species in the flamelet table that are not accessed during the simulation are inactive.

Dissipation Constant

Represents the ratio of velocity and chemical species fluctuation time scales.

Number of Streams

The Steady Laminar Flamelet model allows you to have two streams.

Reference Values

Minimum Allowable Temperature

The smallest temperature value that is permitted anywhere in the continuum.

The Energy models (Coupled Energy, Coupled Solid Energy, Segregated Solid Energy, Segregated Fluid Enthalpy, Segregated Fluid Temperature) limit temperature corrections such that the corrected value does not go below this minimum. If this occurs, a message is printed to the *Output* window.

Maximum Allowable Temperature

The largest temperature value that is permitted anywhere in the continuum.

The Energy models (Coupled Energy, Coupled Solid Energy, Segregated Solid Energy, Segregated Fluid Enthalpy, Segregated Fluid Temperature) limit temperature corrections such that the corrected value does not exceed this maximum. If this occurs, a message is printed to the *Output* window.

Materials and Methods

Turbulent Schmidt Number

σ_t in all applicable scalar transport equations, except when the **Adiabatic** or **Non-Adiabatic** model property, *Separate Turbulent Schmidt Number* is activated. If values are specified separately (for **Turbulent Schmidt Number for Mixture Fraction**, or **Turbulent Schmidt Number for Mixture Fraction Variance**), this **Turbulent Schmidt Number** property setting applies to all instances of the turbulent Schmidt number other than those that are specified separately.

Turbulent Schmidt Number for Mixture Fraction

Available when the **Adiabatic** or **Non-Adiabatic** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,Z}$ that is specifically applied to the mixture fraction Z transport equation Eqn. (3560).

Turbulent Schmidt Number for Mixture Fraction Variance

Available when the **Adiabatic** or **Non-Adiabatic** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\ Z_{\mathrm{var}}}$ that is specifically applied to the mixture fraction variance Z_{var} transport equation Eqn. (3561).

Boundary Settings

Wall Combustion Scalar

Selects the scalars for the wall combustion calculation.

See Wall Combustion Scalar Option.

Region Settings

Applies to any region:

Flamelet Sources Option

Provides the *Flamelet Sources Term* property which when activated creates the following physics conditions:

- **Mixture Fraction Source Option**
- **Mixture Fraction Variance Source Option**

Mixture Fraction Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None No source term is defined.	None.

User Source Term	**Corresponding Physics Values Nodes**
Add to Built-In Source Term	**Mass Source** Allows you to define a new source term for the mass fraction that is associated with the mixture fraction. This source term is added to the existing source term in the mixture fraction transport equation. **Mass Source Pressure Derivative** Allows you to define a new source term to represent the derivative of the **Mass Source** with respect to pressure. This source term is added to the existing source term linearization in the mixture fraction transport equation. **Mixture Fraction User Source** Allows you to define a new source term to add to the existing source term in the mixture fraction transport equation. **Mixture Fraction User Source Jacobian** Allows you to define a new source term linearization to add to the existing source term linearization in the mixture fraction transport equation.

User Source Term	**Corresponding Physics Values Nodes**
Replace Built-In Source Term	**Mass Source** Allows you to define a new source term for the mass fraction that is associated with the mixture fraction. This source term replaces the existing source term in the mixture fraction transport equation. **Mass Source Pressure Derivative** Allows you to define a new source term to represent the derivative of the **Mass Source** with respect to pressure. This source term linearization replaces the existing source term linearization in the mixture fraction transport equation. **Mixture Fraction User Source** Allows you to define a new source term to replace the existing source term in the mixture fraction transport equation. **Mixture Fraction User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the mixture fraction transport equation.

Mixture Fraction Variance Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None No source term is defined.	None.

User Source Term	**Corresponding Physics Values Nodes**
Add to Built-In Source Term	**Mixture Fraction Variance User Source** Allows you to add a new source term to add to the existing sources in the mixture fraction variance transport equation. **Mixture Fraction Variance User Source Jacobian** Allows you to add a new source term linearization to add to the existing sources linearization in the mixture fraction variance transport equation.
Replace Built-In Source Term	**Mixture Fraction Variance User Source** Allows you to define a new source term to replace the existing source term in the mixture fraction variance transport equation. **Mixture Fraction Variance User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the mixture fraction variance transport equation.

PPDF Combustion Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

URF for Mixture Fraction

Appears only when the solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the mixture fraction Z in Eqn. (3560).

URF for Mixture Fraction Variance

Appears only when the solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the mixture fraction variance Z_{var} in Eqn. (3561).

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Separate URF Numbers

When activated, the *Under-Relaxation Factor* property for the solver is removed and replaced by separate URF properties for each relevant transport equation. For example, *URF for Mixture Fraction* and *URF for Mixture Fraction Variance*.

Field Functions

Chemistry Heat Release Rate Indicator

The chemistry heat release rate is $\dot{h}$ in Eqn. (3433) for the partially-premixed SLF model, and Eqn. (3436) for the non-premixed SLF model.

Mixture Fraction 0

Represents the atomic mass fraction that originated from the fuel stream.

Scalar Dissipation Rate

χ in Eqn. (3593).

Adiabatic and Non-Adiabatic Model Properties

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.
- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.

- **Boundaries Only**: Solves for the boundary secondary gradients only.

Flow Boundary Diffusion

When activated, this property includes the flow-boundary diffusion fluxes (or viscous fluxes for flow models) as given by Eqn. (908). This property is activated by default.

Separate Turbulent Schmidt Number

When activated, allows you to specify a different turbulent Schmidt number for each flamelet transport equation that is applicable—such as the transport equations for unnormalized progress variable y Eqn. (3599), unnormalized progress variable variance y_{var} Eqn. (3603), mixture fraction Z Eqn. (3560), and mixture fraction variance Z_{var} Eqn. (3561).

It is only possible to specify custom turbulent Schmidt numbers for y_{var} and Z_{var} when the relevant flamelet table contains multiple points in the y_{var} and Z_{var} table dimensions—and additionally, if the **Transport Equation** method is used to calculate them.

Contents:

Steady Laminar Flamelet Table Reference

This section describes the parameters that you set for the SLF Table which the Steady Laminar Flamelet model uses.

SLF Table Generator

Properties

None

Right-Click Actions

`Import Table`...

Imports a previously saved SLF table.

> **Note:** Since tables are saved in single precision, *Table Precision*—under the **SLF Table Generator** > **Parameters** node—is switched to `Single` after importing a table.

`Delete Table`

Removes a stored table from memory. The flamelet table must be deleted before making changes to the table settings.

`Stop Calculations`

Stops the calculations during the flamelet library generation.

Child Nodes

The SLF Table Generator node contains the following sub-nodes:

- Chemistry Definition
- Fluid Streams (see Fluid Streams Reference)
- Parameters
- SLF Table

Chemistry Definition

The Chemistry Definition describes the chemical reaction mechanism, which is the collection of all species in a reaction—reactants, intermediates, and products—and the corresponding set of all reactions. The Chemistry Definition also includes the thermodynamic properties, as well as, optionally, the transport properties.

Properties

None

Right-Click Actions

`Import Complex Chemistry Definition (Chemkin format)`

Activates a standard *Open* dialog that imports a library file for the complex chemistry definition in Chemkin™ format. Upon importing a chemistry definition, the reactions for the definition appear as sub-nodes of the Chemistry Definition node.

If you import transport data along with the chemical mechanism and thermal data, Simcenter STAR-CCM+ tabulates the molecular transport properties for the Dynamic Viscosity, Molecular Diffusivity, and Thermal Conductivity material properties. You can then choose to use these tabulated molecular transport properties after table generation, in the Multi-Component Gas node, by selecting the `Flamelet Table` option for each of the Material Properties.

`Delete Complex Chemistry Definition`

Removes the species and the corresponding reactions from the chemistry definition.

Parameters

Properties

Table Precision

Specifies the precision—`Single` or `Double`—to which the flamelet table is generated. The default is `Single`.

Child Nodes

Absolute Pressure

Value: The pressure that is used when generating the flamelet table.

Species for Tabulation

Species: Allows you to select which species are stored in the flamelet table. These species are then made available in a simulation, for example, to use for post-processing in contours or reports.

Emissions

Thermal NOx

When activated, the NOx source-term coefficients are calculated and tabulated.

Soot Moment

When activated, the soot moment model source-term coefficients are calculated and tabulated. Creates a **Soot Moments Options** sub-node which allows you to specify the *Nucleation Option* as either:

- **C2H2**, see Eqn. (3748).
- **Single PAH Species (C16H10)**, see Eqn. (3745) and Eqn. (3746). The PAH precursor is recognised as any species which includes either A4 or A3R5 in the species name, or has the composition C16H10.

Numerical Settings

The Numerical Settings node allows you to define the following properties. It also contains the **Table Dimensions** sub-node which you can use to define the dimensions for the flamelet table. See Table Dimensions Reference.

- *Absolute Tolerance*: Specifies the absolute tolerance of the ODE solver.
- *Relative Tolerance*: Specifies the relative tolerance of the ODE solver.
- *Flamelet Relative Tolerance*: The flamelet equations are integrated in time using the ODE solver Absolute Tolerance and Relative Tolerance until steady-state. Steady state is determined when the average residual over all species and temperature and all grid points is less than the Flamelet Relative Tolerance.
- *Initial Scalar Dissipation (/s)*: Specifies the scalar dissipation rate, χ in Eqn. (3412), for the first steady laminar flamelet.
- *Maximum Scalar Dissipation (/s)*: Specifies the largest scalar dissipation, χ in Eqn. (3412), that is allowed. Usually, flamelets extinguish well before this value. See Scalar Dissipation Rate.
- *Scalar Dissipation Multiplier*: The sequence of flamelet scalar dissipation rates are calculated as follows: Starting from the initial scalar dissipation rate, the next scalar dissipation is multiplied by 10/s (if the current scalar dissipation is less than 1/s). Else it is multiplied by the scalar dissipation multiplier, until either the flamelet extinguishes or else the maximum scalar dissipation rate is exceeded. See Scalar Dissipation Rate.

SLF Table

Properties

Save Table in .sim File

When activated, stores the flamelet table in the sim file. When deactivated, the flamelet table is not stored in the .sim file—which is useful to save disk space when using the same flamelet table in different .sim files, or when auto-saving many sim files. If the flamelet table is required for future use, you must export it manually by right-clicking the flamelet table node and selecting Export Table. Then save it separately from the .sim file.

Path for Table Read

Specifies the file path location of the flamelet table file that has been exported from Simcenter STAR-CCM+ and saved previously. Useful to reduce the .sim file size and save disk space when several .sim files use the same flamelet table.

Verbosity

When activated, if selected tolerance criteria are not met in adaptive grid generation steps, Simcenter STAR-CCM+ prints a summary of tolerance warnings to the *Output* window at each step during the table generation.

For example:

```
WARNING: For 'Heat Loss Ratio' the   maximum error of 0.00652988 is
greater than the specified tolerance of 0.0001. To achieve the prescribed
tolerance, delete the table, increase the maximum number of points
(currently 9) and regenerate the table.
```

When deactivated, all of the warning messages about exceeding the defined tolerance for adaptive table dimensions are hidden.

Right-Click Actions

`Generate Flamelet Library and Construct Table`

Generates steady laminar flamelet libraries and constructs the presumed probability density function (PPDF) table.

`Print Estimated Maximum Table Size`

Prints the estimated maximum table size (in KB) in the output window. This value also appears as a read-only property of the **Table Dimensions** node.

`Export Table`

Saves a table that is stored in the memory of Simcenter STAR-CCM+ to a file with extension `.tbl`.

`Delete Table`

Removes a stored table from memory. The flamelet table must be deleted before making changes to the table settings.

`Stop Calculations`

Stops the calculations during the flamelet library generation.

`Print Table Summary`

The *Output* window displays a summary of the table parameters and conditions with which the table was built. When running the simulation, if the current parameters and conditions differ from those that were specified when the table was built, a warning is displayed in the *Output* window at each iteration.

Parameters and conditions are not displayed for tables that are imported from Simcenter STAR-CCM+ versions prior to 2410, or from tables that are constructed using DARS libraries.

Child Nodes

Final Table Grid Size

Contains sub-nodes for each of the table dimensions. Each table dimensions sub-node displays the read only value, *Number of Grid Points*, that are used from the data for that parameter. The values are specified before building the table by defining settings under the **Table Dimensions** node. See Table Dimensions Reference.

SLF XY Plots

To visualize the steady laminar flamelet table, you can create an XY plot—right-click this node and select New Plot. See Flamelet Table XY Plots Reference.

Flamelet Generated Manifold Model Reference

The Flamelet Generated Manifold (FGM) model is designed to approximate complex chemical mechanisms with a reduced computational cost.

FGM Model

For simulations involving combustion, it is often important to include a detailed reaction mechanism, which has many reactions and many species. Inclusion of such a mechanism in a CFD simulation with realistic geometries, however, inevitably leads to a large computational cost.

In the FGM model, the effects of detailed chemistry on combustion are stored in a Flamelet table and the required values are retrieved during the CFD simulation. A progress variable is used to facilitate interactions between CFD computation and the Flamelet table.

FGM Model Reference

Theory	See Flamelet Generated Manifold.
Provided By	**[physics continuum]** > **Models** > *Flamelet Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Flamelet Generated Manifold (FGM)**
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet**
Properties	Key properties are: **FGM Constant, Alpha**. See FGM Model Properties.

Activates	Physics Models	**FGM Reaction** and **Ideal Gas Equation of State for FGM**
	Model Controls (child nodes)	**Mixture Fraction Variance** **Progress Variable Variance** See Model Controls
	Material Properties	See Materials and Methods
	Initial Conditions	**Mixture Fraction Profile** and **Mixture Fraction Variance Profile**. See Initial Conditions.
	Boundary Settings	**Wall Combustion Scalar Option**. See Boundary Settings.
	Region Settings	**Active Reactions Option**, **Flamelet Sources Option**. See Region Settings.
	Other Continuum Nodes	• **FGM Table**. See FGM Table Reference. • The **Ignitors** node provides the right-click option to create a **Progress Variable Ignitor**. See Ignitors.
	Solvers	FGM Combustion
	Field Functions	Chemistry Heat Release Rate Indicator, Combustion Scalar Diffusion Coefficient, Heat Loss Ratio, Mach Number, Mixture Fraction 0, Mixture Fraction Variance 0, Progress Variable. See Field Functions.
	Simulation Operations	See Run Flamelet Table Generator.

Flamelet Generated Manifold (FGM) Model Properties

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

FGM Constant, Alpha

A scaling factor multiplying the progress variable source term.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.

- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.
- **Boundaries Only**: Solves for the boundary secondary gradients only.

Flow Boundary Diffusion

When activated, diffusion is calculated across the flow boundary for all combustion scalars (for example, mixture fraction, mixture fraction variance, and progress variable).

Separate Turbulent Schmidt Number

When activated, allows you to specify a different turbulent Schmidt number for each flamelet transport equation that is applicable—such as the transport equations for unnormalized progress variable y Eqn. (3599), unnormalized progress variable variance y_{var} Eqn. (3603), mixture fraction Z Eqn. (3560), and mixture fraction variance Z_{var} Eqn. (3561).

It is only possible to specify custom turbulent Schmidt numbers for y_{var} and Z_{var} when the relevant flamelet table contains multiple points in the y_{var} and Z_{var} table dimensions—and additionally, if the **Transport Equation** method is used to calculate them.

Model Controls

Mixture Fraction Variance

Available when the Large Eddy Simulation (LES) turbulence model is selected, and when the *Maximum Number of Grid Points* property within the **FGM Table Generator** > **Parameters** > **0D Ignition Numerical Settings** > **Table Dimensions** > **Mixture Fraction Variance** node is set to a value greater than 1.

Method	**Corresponding Method Node**
Transport Equation Computes the mixture fraction variance using the standard Simcenter STAR-CCM+ calculations.	None.
Algebraic Relationship Computes the mixture fraction variance using Eqn. (3571).	**Algebraic Relationship**—allows you to specify the model constant, c_v, in Eqn. (3571).

Progress Variable Variance

Available when the Large Eddy Simulation (LES) turbulence model is selected, and when the *Maximum Number of Grid Points* property, within the **FGM Table Generator** > **Parameters** > **0D Ignition Numerical Settings** > **Table Dimensions** > **Progress Variable Variance** node, is set to a value greater than 1.

Method	**Corresponding Method Node**
Transport Equation Computes the progress variable variance using a transport equation, Eqn. (3603).	None.

Algebraic Relationship

Computes the progress variable variance using Eqn. (3602).

Algebraic Relationship—allows you to specify the Cv model constant, c_v, in Eqn. (3602).

Materials and Methods

Molecular Weight

The Molecular Weight *Method* is set to **Flamelet Table** by default. This setting specifies that all values for Molecular Weight are taken from the values in the FGM Flamelet Table.

Specific Heat

The Specific Heat *Method* is set to **Flamelet Table** by default. This setting specifies that all values for Specific Heat are taken from the values in the FGM Flamelet Table.

Turbulent Schmidt Number

σ_t in all applicable scalar transport equations, except when the **Adiabatic** or **Non-Adiabatic** model property, *Separate Turbulent Schmidt Number* is activated. If values are specified separately (for **Turbulent Schmidt Number for Mixture Fraction**, or **Turbulent Schmidt Number for Mixture Fraction Variance**), this **Turbulent Schmidt Number** property setting applies to all instances of the turbulent Schmidt number other than those that are specified separately.

Turbulent Schmidt Number for Mixture Fraction

Available when the **Adiabatic** or **Non-Adiabatic** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,Z}$ that is specifically applied to the mixture fraction Z transport equation Eqn. (3560).

Turbulent Schmidt Number for Mixture Fraction Variance

Available when the **Adiabatic** or **Non-Adiabatic** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,Z_{\mathrm{var}}}$ that is specifically applied to the mixture fraction variance Z_{var} transport equation Eqn. (3561).

Turbulent Schmidt Number for Progress Variable

Available when the **Flamelet Generated Manifold (FGM)** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,y}$ that is specifically applied to the unnormalized progress variable y transport equation Eqn. (3599).

Turbulent Schmidt Number for Progress Variable Variance

Available when the **Flamelet Generated Manifold (FGM)** model property *Separate Turbulent Schmidt Number* is activated.

Allows you to specify the turbulent Schmidt number $\sigma_{t,\,y_{\mathrm{var}}}$ that is specifically applied to the unnormalized progress variable variance y_{var} transport equation Eqn. (3603).

Initial Conditions

Mixture Fraction

The mixture fraction is the atomic mass fraction that originated from the fuel stream. 1.0 is equal to 100%. To initialize with pure oxidizer, maintain the default of 0.0. For inflows where the mixture is unburnt, the Mixture Fraction Profile is the mass fraction of the fuel.

Mixture Fraction Variance

The mixture fraction variance is a measure of turbulent fluctuations in the local mixture fraction values. It is a scalar quantity whose initial and boundary condition values are entered in the Properties window as a scalar array profile. In simulations that use the Large Eddy Simulation (LES) model, you can select one of two methods for mixture fraction variance:

- **Transport Equation**: Uses standard Simcenter STAR-CCM+ calculations.
- **Algebraic Relationship**: Activates the Algebraic Relationship node which allows you to set values for the model constant, C_v in Eqn. (3603), and the Internal Dissipation Constant, C_d in Eqn. (3604).

Boundary Settings

Wall

Wall Combustion Scalar

Selects the scalars for the wall combustion calculation.

See Wall Combustion Scalar Option.

Region Settings

Applies to any region:

Active Reactions Option

Activates or deactivates chemical reactions in this region.

Flamelet Sources Option

Provides the *Flamelet Sources Term* property which when activated creates the following physics conditions:

- **Mixture Fraction Source Option**
- **Mixture Fraction Variance Source Option**
- **Progress Variable Source Option**
- **Progress Variable Variance Source Option**

Progress Variable Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None	No source term is defined.

User Source Term	**Corresponding Physics Values Nodes**
Add to Built-In Source Term	**Progress Variable User Source** Allows you to add a new source term to the existing sources in the progress variable transport equation. **Progress Variable User Source Jacobian** Allows you to add a new source term linearization to the existing sources in the progress variable transport equation.
Replace Built-In Source Term	**Progress Variable User Source** Allows you to define a new source term to replace the existing source term in the progress variable transport equation. **Progress Variable User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the progress variable transport equation.

Progress Variable Variance Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None	No source term is defined.
Add to Built-In Source Term	**Progress Variable Variance User Source** Allows you to add a new source term to the existing sources in the progress variable variance transport equation. **Progress Variable Variance User Source Jacobian** Allows you to add a new source term linearization to the existing sources linearization in the progress variable variance transport equation.

User Source Term	**Corresponding Physics Values Nodes**
Replace Built-In Source Term	**Progress Variable Variance User Source** Allows you to define a new source term to replace the existing source term in the progress variable variance transport equation. **Progress Variable Variance User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the progress variable variance transport equation.

Mixture Fraction Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None No source term is defined.	None.

User Source Term	**Corresponding Physics Values Nodes**
Add to Built-In Source Term	**Mass Source** Allows you to define a new source term for the mass fraction that is associated with the mixture fraction. This source term is added to the existing source term in the mixture fraction transport equation. **Mass Source Pressure Derivative** Allows you to define a new source term to represent the derivative of the **Mass Source** with respect to pressure. This source term is added to the existing source term linearization in the mixture fraction transport equation. **Mixture Fraction User Source** Allows you to define a new source term to add to the existing source term in the mixture fraction transport equation. **Mixture Fraction User Source Jacobian** Allows you to define a new source term linearization to add to the existing source term linearization in the mixture fraction transport equation.

User Source Term	**Corresponding Physics Values Nodes**
Replace Built-In Source Term	**Mass Source** Allows you to define a new source term for the mass fraction that is associated with the mixture fraction. This source term replaces the existing source term in the mixture fraction transport equation. **Mass Source Pressure Derivative** Allows you to define a new source term to represent the derivative of the **Mass Source** with respect to pressure. This source term linearization replaces the existing source term linearization in the mixture fraction transport equation. **Mixture Fraction User Source** Allows you to define a new source term to replace the existing source term in the mixture fraction transport equation. **Mixture Fraction User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the mixture fraction transport equation.

Mixture Fraction Variance Source Option

Available when the region condition **Flamelet Sources Option** has the property *Flamelet Sources Term* activated.

User Source Term	**Corresponding Physics Values Nodes**
None No source term is defined.	None.

User Source Term	**Corresponding Physics Values Nodes**
Add to Built-In Source Term	**Mixture Fraction Variance User Source** Allows you to add a new source term to add to the existing sources in the mixture fraction variance transport equation. **Mixture Fraction Variance User Source Jacobian** Allows you to add a new source term linearization to add to the existing sources linearization in the mixture fraction variance transport equation.
Replace Built-In Source Term	**Mixture Fraction Variance User Source** Allows you to define a new source term to replace the existing source term in the mixture fraction variance transport equation. **Mixture Fraction Variance User Source Jacobian** Allows you to define a new source term linearization to replace the existing source term linearization in the mixture fraction variance transport equation.

FGM Combustion Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

URF for Mixture Fraction

Appears only when the solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the mixture fraction Z in Eqn. (3560).

URF for Mixture Fraction Variance

Appears only when the solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the mixture fraction variance Z_{var} in Eqn. (3561).

URF for Progress Variable

Appears only when the flamelet solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the progress variable y in Eqn. (3598).

URF for Progress Variable Variance

Appears only when the flamelet solver property *Separate URF Numbers* is activated, and if using the Flamelet Generated Manifold model, the model property *Progress Variable Variance* is set to **Transport Equation**.

Under-relaxation factor for the progress variable variance y_{var} in Eqn. (3603).

URF for Flame Area Density

Available only with the **Coherent Flame Model** model.

Appears only when the flamelet solver property *Separate URF Numbers* is activated.

Under-relaxation factor for the flame area density variance Σ in Eqn. (3629).

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Separate URF Numbers

When activated, the *Under-Relaxation Factor* property for the solver is removed and replaced by separate URF properties for each relevant transport equation. For example, *URF for Mixture Fraction*, *URF for Mixture Fraction Variance*, and *URF for Progress Variable Variance*.

Field Functions

Burnt Progress Variable

The burnt progress variable, y_b in Eqn. (3601).

Chemistry Heat Release Rate Indicator

The chemistry heat release rate is $\dot{h}$ in Eqn. (3433).

Combustion Scalar Diffusion Coefficient

Γ_y in Eqn. (3600)—for the unnormalized progress variable.

Progress Variable

The progress variable, c in Eqn. (3601).

Unburnt Progress Variable

The unburnt progress variable, y_u in Eqn. (3601).

Unnormalized Progress Variable

The unnormalized progress variable, y in Eqn. (3598).

Unnormalized Progress Variable Variance

The unnormalized progress variable variance, y_{var} in Eqn. (3602).

Contents:

FGM Table Reference

The Flamelet Generated Manifold (FGM) model uses the table that is generated by the FGM Table Generator.

FGM Table Generator

Properties

None

Right-Click Actions

`Import Table`...

Imports a previously saved FGM table.

Note: Since tables are saved in single precision, *Table Precision*—under the **FGM Table Generator** > **Parameters** node—is switched to `Single` after importing a table.

`Delete Table`

Removes a stored table from memory. The flamelet table must be deleted before making changes to the table settings.

`Stop Calculations`

Stops the calculations during the flamelet library generation.

Child Nodes

The FGM Table Generator node contains the following sub-nodes:

- Chemistry Definition
- Fluid Streams (see Fluid Streams Reference)
- Reactor Type

- Parameters
- FGM Table

Chemistry Definition

The Chemistry Definition describes the chemical reaction mechanism, which is the collection of all species in a reaction—reactants, intermediates, and products—and the corresponding set of all reactions. The Chemistry Definition also includes the thermodynamic properties, as well as, optionally, the transport properties. Including the transport properties file can increase accuracy for low Reynolds number flows where laminar mixture viscosity and thermal conductivity are comparable to their corresponding turbulent values, and also when tabulating laminar flame speeds where the simulation conditions are outside the range of the built-in correlations.

Properties

None

Right-Click Actions

`Import Complex Chemistry Definition (Chemkin format)`

Activates a standard *Open* dialog that imports files for the complex chemistry definition in Chemkin™ format. Upon importing a chemistry definition, the reactions for the definition appear as sub-nodes of the Chemistry Definition node.

If you import transport data along with the chemical mechanism and thermal data, Simcenter STAR-CCM+ tabulates the molecular transport properties for the Dynamic Viscosity, Molecular Diffusivity, and Thermal Conductivity material properties. You can then choose to use these tabulated molecular transport properties after table generation, in the Multi-Component Gas node, by selecting the `Flamelet Table` option for each of the Material Properties.

`Delete Complex Chemistry Definition`

Removes the reactions and species in the chemistry definition.

Reactor Type

Option

`0D Ignition`

FGM tables are generated using a 0D Constant Pressure reactor. These flamelets are the fastest and most stable to generate, but typically tend to over-predict intermediate species such as OH and CO.

See Governing Equations for 0D Ignition Reactor Type .

`1D Premixed Strained`

1D opposed flow premixed flamelets are solved in progress variable space. This reactor type is the most appropriate for solving perfectly-premixed or partially-premixed turbulent flames.

See Governing Equations for 1D Premixed Strained Reactor Type .

`1D Premixed Freely Propagating`

1D freely propagating premixed flamelets are solved in progress variable space.

This reactor type is the most appropriate for solving premixed flames when using the Turbulent Flame speed Closure (TFC) model or Coherent Flame Model (CFM) and the laminar flame speed is not accurately modeled by the Simcenter STAR-CCM+ laminar flame speed correlations, since the laminar flame speed is computed and tabulated during flamelet generation.

See Governing Equations for 1D Premixed Freely Propagating Reactor Type.

Parameters

Properties

Progress Variable Definition

Allows three ways to define the weights W_k of the un-normalized progress variable y as defined by Eqn. (3598). Ideally, the set of species weights results in the progress variable increasing monotonically from unburnt to burnt.

- **Species Weights**: Adds a **Species Weights** sub-node which allows you to define the individual progress variable species weights W_k manually. You select species that correspond to the typical products of the combustion reaction.
- **Chemical Enthalpy**: The progress variable species weights, W_k are set to the chemical formation enthalpies (h) of each species. Values for h_k are taken from the thermodynamic properties file which is imported as part of the reaction mechanism. See Reaction Mechanism Formats: Gas / Surface Thermodynamic Properties Files.
- **Optimal Weights**: The optimal weights are calculated to minimize the gradients of the tabulated variables (ϕ) with respect to the unnormalized progress variable y, as well as ensuring that the progress variable increases monotonically through the flamelet. After optimization, the species weights are shown in the **Species Weights** sub-node.

Table Precision

Specifies the precision—`Single` or `Double`—to which the flamelet table is generated. The default is `Single`.

Child Nodes

Absolute Pressure

Value

The pressure that is used when generating the FGM table.

Species for Tabulation

Species

Allows you to select which species are stored in the flamelet table. These species are then made available in a simulation, for example, to use for post-processing in contours or reports.

Emissions

Thermal NOx

When activated, NOx source-term coefficients are calculated and tabulated.

Soot Moment

When activated, the soot moment model source-term coefficients are calculated and tabulated. Creates a **Soot Moments Options** sub-node which allows you to specify the *Nucleation Option* as either:

- **C2H2**, see Eqn. (3748).
- **Single PAH Species (C16H10)**, see Eqn. (3745) and Eqn. (3746). The PAH precursor is recognised as any species which includes either A4 or A3R5 in the species name, or has the composition C16H10.

Numerical Settings

Defines the following properties, depending upon the option that is selected for Reactor Type. Also contains the **Table Dimensions** sub-node which you can use to set the dimensions for the flamelet table. See Table Dimensions Reference.

Properties	Reactor Type		
	0D Ignition	1D Premixed Freely Propagating	1D Premixed Strained
Minimum Temperature	✔	✔	✔
Absolute ODE Tolerance	✔	✔	✔
Relative ODE Tolerance	✔	✔	✔
Flamelet Convergence Tolerance		✔	✔
Max Dissipation Rate			✔

Minimum Temperature

Specifies the minimum temperature for enthalpy normalization in the flamelet table.

Absolute ODE Tolerance

Specifies the absolute tolerance of the ODE solver.

Relative ODE Tolerance

Specifies the relative tolerance of the ODE solver.

Flamelet Convergence Tolerance

The 1D premixed flamelet equations are integrated in time using the ODE solver Absolute Tolerance and Relative Tolerance until steady-state. Steady-state is determined when the average residual over all post-processing species and temperatures, and over all grid points, is less than the Flamelet Convergence Tolerance.

Max Dissipation Rate

The maximum dissipation rate of the normalized progress variable at stoichiometric conditions $\chi_{Z,\mathrm{sto}}$, that is used to determine the progress variable dissipation rate using Eqn. (3610) and Eqn. (3609). The default value of 1000 (s^{-1}) is approximately the scalar dissipation rate of a freely propagating flame.

Analytical Jacobian

When activated, an analytical Jacobian is used in the ODE solver instead of the numerical Jacobian.

Species Weights

The following values for the progress variable species weights, W_k in Eqn. (3598), are set by default. However, these values can be edited manually prior to generating the table.

- If CO and CO2 are present in the mechanism, they are both set to 1.0 and all other species weights are set to 0.0.
- If neither CO or CO2 are present in the mechanism, but H2 and H2O are present (for example, during hydrogen combustion), H2O is set to 1.0 and all other species weights are set to 0.0.

Heat Loss Ratio Range

Specifies the heat loss ratio range. You can increase the enthalpy space that is covered in the Flamelet table in response to heat loss ratio warnings, or decrease it for better resolution. For example, if your simulation involves heat loss only, with no heat gain, you can set the minimum heat loss ratio limit to 0 and the maximum heat loss ratio to 1.0.

You can set either the minimum heat loss ratio limit or the maximum heat loss ratio limit to 0, but you cannot have both set to 0 at the same time.

Minimum Heat Loss Ratio

Sets the minimum heat loss ratio limit.

Maximum Heat Loss Ratio

Sets the maximum heat loss ratio limit. However, if the resulting minimum temperature drops below a physical limit, the temperature is clipped to the table minimum temperature that is specified at the table generation.

After a table is generated, these values cannot be changed unless the table is deleted first.

FGM Table

The FGM Table node has the following options available from the context menu:

Properties

Save Table in .sim File

When activated, stores the flamelet table in the sim file. When deactivated, the flamelet table is not stored in the .sim file—which is useful to save disk space when using the same flamelet table in different .sim files, or when auto-saving many sim files. If the flamelet table is required for future use, you must export it manually by right-clicking the flamelet table node and selecting Export Table. Then save it separately from the .sim file.

Path for Table Read

Specifies the file path location of the flamelet table file that has been exported from Simcenter STAR-CCM+ and saved previously. Useful to reduce the .sim file size and save disk space when several .sim files use the same flamelet table.

Verbosity

When activated, if selected tolerance criteria are not met in adaptive grid generation steps, Simcenter STAR-CCM+ prints a summary of tolerance warnings to the *Output* window at each step during the table generation.

For example:

```
WARNING: For 'Heat Loss Ratio' the   maximum error of 0.00652988 is
greater than the specified tolerance of 0.0001. To achieve the prescribed
tolerance, delete the table, increase the maximum number of points
(currently 9) and regenerate the table.
```

When deactivated, all of the warning messages about exceeding the defined tolerance for adaptive table dimensions are hidden.

Right-Click Actions

`Generate FGM Library and Construct Table`

Generates the FGM library and constructs the FGM table (performs PDF integrations) in Simcenter STAR-CCM+ using the properties and table dimensions that are specified under the FGM table node. The progress is displayed in the *Output* window.

`Import FGM User Library File and Construct Table...`

Imports the FGM user library file and constructs the FGM table (performs PDF integrations) in Simcenter STAR-CCM+ using the properties and table dimensions that are specified under the FGM table node. The progress is displayed in the *Output* window. See Loading Library Tables.

`Print Estimated Maximum Table Size`

Prints the estimated maximum table size (in KB) in the output window. This value also appears as a read-only property of the **Table Dimensions** node.

`Export Table`

Saves the FGM table that is stored in the memory of Simcenter STAR-CCM+ to a file with extension `.tbl`.

Delete Table

Removes a stored table from memory. The flamelet table must be deleted before making changes to the table settings.

Stop Calculations

Stops the calculations during the flamelet library generation.

Print Table Summary

The *Output* window displays a summary of the table parameters and conditions with which the table was built. When running the simulation, if the current parameters and conditions differ from those that were specified when the table was built, a warning is displayed in the *Output* window at each iteration.

Parameters and conditions are not displayed for tables that are imported from Simcenter STAR-CCM+ versions prior to 2410, or from tables that are constructed using DARS libraries.

Child Nodes

Final Table Grid Size

Contains sub-nodes for each of the table dimensions. Each table dimensions sub-node displays the (read only) *Number of Grid Points* that are used from the data for that parameter. The values are specified before building the table by defining settings under the **Table Dimensions** node. See Table Dimensions Reference.

FGM XY Plots

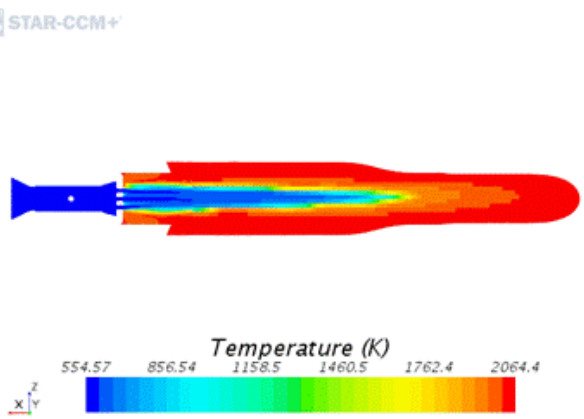
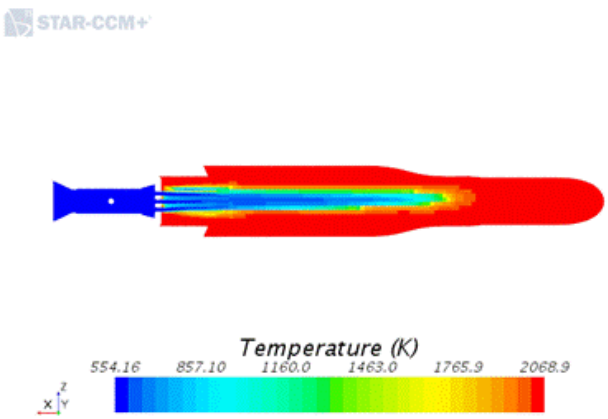
To visualize the flamelet generated manifold flamelet table, you can create an XY plot. Right-click this node and select New Plot. See Flamelet Table XY Plots Reference.

Restoring the Premixed FGM Model

The Premixed Flamelet Generated Manifold (FGM) model in Simcenter STAR-CCM+ v.11.04 is superceded by a Partially Premixed version. You can restore the Premixed model settings as described in this section.

As part of a plan to improve and simplify the procedure for selecting combustion models, the Premixed version of the FGM model is discontinued in Simcenter STAR-CCM+ v.11.04.

When loading a simulation in Simcenter STAR-CCM+ v.11.04 or later that was saved in a version of Simcenter STAR-CCM+ before v11.04, the Premixed FGM model behaves as a Partially-Premixed FGM model. Several settings are defined differently and must be set up again. The following images show a comparison of the temperatures on the cross section of a flame holder.

Premixed FGM 11.02	Premixed FGM 11.04 (Partially Pre-Mixed)
	

Simcenter STAR-CCM+ v.11.04 provides the FGM model as an option for Premixed Combustion. However, this model is the same as that provided for Partially-Premixed combustion. Further steps are required to restore the premixed behaviour that was available in Simcenter STAR-CCM+ v.11.02 and earlier. These steps are as follows:

You can restore the settings of the deprecated Premixed combustion model, using the following procedure:

1. Redefine the reacting fluid stream to match the Premixed set-up.
   a) Select the **[Continuum]** > **Fluid Stream Manager** > **Fuel Stream** node and set the *Fluid Stream Components* as the Premixed mixture.
   b) Select the **Fuel Stream** node and set the *Temperature of the Stream* using the temperature from Simcenter STAR-CCM+ v11.02 that is set for the inlet boundary of the fuel/air mixture.
   c) Select the **[Continuum]** > **Fluid Stream Manager** > **Oxidizer Stream** node and set the *Fluid Stream Components* as Air.
   d) Select the **Oxidizer Stream** node and set the *Temperature of the Stream* using the temperature from Simcenter STAR-CCM+ v11.02 that is set for the inlet boundary of the fuel/air mixture.

Any FGM Table parameters that were set in the simulation before Simcenter STAR-CCM+ v11.04, must be redefined.

2. Create an FGM table in DARS and construct the FGM table in Simcenter STAR-CCM+. It is not possible to use a Premixed FGM table in Simcenter STAR-CCM+ v.11.04 or later. See FGM Table.
   When creating the FGM table in DARS:
   - Set the Fuel Composition to the premixed mixture and the oxidizer to air.
   - Set the Fuel Temperature to the temperature that is set for the inlet boundary of the fuel/air mixture in Simcenter STAR-CCM+ v11.02.
   - Set the Pressure to the absolute pressure that is specified in Simcenter STAR-CCM+.
3. Select the **[Physics]** > **Initial Conditions** > **Mixture Fraction Profile** node and specify the *Value* as `1.0`.
4. Select the **Models** > **Flamelet Generated Manifold** > **Progress Variable Variance** node and set the *Method* that you require.
5. To restore the Ignitor:

a) Right-click the **[Continuum]** > **Ignitors** node and select **New**.
b) Select the **ProgressVariableIgnitor 1** node and specify the necessary properties.
c) If the **ProgressVariableIgnitor 1** node *Activator* is set to **Pulse**, select the **Pulse** sub-node and specify the necessary properties.

6. For all inlet and outlet boundaries within each physics continuum, select the **[Boundary]** > **Physics Values** > **Mixture Fraction Profile** node and specify the *Value* as `1.0`.

FGM Reaction Model Reference

The FGM Reaction model is selected automatically with the Flamelet Generated Manifold model.

FGM Reaction Model Reference

Theory	See Flamelet Generated Manifold.	
Provided By	**[physics continuum]** > **Models** > *FGM Reaction*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **FGM Reaction**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** *Flamelet Models*: **Flamelet Generated Manifold (FGM)**	
Properties	Key properties are: **Dissipation Constant** and **Number of Streams**. See FGM Reaction Model Properties.	
Activates	Field Functions	Heat Loss Ratio, Mixture Fraction 0, Mixture Fraction Variance 0, Progress Variable Variance, Unnormalized Progress Variable Variance. See Field Functions.

FGM Reaction Model Properties

Dissipation Constant

Represents the ratio of velocity and chemical species fluctuation time scales.

Number of Streams

You can choose the number of streams.

Field Functions

Heat Loss Ratio

γ in Eqn. (3586). When using the Inert Stream model, heat losses or gains from the fluid stream are also accounted for. See Inert Streams.

Mixture Fraction 0

Represents the atomic mass fraction that originated from the fuel stream.

Mixture Fraction Variance 0

Represents the turbulent fluctuations in the fuel mixture fraction values.

Progress Variable Variance

c_{var}, in Eqn. (3398).

Unnormalized Progress Variable Variance

y_{var} in Eqn. (3602).

FGM Kinetic Rate Model Reference

The FGM Kinetic Rate model takes the progress variable source term from the FGM table.

The FGM Kinetic Rate model uses the chemical kinetic rate for the progress variable equation source term, and should be used when chemical kinetic effects, such as ignition, extinction/quenching are important. This model is recommended for Large Eddy Simulation (LES).

FGM Kinetic Rate Model Reference

Theory	See Flamelet Generated Manifold.
Provided By	**[physics continuum]** > **Models** > *Progress Variable Source*
Example Node Path	**Continua** > **Physics 1** > **Models** > **FGM Kinetic Rate**
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** *Flamelet Models*: **Flamelet Generated Manifold (FGM)** *FGM Reaction*: **FGM Rection**

Table Dimensions Reference

Different table dimensions (grid resolution) sub-nodes are available for each flamelet table.

You can specify the grid resolution for a flamelet table using the **[Table Generator]** > **Parameters** > **[Numerical Settings]** > **Table Dimensions** node.

When trying to reach a flamelet table grid independent solution, you can refine the grid resolution—for adaptive gridding tables you can decrease the tolerance, or for fixed tables you can increase the number of data points—then re-converge the solution until it stops changing.

Flamelet Table Type	Available Table Dimensions
Flamelet Generated Manifold (FGM), (with two streams)	**Heat Loss Ratio**, **Mixture Fraction**, **Mixture Fraction Variance**, **Progress Variable**, **Progress Variable Variance** (useful when using Premixed).
Flamelet Generated Manifold (FGM), (with three streams)	**Heat Loss Ratio**, **Mixture Fraction 0**, **Mixture Fraction Variance 0**, **Mixture Fraction 1**, **Mixture Fraction Variance 1**, **Progress Variable**, **Progress Variable Variance** (useful when using Premixed)

Flamelet Table Type	Available Table Dimensions
Steady Laminar Flamelet (SLF)	**Heat Loss Ratio**, **Mixture Fraction**, **Mixture Fraction Variance**
Chemical Equilibrium (with two streams)*	**Heat Loss Ratio**, **Mixture Fraction**, **Mixture Fraction Variance**
Chemical Equilibrium (with three streams)*	**Heat Loss Ratio**, **Mixture Fraction 0**, **Mixture Fraction 1**, **Mixture Fraction Variance 0**, **Mixture Fraction Variance 1**

*When using the Non-Adiabatic model, the **Heat Loss Ratio** table dimension is also available to specify.

- **Mixture Fraction**: Data points which represent the mixture fraction, Z. See Mixture Fraction.
- **Mixture Fraction Variance**: Data points which represent the turbulent fluctuations in the local mixture fraction values, Z_{var}.
- **Progress Variable**: Data points which represent the progress of the combustion, c.
- **Progress Variable Variance**: Data points which represent the fluctuations in the progress of the combustion, c_{var}.
- **Mixture Fraction 0**: Data points which represent the stoichiometry of the first stream ratio, Z_0.
- **Mixture Fraction 1**: Data points which represent the stoichiometry of the second stream ratio, Z_1.
- **Mixture Fraction Variance 0**: Data points which represent the turbulent fluctuations in the mixture fraction values of the first stream, $Z_{0,\text{var}}$.
- **Mixture Fraction Variance 1**: Data points which represent the turbulent fluctuations in the mixture fraction values of the second stream, $Z_{1,\text{var}}$.
- **Heat Loss Ratio**: Data points which represent the heat loss ratio (enthalpy), γ in Eqn. (3586). When using the Inert Stream model, heat losses or gains from the fluid stream are also accounted for. See Inert Streams.

Table Dimensions Properties

Maximum Table Size Estimate

Displays the read-only value for the estimated maximum table size.

Each of the Table Dimension sub-nodes has the following property:

Use Adaptive Number of Grid Points

Allows you to specify if adaptive gridding is used for this table dimension. For more details of how this feature adapts tables, see Flamelet Tables. If the table is populated, the property cannot be changed unless you delete the table.

- **Activated**: Simcenter STAR-CCM+ creates a non-uniform grid for this table dimension by placing table points so that table interpolation is accurate to the tolerance that you specify. You can set the *Maximum Number of Grid Points* property which appears, along with the interpolation *Tolerance* property which is used to calculate a normalized tolerance.
- **Deactivated**: You set a specified value of the *Number of Grid Points* for the table dimension. Simcenter STAR-CCM+ clusters grid points at stochiometric values for the mixture fraction grid, but uses equal spacing for the other dimensions of variance, reaction progress (Progress Variable) and enthalpy (Heat Loss Ratio).

Note: When the *Maximum Number of Grid Points* for **Mixture Fraction Variance** and **Progress Variable Variance** is set to a value greater than 1, the transport equation is solved.

Flamelet Table XY Plots Reference

You can create XY Plots to visualize the values that are stored in a flamelet table for each variable. Simcenter STAR-CCM+ provides two methods of extracting the data from the multi-dimensional table. The first method interpolates and plots the data from the table based on the specified values of variables such as Heat Loss Ratio, Mixture Fraction, Mixture Fraction Variance etc. The second method plots only the actual points stored in the table.

[Flamelet Model] XY Plots

Properties

None.

Right-Click Actions

New Plot

Creates an XY Plot which allows you to visualize the variable that you select from the stored flamelet table —appears as a **[Variable]** child node. Note that for the Three Stream Tables there are two Mixture Fractions.

The following XY plots are available to specify:

ACoeff

Thermal NOx coefficient A in Eqn. (3693).

BCoeff

Thermal NOx coefficient B in Eqn. (3693).

CCoeff

Thermal NOx coefficient C in Eqn. (3693).

DCoeff

Thermal NOx coefficient D in Eqn. (3693).

Density

Dynamic Viscosity

Enthalpy

Enthalpy h is defined as sensible (thermal) enthalpy h_{sens}, plus chemical (heat of formation) enthalpy h_{chem}.

Laminar Flame Speed

Laminar flame speed, S_u in Eqn. (3614). Available when the flamelet table *Reactor Type* is set to **1D Premixed Freely Propagating**.

Mass Fraction of [SPECIES]

Mass fraction of the [species] that is set as a *Species For Tabulation* in the flamelet table.

Mixture Fraction 0

The mixture fraction Z_0 in Eqn. (3556). When a third stream is specified, plots normalize the bottom axis of mixture fraction by $\frac{Z_0}{(1-Z_1)}$ so that the axis ranges from 0 to 1.

Mixture Fraction 1

(Only available when a third stream is specified). The secondary mixture fraction Z_1 in Eqn. (3557). The tables are normalized, so the value of mixture fraction ranges from 0 to 1. When plotting table values versus secondary mixture fraction, the bottom axis of the plot that is fixed when extracting the data is $\frac{Z_1}{(1-Z_0)}$.

Mixture Fraction Variance 0

Mixture Fraction Variance 1

(Only available when a third stream is specified).

Molecular Diffusivity

Molecular Weight

Progress Variable Source Term

The unnormalized progress variable source term $\dot{\omega}_y$ in Eqn. (3599). Units of 1/s.

Progress Variable Source Term Jacobian

The gradient of the source term, which is the Jacobian of the FGM kinetic source term $\dot{\omega}_y$ in Eqn. (3599). That is the derivative of progress variable source term with respect to the unnormalized progress variable, y.

[SPECIES]

Sensible Enthalpy

The sensible enthalpy h_{sens} in Eqn. (3587).

Specific Heat

C_p

Temperature

Thermal Conductivity

Child Nodes

[Variable]

Properties

The flamelet table XY plots share some of the properties of the regular XY plots, with the addition of the properties that are described below. See Plot Properties Lookup.

Variable Name

Displays the read-only name of the variable that was chosen to plot.

X-Axis Variable

Allows you to select from the grid resolution variables that are available which is used for the X-axis. For example, Heat Loss Ratio, Mixture Fraction, Mixture Fraction Variance, etc.

Right-Click Actions

The flamelet table XY plots share some of the right-click actions of the regular XY plots, with the addition of the right-click actions that are described below. See Plot Pop-Up Menu.

Add New Table View for Plotting

Activates a dialog in which you can choose to specify either values or table points to plot.

- In the *Select Values to Plot* tab, you can set specific values for the variables and the table is interpolated to these values. Since the points are interpolated, they appear equally spaced.
- In the *Select Table Points to Plot* tab, you can set the actual grid points to plot for the variables.

Child Nodes

Data Series

See Managing Data in a Plot.

Axes

See Axis Properties Reference.

Legend

See Legend Properties Reference.

Fluid Streams Reference

You can define the fluid streams for a reacting flow within each of the flamelet table generators.

Fluid Streams

Number of Streams

You can choose to have either two or three streams.

Note: It is not possible to specify a third stream when using the Steady Laminar Flamelet model.

Number of Streams	**Resulting Child Nodes**
2	• **Oxidizer** • **Fuel**
3	• **Oxidizer** • **Fuel** • **Second Stream**

All three flamelet models allow you to define an additional inert stream using the Inert Stream model. See Inert Streams.

The mass fractions of all components within a fluid stream must add up to 1.0. For example, at a boundary, the combined inert (mass) fraction and mixture (mass) fraction must be less than 1.0. The remaining mass fraction accounts for the oxidizer.

Each of the streams has the following Properties:

Fluid Stream Components

Allows you to select the fluid stream components for the selected fluid stream. You can select the fluid stream components from a list of the components that are already specified within the Multi-Component Gas or Multi-Component Liquid models.

Composition Specification

Allows you to specify the composition of the fluid stream using Mass fraction or Mole fraction.

Temperature

Allows you to set the temperature of the fluid stream.

Coherent Flame Model Reference

The Coherent Flame Model is a flame positioning model which you can use with any of the flamelet combustion models—Chemical Equilibrium, Steady Laminar Flamelet, or Flamelet Generated Manifold.

In this model, a flame area density and a progress variable on the grid are tracked through transport equations. The mean species concentrations come from the underlying combustion model—Chemical Equilibrium, Steady Laminar Flamelet, or Flamelet Generated Manifold. A mean enthalpy transport equation is also solved. The mean temperature, density, and viscosity are then calculated knowing the mean enthalpy and species concentrations.

Coherent Flame Model Reference

Theory	See Flame Propagation.

Provided By	• When using the FGM model: **[physics continuum]** > **Models** > *Progress Variable Source* • When using the Chemical Equilibrium or SLF model: **[physics continuum]** > **Models** > *Flame Propagation*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Coherent Flame Model (CFM)**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** then either: • *Flamelet Models*: **Flamelet Generated Manifold (FGM)** • *Flamelet Models*: **Chemical Equilibrium** or **Steady Laminar Flamelet** *Flame Type*: **Partially-Premixed Flame**	
Properties	Key properties are the coefficients α, β, a, and B. See Coherent Flame Model (CFM) Properties.	
Activates	Model Controls (child nodes)	Laminar Flame Speed
	Initial Conditions	Flame Area Density Progress Variable See Initial Conditions.
	Boundary Inputs	Flame Area Density Progress Variable See Boundary Settings.
	Region Settings	Active Reactions Option. See Region Settings.
	Other Continuum Nodes	The **Ignitors** node provides the right-click option to create a **Flame Area Density Ignitor**. See Ignitors.
	Solvers	When using the FGM model see FGM Combustion. When using the Chemical Equilibrium or SLF model, the CFM Combustion Solver is activated. See CFM Combustion Solver Properties.
	Monitors	**Fad**: Flame Area Density **ProgVarCFM:** Progress Variable CFM
	Field Functions	Flame Area Density Progress Variable Progress Variable Variance Unnormalized Progress Variable CFM Unnormalized Progress Variable Variance See Field Functions.

Coherent Flame Model (CFM) Properties

Convection

Sets the discretization scheme that Simcenter STAR-CCM+ uses for computing the convection flux on a cell face in appropriate transport equations. More information is given in the related topic for the Convection Term:

- **1st-Order**: First-order upwind scheme. This scheme scales the transported quantity by the upstream or downstream mass flowrate depending on flow direction. Only use when a higher-order scheme fails to give convergence, or in order to obtain an initial solution before switching to a higher-order scheme.
- **2nd-Order**: Second-order upwind scheme. This scheme introduces linear interpolation of cell values on either side of the upstream or downstream face. Using this scheme can lead to poorer convergence properties, but gives accuracy as good as or better than the first-order scheme.

Secondary Gradients

There are two sources of secondary gradients in Simcenter STAR-CCM+ flow solvers:

- boundary secondary gradients for diffusion
- interior secondary gradients at cell faces

Use this property to control which gradients are included in the solver. **On** gives both gradients while **Off** excludes them. **Interior Only** and **Boundaries Only** select the corresponding gradients.

Flow Boundary Diffusion

When activated, diffusion is calculated across the flow boundary for all combustion scalars (for example, mixture fraction, mixture fraction variance, and progress variable).

The following properties are also available when using the Chemical Equilibrium model or the Steady Laminar Flamelet model.

CFM Constant, Alpha

Coefficient α, from Eqn. (3628).

CFM Constant, Beta

Coefficient β, from Eqn. (3628).

CFM Constant, A

Coefficient a, from Eqn. (3628).

CFM Constant, B

Coefficient B, from Eqn. (3635).

Laminar Flame Speed

Laminar Flame Speed

Provides options for controlling the unstrained laminar flame speed. Unavailable when the Turbulent Flame-Speed Closure (TFC) *Source Option* property is set to `User Defined Source`.

Method	Corresponding Method Node
Flamelet Table Laminar Flame Speed Available when the FGM model is used and the Reactor Type is set to **1D Premixed Freely Propagating**.	Uses the laminar flame speed that is stored in the flamelet table generated by the FGM Table Generator. See FGM Table. Activates the **Flamelet Table Laminar Flame Speed** node.
Gulder Laminar Flame Speed	Uses the Gülder laminar flame speed correlation Eqn. (3645). Activates the **Gulder Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Metghalchi Laminar Flame Speed	Uses the Metghalchi laminar flame speed correlation Eqn. (3639). Activates the **Metghalchi Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Universal Laminar Flame Speed	Simcenter STAR-CCM+ identifies the best laminar flame speed correlation for each individual fuel in a mixture of fuels and then uses the Hirasawa method to calculate the laminar flame speed of the blended mixture of fuels that are specified Eqn. (3637). Hydrocarbons, alcohols, hydrogen and ammonia are considered as fuels. Activates the **Universal Laminar Flame Speed** node.
User Defined Laminar Flame Speed	Allows you to specify the unstrained laminar flame speed. Activates the **User Defined Laminar Flame Speed** node.

Initial Conditions

Flame Area Density

The initial flame area per unit volume. Σ in Eqn. (3629).

Progress Variable

You specify an initial progress variable between 0.0 (unburnt) and 1.0 (fully burnt).

Boundary Settings

Flow Boundaries (except outlet)

Flame Area Density

The flame area per unit volume. Σ in Eqn. (3629).

Progress Variable

You specify a progress variable between 0.0 (unburnt) and 1.0 (fully burnt).

Wall Boundary

Wall Combustion Scalar

Selects the scalars for the wall combustion calculation.

See Wall Combustion Scalar Option.

Region Settings

Applies to any region:

Active Reactions Option

Activates or deactivates chemical reactions in this region.

CFM Combustion Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence and do not decrease, reduce the under-relaxation factor for the relevant solvers. The default value is 0.9.

Reconstruction Frozen

When activated, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is deactivated by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When activated, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. Deactivated by default.

Field Functions

Flame Area Density

Σ in Eqn. (3629).

Progress Variable

c in Eqn. (3397).

Progress Variable Variance

c_{var} in Eqn. (3398).

Unnormalized Progress Variable CFM

y in Eqn. (3395).

Unnormalized Progress Variable Variance

y_{var} in Eqn. (3396).

Contents:

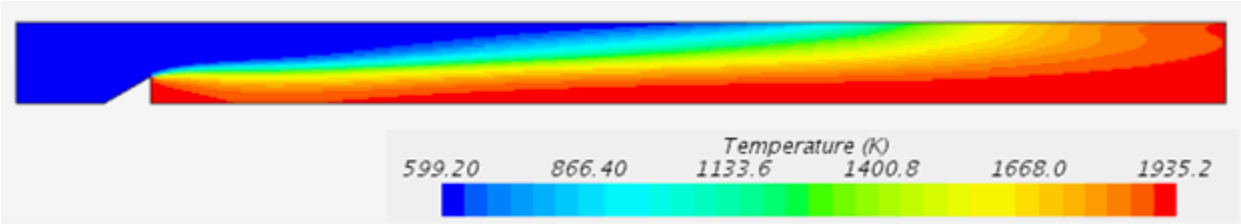
Restoring the Premixed Coherent Flame Model

The Premixed Coherent Flame Model (CFM) in Simcenter STAR-CCM+ v.11.06 is restored to the Flamelet Generated Manifold (FGM) model with the Coherent Flame Model (CFM) flame propagation model. You can restore the Premixed model settings as described in this section.

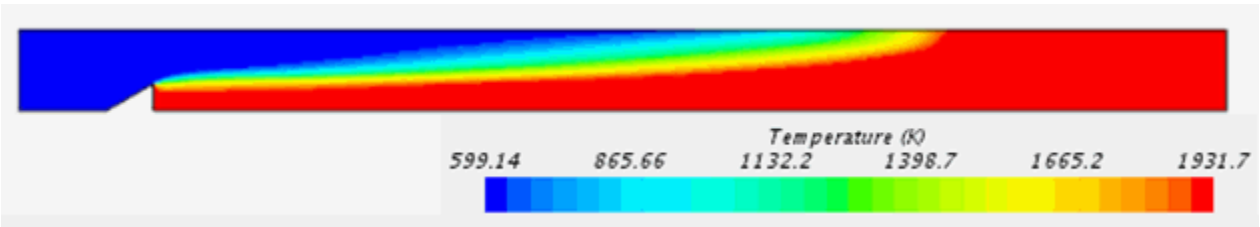
As part of a plan to improve and simplify the procedure for selecting combustion models, the Premixed CFM model is discontinued in Simcenter STAR-CCM+ v.11.06.

When loading a simulation in Simcenter STAR-CCM+ v.11.06 or later that was saved in a version of Simcenter STAR-CCM+ before v11.06, the Premixed CFM model is restored to the Flamelet Generated Manifold (FGM) model with the Coherent Flame Model (CFM) flame propagation model. Several settings are defined differently and must be set up again. The following images show a comparison of the temperatures on the cross section of a flame holder.

Premixed CFM 11.04



Premixed FGM 11.06 (Partially Pre-Mixed)



Simcenter STAR-CCM+ v.11.06 provides the FGM model as an option for Premixed Combustion. However, this model is the same as that provided for Partially-Premixed combustion. Further steps are required to restore the

premixed behaviour that was available in Simcenter STAR-CCM+ v.11.04 and earlier. These steps are as follows:

You can restore the settings of the deprecated Premixed combustion model, using the following procedure:

1. Redefine the reacting fluid stream to match the Premixed set-up.
   a) Select the **[Continuum]** > **FGM Table Generator** > **Fluid Streams** node and set the *Fluid Stream Components* as the Premixed mixture.
   b) Select the **Fluid Streams** node and set the *Temperature of the Stream* using the temperature from Simcenter STAR-CCM+ v11.04 that is set for the inlet boundary of the fuel/air mixture.
   c) Select the **[Continuum]** > **FGM Table Generator** > **Fluid Streams** > **Oxidizer Stream** node and set the *Fluid Stream Components* as Air.
   d) Select the **Oxidizer Stream** node and set the *Temperature of the Stream* using the temperature from Simcenter STAR-CCM+ v11.04 that is set for the inlet boundary of the fuel/air mixture.

Any FGM Table parameters that were set in the simulation before Simcenter STAR-CCM+ v11.06, must be redefined.

2. Create an FGM table using **[Continuum]** > **FGM Table Generator**.
   - Set the Fuel Composition to the premixed mixture and the oxidizer to air.
   - Set the Fuel Temperature to the temperature that is set for the inlet boundary of the fuel/air mixture in Simcenter STAR-CCM+ v11.04.
   - Set the Pressure to the absolute pressure that is specified in Simcenter STAR-CCM+.
3. Select the **[Physics]** > **Initial Conditions** > **Mixture Fraction Profile** node and specify the *Value* as `1.0`.
4. Select the **Models** > **Flamelet Generated Manifold** > **Progress Variable Variance** node and set the *Method* that you require.
5. To restore the Ignitor:
   a) Right-click the **[Continuum]** > **Ignitors** node and select **New**.
   b) Select the **ProgressVariableIgnitor 1** node and specify the necessary properties.
   c) If the **ProgressVariableIgnitor 1** node *Activator* is set to **Pulse**, select the **Pulse** sub-node and specify the necessary properties.
6. For all inlet and outlet boundaries within each physics continuum, select the **[Boundary]** > **Physics Values** > **Mixture Fraction Profile** node and specify the *Value* as `1.0`.

Turbulent Flame Speed Closure (Flamelet) Model Reference

The Turbulent Flame Speed Closure (Flamelet) model is a flame positioning model which you can use with any of the flamelet combustion models—Chemical Equilibrium, Steady Laminar Flamelet (SLF), or Flamelet Generated Manifold (FGM).

This model provides a choice of correlations for turbulent flame speed:

- Zimont, the most widely used option for constant pressure combustion simulations
- Peters, commonly for internal combustion engines
- User Defined, a scalar profile

Turbulent Flame Speed Closure (Flamelet) Model Reference

Theory	See Turbulent Flame Speed.

Provided By	• When using the FGM model: **[physics continuum]** > **Models** > *Progress Variable Source* • When using the Chemical Equilibrium or SLF model: **[physics continuum]** > **Models** > *Flame Propagation*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Turbulent Flame Speed Closure (TFC)**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** *Flamelet Models*: **Flamelet Generated Manifold (FGM)**, **Chemical Equilibrium**, or **Steady Laminar Flamelet** For Chemical Equilibrium and Steady Laminar Flamelet only, *Flame Type*: **Partially-Premixed Flame**	
Properties	Key properties are: *Convection* and *Source Option*. See Turbulent Flame Speed Closure (Flamelet) Model Properties.	
Activates	Model Controls (child nodes)	The TFC model contains sub-nodes for a rate coefficient, turbulent flame speed options, and laminar flame properties. See the following: • Bounded Differencing • TFC Rate Coefficient, A • Laminar Flame Speed • Turbulent Flame Speed • Zimont Turbulent Flame Speed • Peters Turbulent Flame Speed • User Defined Turbulent Flame Speed • User Defined Source
	Initial Conditions	Progress Variable See Initial Conditions.
	Boundary Inputs	Progress Variable See Boundary Settings.
	Region Settings	Active Reactions Option. See Region Settings.
	Other Continuum Nodes	The **Ignitors** node provides the right-click option to create a **Progress Variable Ignitor**. See Ignitors.
	Solvers	When using the FGM model see FGM Combustion. When using the Chemical Equilibrium or SLF model, the TFC Combustion Solver is activated. See TFC Combustion Solver Properties.
	Monitors	**ProgVarTFC**: Progress Variable TFC
	Field Functions	Progress Variable, Progress Variable Variance, Unnormalized Progress Variable TFC, Unnormalized Progress Variable Variance. See Field Functions.

Turbulent Flame Speed Closure (Flamelet) Model Properties

Convection

Sets the discretization scheme that Simcenter STAR-CCM+ uses for computing the convection flux on a cell face in appropriate transport equations. More information is given in the related topic for the Convection Term:

- **1st-Order**: First-order upwind scheme. This scheme scales the transported quantity by the upstream or downstream mass flow rate depending on flow direction. Only use when a higher-order scheme fails to give convergence, or in order to obtain an initial solution before switching to a higher-order scheme.
- **2nd-Order**: Second-order upwind scheme. This scheme introduces linear interpolation of cell values on either side of the upstream or downstream face. Using this scheme can lead to poorer convergence properties, but gives accuracy as good as or better than the first-order scheme.
- **MUSCL 3rd-Order/CD**: Third-order upwind scheme. This scheme, which is valid for both steady and unsteady simulations, uses bounded differencing with an upwind blending factor to control the numerical dissipation in the scheme.

Secondary Gradients

There are two sources of secondary gradients in Simcenter STAR-CCM+ flow solvers:

- boundary secondary gradients for diffusion
- interior secondary gradients at cell faces

Use this property to control which gradients are included in the solver. **On** gives both gradients while **Off** excludes them. **Interior Only** and **Boundaries Only** select the corresponding gradients.

Flow Boundary Diffusion

When activated, diffusion is calculated across the flow boundary for all combustion scalars (for example, mixture fraction, mixture fraction variance, and progress variable).

Bounded Differencing

Only available when the **Turbulent Flame Speed Closure (TFC)** model property, *Convection*, is set to **MUSCL 3rd-Order/CD**.

Upwind Blending Factor

Specifies the proportion of upwind differencing, ς_{ubf} related to Eqn. (900).

The default value of this property is 1.0. Use lower values to reduce the numerical dissipation of the scheme.

Coefficient from Eqn. (3622). Unavailable when the Turbulent Flame-Speed Closure (TFC) *Source Option* property is set to `User Defined Source`.

Laminar Flame Speed

Laminar Flame Speed

Provides options for controlling the unstrained laminar flame speed. Unavailable when the Turbulent Flame-Speed Closure (TFC) *Source Option* property is set to `User Defined Source`.

Method	Corresponding Method Node
Flamelet Table Laminar Flame Speed Available when the FGM model is used and the Reactor Type is set to **1D Premixed Freely Propagating**.	Uses the laminar flame speed that is stored in the flamelet table generated by the FGM Table Generator. See FGM Table. Activates the **Flamelet Table Laminar Flame Speed** node.
Gulder Laminar Flame Speed	Uses the Gülder laminar flame speed correlation Eqn. (3645). Activates the **Gulder Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Metghalchi Laminar Flame Speed	Uses the Metghalchi laminar flame speed correlation Eqn. (3639). Activates the **Metghalchi Laminar Flame Speed** node which allows you to select a fuel using the *Fuel Name* property.
Universal Laminar Flame Speed	Simcenter STAR-CCM+ identifies the best laminar flame speed correlation for each individual fuel in a mixture of fuels and then uses the Hirasawa method to calculate the laminar flame speed of the blended mixture of fuels that are specified Eqn. (3637). Hydrocarbons, alcohols, hydrogen and ammonia are considered as fuels. Activates the **Universal Laminar Flame Speed** node.
User Defined Laminar Flame Speed	Allows you to specify the unstrained laminar flame speed. Activates the **User Defined Laminar Flame Speed** node.

Flame Speed Multiplier

Available for all Laminar Flame Speed (LFS) methods.

Allows you to multiply the LFS with a scale factor. The flame speed multiplier is applied to S_l obtained from any of the LFS methods in Turbulent Flame Speed Closure .

Increasing the multiplier will increase the LFS and therefore the Turbulent Flame Speed. The recommended value ranges from 0.5 to 2. The default of 1 indicates that no multiplier is applied.

You select the turbulent flame speed method within the **Turbulent Flame Speed Closure (TFC)** > **Turbulent Flame Speed** node.

Method

Method	Corresponding Method Node
Turbulent Flame Speed - Zimont Selects the Zimont method (Eqn. (3646)) for calculating the turbulent flame speed source term.	**Zimont Turbulent Flame Speed** *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Specify a setting from `0` (fully extinguished) to `1` (no effect). See Turbulent Flame Speed. *Unburnt Thermal Diffusivity Control* The unburnt thermal diffusivity is defined as the laminar thermal conductivity divided by the product of specific heat and density, evaluated at the unburnt state. • **Flamelet Table** The above properties are interpolated from the flamelet table. • **User Defined Profile** Allows you to set this diffusivity as a scalar profile. Activates the **User Defined Unburnt Thermal Diffusivity** node. • **Power Law** Determines the diffusivity using Eqn. (3552). *Flame Stretch Effect* When activated, uses the flame stretch factor G (Eqn. (3647)), which takes the flame stretch effect into account by representing the probability of unquenched flamelets. Activates the **Flame Stretch Effect** node. **Sub-Nodes** **Flamelet Table** This node serves as a placeholder to indicate that the flamelet table provides values for the unburnt thermal diffusivity. **User Defined Unburnt Thermal Diffusivity** Use the **Unburnt Thermal Diffusivity Profile** sub-node of this node to set this diffusivity as a scalar profile.

Method	Corresponding Method Node
Peters Turbulent Flame Speed Selects the Peters method (Eqn. (3651)) for calculating the turbulent flame speed source term.	**Peters Turbulent Flame Speed** *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Select a setting from `0` (fully extinguished) to `1` (no effect). *Constant, A1* Coefficient A_1, from Eqn. (3652) *Constant, A4* Coefficient A_4, from Eqn. (3652) *Constant, B1* Coefficient B_1, from Eqn. (3652) *Constant, B3* Coefficient B_3, from Eqn. (3652) *Ewald's Corrector Constant* c_{ew}, from Eqn. (3652)
User Defined Turbulent Flame Speed Selects the User-Defined method for calculating the turbulent flame speed source term.	**User Defined Turbulent Flame Speed** *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Select a setting from `0` (fully extinguished) to `1` (no effect). **Sub-Nodes** **Turbulent Flame Speed Profile** Scalar profile value.

Method	Corresponding Method Node
User Defined Source Selects the User-Defined Source method for calculating the turbulent flame speed source term.	**User Defined Source** Progress variable source term. *Wall Effect Constant* Uses wall effects to model the quenching of the flame at walls. Specify a setting from `0` (fully extinguished) to `1` (no effect). **Sub-Nodes** **User Source Profile** Defines the Turbulent Flame-Speed Closure (TFC) progress variable source term. **User Source Jacobian Profile** Defines the Turbulent Flame-Speed Closure (TFC) progress variable Jacobian source term.

Initial Conditions

Progress Variable

You specify a progress variable between 0.0 (unburnt) and 1.0 (fully burnt).

Boundary Settings

Flow Boundaries

Flow boundaries except the Outlet have the **Progress Variable** physics value, a scalar profile, available by default.

Wall Boundary

Wall Combustion Scalar

Selects the scalars for the wall combustion calculation.

See Wall Combustion Scalar Option.

Region Settings

Applies to all regions:

Active Reactions Option

Activates or deactivates chemical reactions in this region.

TFC Combustion Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence and do not decrease, reduce the under-relaxation factor for the relevant solvers. The default value is 0.8.

Reconstruction Frozen

When activated, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is deactivated by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When activated, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. Deactivated by default.

Field Functions

The following field functions are only available when the TFC model is selected with a flamelet model.

Progress Variable

c, in Eqn. (3601).

Progress Variable Variance

c_{var}, in Eqn. (3398).

Unnormalized Progress Variable

y in Eqn. (3598).

Unnormalized Progress Variable Variance

y_{var} in Eqn. (3602).

Contents:

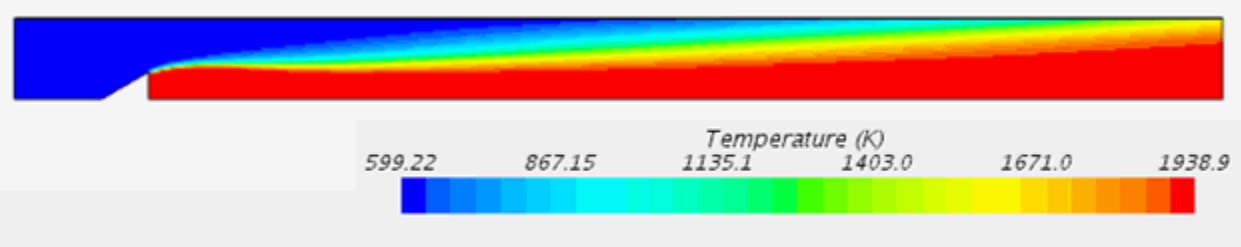
Restoring the Premixed Turbulent Flame-Speed Closure Model

The Premixed Turbulent Flame-Speed Closure (TFC) model in Simcenter STAR-CCM+ v.11.06 is restored to the Flamelet Generated Manifold (FGM) model with the Turbulent Flame-Speed Closure (TFC) flame propagation model. You can restore the Premixed model settings as described in this section.

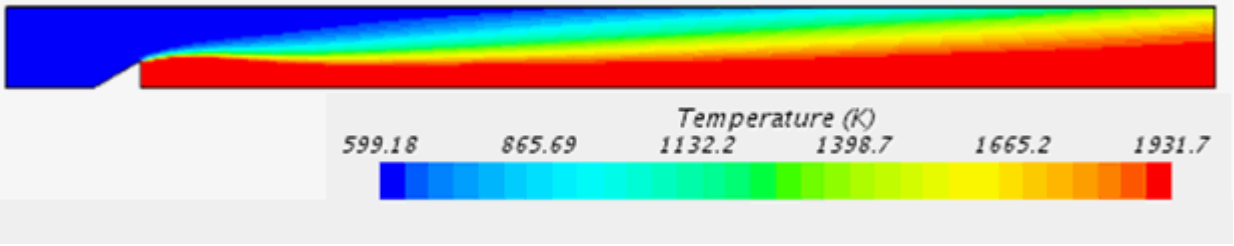
As part of a plan to improve and simplify the procedure for selecting combustion models, the Premixed TFC model is discontinued in Simcenter STAR-CCM+ v.11.06.

When loading a simulation in Simcenter STAR-CCM+ v.11.06 or later that was saved in a version of Simcenter STAR-CCM+ before v11.06, the Premixed TFC model is restored to the Flamelet Generated Manifold (FGM) model with the Turbulent Flame-Speed Closure (TFC) flame propagation model. Several settings are defined differently and must be set up again. The following images show a comparison of the temperatures on the cross section of a flame holder.

Premixed TFC 11.04



Premixed FGM 11.06 (Partially Pre-Mixed)



Simcenter STAR-CCM+ v.11.06 provides the FGM model as an option for Premixed Combustion. This model is the same as that provided for Partially-Premixed combustion. Further steps are required to restore the premixed behaviour that was available in Simcenter STAR-CCM+ v.11.04 and earlier. These steps are as follows:

You can restore the settings of the deprecated Premixed combustion model, using the following procedure:

1. Redefine the reacting fluid stream to match the Premixed set-up.
    a) Select the **[Continuum]** > **FGM Table Generator** > **Fluid Streams** node and set the *Fluid Stream Components* as the Premixed mixture.
    b) Select the **Fluid Streams** node and set the *Temperature of the Stream* using the temperature from Simcenter STAR-CCM+ v11.04 that is set for the inlet boundary of the fuel/air mixture.
    c) Select the **[Continuum]** > **FGM Table Generator** > **Fluid Streams** > **Oxidizer Stream** node and set the *Fluid Stream Components* as Air.
    d) Select the **Oxidizer Stream** node and set the *Temperature of the Stream* using the temperature from Simcenter STAR-CCM+ v11.04 that is set for the inlet boundary of the fuel/air mixture.

Any FGM Table parameters that were set in the simulation before Simcenter STAR-CCM+ v11.06, must be redefined.

2. Create an FGM table using the **[Continuum]** > **FGM Table Generator**.
   - Set the Fuel Composition to the premixed mixture and the oxidizer to air.
   - Set the Fuel Temperature to the temperature that is set for the inlet boundary of the fuel/air mixture in Simcenter STAR-CCM+ v11.04.
   - Set the Pressure to the absolute pressure that is specified in Simcenter STAR-CCM+.
3. Select the **[Physics]** > **Initial Conditions** > **Mixture Fraction Profile** node and specify the *Value* as `1.0`.
4. Select the **Models** > **Flamelet Generated Manifold** > **Progress Variable Variance** node and set the *Method* that you require.
5. To restore the Ignitor:
   a) Right-click the **[Continuum]** > **Ignitors** node and select **New**.
   b) Select the **ProgressVariableIgnitor 1** node and specify the necessary properties.
   c) If the **ProgressVariableIgnitor 1** node *Activator* is set to **Pulse**, select the **Pulse** sub-node and specify the necessary properties.
6. For all inlet and outlet boundaries within each physics continuum, select the **[Boundary]** > **Physics Values** > **Mixture Fraction Profile** node and specify the *Value* as `1.0`.

Wall Combustion Scalar Option

Boundary condition available for the Flamelet Generated Manifold (FGM) model, the Steady Laminar Flamelet (SLF) model, the Chemical Equilibrium (CE) model, the Polymerization model, and some emissions models. Selects the scalars for the wall combustion calculation.

Wall Combustion Scalar Option

Wall Combustion Scalar	Corresponding Value Nodes
Zero Flux Corresponds to an impermeable wall.	None
Specified Value Values that are specified for the corresponding physics values nodes are prescribed at the wall. For the Polymerization model, see Polymerization Model Reference: Boundary Settings	**Mixture Fraction Profile** The mixture fraction is a measure of the local fuel/oxidizer ratio in a combustion system consisting of separate fuel and oxidizer streams. The Mixture Fraction Profile represents the reacting proportion of a fluid stream—the atomic mass fraction that originated from the fuel stream. 1.0 is equal to 100%. To initialize with pure oxidizer, maintain the default of 0.0. For inflows where the mixture is unburnt, the Mixture Fraction Profile is the mass fraction of the fuel. **Mixture Fraction Variance Profile** The mixture fraction variance is a measure of turbulent fluctuations in the local mixture fraction values.

	Progress Variable Not available when using the non-premixed SLF or CE models. The progress variable is a dimensionless parameter, Eqn. (3601), that shows the progress of the combustion. The Constant value is 0 for the unburnt state and 1 for the fully burnt state. **Flame Area Density** Only available when using the CFM model. The flame area per unit volume, Σ in Eqn. (3621). Additional physics value nodes appear when the following soot or NOx models are selected: • Soot Moments model: **Soot Moment Profile** • Soot Two-Equation model: **Soot Scaled Mass Density Profile** and **Soot Scaled Number Density Profile** • NOx Emission model: **Nitrogen Oxide** • NOx Fuel model: **Ammonia**, **Hydrogen Cyanide**
Specified Flux Specifies the mass flux through the wall. It is assumed that the mixture fraction variance and the progress variable (for the FGM, TFC, and CFM models) is 0.0. Therefore, the specified wall flux is always treated as unburnt mixture. Activates the physics condition node, **Wall Flux Temperature Specification**	**Mass Flux** The mass flow rate per unit area at the boundary. **Mixture Fraction Profile** The default of 0.0 implies pure oxidizer, 1.0 implies pure fuel. **Static Temperature** The Static Temperature of the associated mass flux.

Wall Flux Temperature Specification

Based on the following specification, enthalpy due to the wall flux is added to the system.

Wall Flux Temperature Specification	Corresponding Value Node
Specified Value	**Static Temperature** The Static Temperature of the associated mass flux.
Wall Value The temperature of the mass flux entering the domain is taken as the wall temperature.	None

Emissions

Emissions are unwanted pollutant species that are by-products of reactions. There are two options to model pollutant species in Simcenter STAR-CCM+. When using the Complex Chemistry model, you can include the pollutant species in the chemical mechanism. For all other models, in particular Flamelet models and the Eddy Break-Up (EBU) model, separate transport equations for the pollutant species are solved.

When modeling NOx emissions using a Flamelet model for which you import a chemical mechanism that contains NOx species, these NOx species should not be selected as species for post-processing within the flamelet table. NOx species should not be stored directly in flamelet tables since NOx species form slowly and are therefore not compatible with the flamelet approximation. A dedicated emissions option is provided within the parameters of the flamelet table generator, which ensures that NOx emissions are transported and calculated accurately.

Simcenter STAR-CCM+ has the following pollutant models:

- NOx Emission
  - NOx Fuel
  - NOx Thermal
  - NOx Prompt
- Soot Emissions
  - Soot Moments
  - Soot Two-Equation
  - Soot Sections

NOx Emission Model

Although oxides of nitrogen (NOx) are created naturally from atmospheric nitrogen during thunderstorms, transportation and industries that burn fossil fuels create more significant NOx emissions. NOx emissions contribute significantly to the creation of acid rain. It is therefore important to develop technologies which produce lower levels of NOx emissions wherever possible.

When using any of the reacting flow models, you can activate the optional NOx Emission model. This model provides a tool to predict the NOx production from various sources and helps in the design of NOx control measures.

The NOx Emission model solves the transport equation for the concentration of NOx, using the Fuel NOx model and/or the NOx Thermal model to contribute to the NOx reactive source term. You can also additionally use the NOx Prompt model.

- The NOx Fuel model contributes the NOx emission arising from fuels such as heavy liquids and coal which release fuel-bound nitrogen during combustion. Therefore, when modeling emissions that are resultant from burning these fuels, use the Fuel NOx model in addition to the Thermal NOx model. In Lagrangian phases, you can use the Fuel NOx model for liquid fuel or coal. In addition to liquid fuels and coal, Simcenter STAR-CCM+ allows you to model Fuel NOx for a purely gaseous fuel. For pure gas fuel, you can introduce the intermediate species, HCN and/or NH3, arising from the fuel directly at the inlet boundary.
- The NOx Thermal model contributes the NOx emission that is formed from N2 and O2 or OH under lean fuel conditions and at high temperatures, using the three-step extended Zeldovich reaction mechanism. Thermal NOx is dominant in hydrocarbon flames. For combustion set-ups that do not use the Complex

Chemistry model, the concentrations of species are computed during the flamelet table generation and are taken directly from the flamelet table for each iteration. When using the Complex Chemistry model, the source terms are computed at each iteration.

- The NOx Prompt model contributes the NOx emission arising from processes that are not accounted for by the NOx Fuel or NOx Thermal models. For example, atmospheric nitrogen reacting with intermediate species of combustion such as C, CH, and CH2 radicals. Such contributions are generated during low-temperature combustion.

NOx is considered to be a passive scalar, not influencing density calculations. Therefore, in steady-state simulations, use the NOx Emission model as a post-processing tool, that is, activate it after the flow field has converged. In transient simulations, to model the evolution of NOx accurately, activate this model from the beginning.

Soot Emissions Model

The formation and emission of carbonaceous particles is often observed during the combustion of hydrocarbons. These particulates, called soot, are identified in flames and fires as yellow luminescence. In gas turbines, internal combustion engines and other practical combustion devices, the formation of soot is mostly a product of incomplete combustion.

Apart from the resulting loss in combustion efficiency, a serious effect of soot formation is the health hazard. On the other hand, there are situations where the presence or generation of soot is required. For example, generation of carbon black is needed in the production of automobile tires. In furnaces for industrial application or in heat generators, the intermediate formation of soot is required to augment the heat transfer by radiation. The soot, however, must undergo oxidation before the exhaust is released into the environment.

It is widely accepted that the formation of soot is a complex process which consists of the following:

- Fuel pyrolysis and oxidation reactions
- Formation of polycyclic aromatic hydrocarbons (PAH)
- Inception of first particles
- Growth of soot particles due to reaction with gas-phase species
- Coagulation of particles
- Oxidation of soot particles and intermediates

Soot Moments Model

The method of moments is based on the fact that solving an infinite set of equations for the statistical moments of the PSDF is equivalent to the direct simulation of the PSDF. Additionally, it can be shown that often the accuracy using only a few moments is sufficiently high. Usually, a set of equations for the first few moments is applied, where the accuracy of the approach increases with the number of moments that are used. The main advantages are:

- Computational efficiency
- The ability to extract major features of the PSDF from the moments, such as:
  - Soot volume fraction
  - Mean number density
  - Total surface
  - Mean diameter

The Soot Moments model in Simcenter STAR-CCM+ can solve up to four moments: Moment 0, 1, 2, and 3. The model is compatible with the Complex Chemistry, Steady Laminar Flamelet (SLF), and Flamelet Generated Manifold (FGM) combustion models.

Soot Two-Equation Model

Simcenter STAR-CCM+ provides a **Soot Two-Equation** model that is based on a technique that is called the Moss-Brookes-Hall (MBH) soot model.

The Soot Two-Equation model is a semi-empirical soot model that is based on four physical processes of soot formation:

- Nucleation / Inception
- Coagulation
- Surface growth
- Oxidation

The Soot Two-Equation model allows you to implement any two-equation soot model by setting the built-in source terms to zero, and then specifying new source terms for each of the four physical processes of soot formation.

When you activate the Soot Two-Equation model with the Eddy Break-up (EBU) model, the fluid stream manager becomes available. The fluid stream manager lets you define the fuel and oxidizer streams.

In Simcenter STAR-CCM+ the Soot Two-Equation model offers a choice of nucleation options in its properties: Acetylene-based and PAH-based.

To access the properties of the **Soot Two-Equation** model, select the **Soot Two-Equation** node.

Soot Sections

The Sectional method is based on a description of sections containing soot particles of equal volume, allowing a volume-based discretization of particle sizes together with conservation of the soot number density and mass. A number of sections are transported in the section model.

Contents:

Emissions Workflow

Follow the steps in this workflow to simulate NOx and/or Soot emissions.

Before following this workflow, make sure that you have completed the model selection steps from the Reacting Flow General Workflow, and one of the following specific detailed workflows:

- Flamelet Workflow
- Reacting Species Transport Workflow
- Surface Chemistry Workflow

This emissions workflow is not suitable for use with the Interphase workflow. The Interphase workflow describes how to use emissions models that are specific to the Lagrangian phase.

The NOx Emission model requires species and enthalpy models to be activated, so a flow model must be selected unless one is already selected with the combustion model. **Segregated Flow** is the recommended choice when using the NOx Emission model.

1. For the physics continuum that represents the reacting flow, select the following models—in addition to the models that are previously selected, with **Auto-Select recommended models** activated:

Group Box	Model
Optional Models	You can select one or both of these models. ◦ **NOx Emission**: provides a framework for modeling the NOx transport equation by providing a tool to predict the NOx production from various sources. ◦ **Soot Emissions**
Specific NOx Models (available when NOx Emission is activated)	You can select one or more of the NOx models to calculate the reactive source term in the NOx transport equation. ◦ **NOx Fuel**: contributes the NOx emission that arise from the fuel portion. You can use this model for a pure gas-phase combustion. The NOx Fuel model transports three passive scalars: NO, NH3, and HCN. When this model is selected, HCN and NH3 boundary conditions are available for you to specify the inlet composition. ◦ **NOx Thermal**: contributes to the source term by using the three-step extended Zeldovich reaction mechanism. ◦ **NOx Prompt**: contributes the NOx emission that arise from the reaction of hydrocarbon fragments and molecular nitrogen. Often produced in combustion environments with relatively low-temperature and fuel-rich conditions—as in staged combustion systems and gas turbines.
Thermal NOx Models (available when NOx Thermal is activated)	For combustion set-ups that do not use the Complex Chemistry model, the NOx Thermal model uses the coefficients—A, B, C, and D, in Eqn. (3692)—that are stored in the flamelet table, to compute the averaged reactive source term in the NOx transport equation. When using the Complex Chemistry model, the Complex Chemistry model computes the source terms at each iteration.
Soot Emissions Model (available when Soot Emissions is activated)	You can select only one Soot model. ◦ **Soot Moments**: uses the Method of Moments technique to calculate the soot particle size distribution function (PSDF). Can solve up to four moments: Moment 0, 1, 2, and 3. ◦ **Soot Two-Equation**: solves transport equations for scaled number density and scaled mass density based on the Moss-Brookes-Hall (MBH) technique. ◦ **Soot Sections**: solves a soot mass fraction transport equation for each section, based on a description of sections containing soot particles of equal volume, allowing a volume-based discretization of particle sizes together with conservation of the soot number density and mass.

2. The Soot Sections model provides options to create various reports.
   For instructions on plotting the particle size distribution for soot sections, see Plotting Soot Sectional Particle Size Distribution.

3. Return to the specific detailed workflow that you are following.

Contents:

Plotting Soot Sectional Particle Size Distributions

You can visualize automatically updated soot post-processing data through plots as a function of iteration or time step.

These instructions are intended as an optional addition to the Emissions Workflow when using the Soot Sections model.

Create the table.

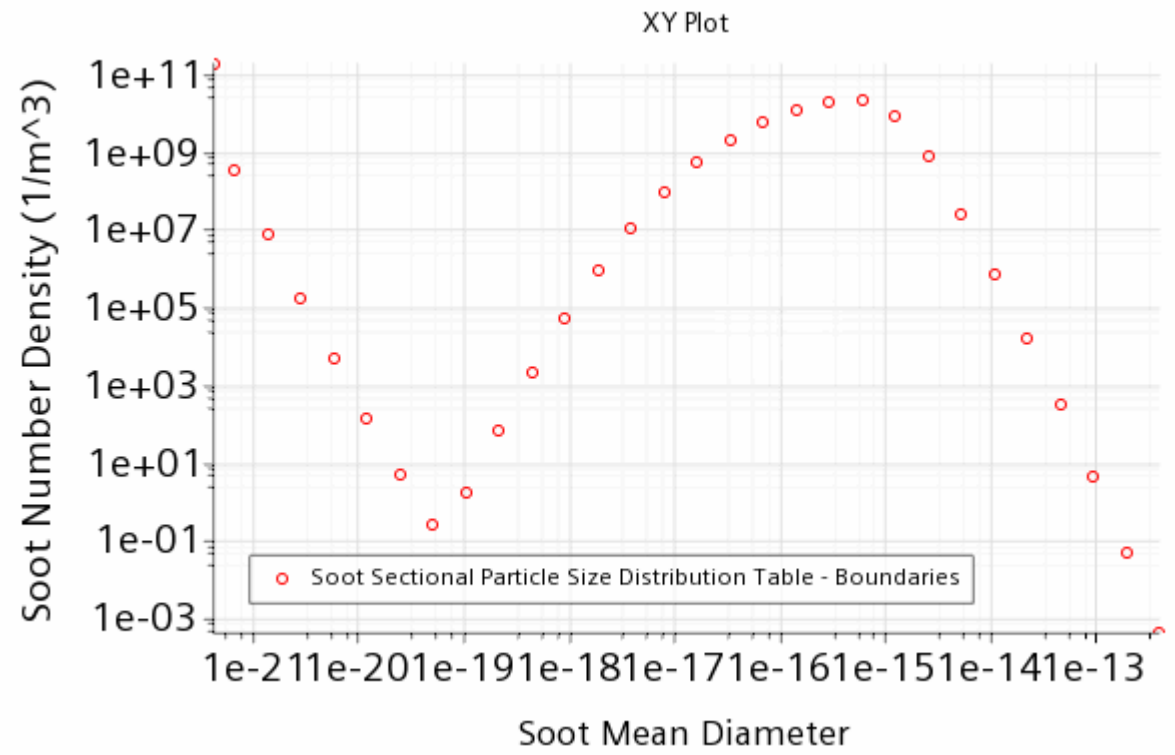
1. a) Right-click the **Tools** > **Tables** node and select either:
   - **New Table** > **Soot Sectional Particle Size Distribution Table - Boundaries**
   - **New Table** > **Soot Sectional Particle Size Distribution Table - Regions**

   b) Select the **Tools** > **Tables** > **[soot sectional particle size distribution table]** node and set *Parts* to the region or boundary for which you want to visualize the soot sectional particle size distribution.

   c) Select the **Tools** > **Tables** > **[soot sectional particle size distribution table]** > **Update** node and activate *Auto Extract*.
2. To create the plot, right-click the **Plots** node and select **New Plot** > **XY Plot**.
3. To visualize the tabular data on the plot:
   a) Right-click the **Tools** > **Tables** > **[Soot Sectional Particle Size Distribution Table]** node and select **Extract**.

   b) Right-click the **Plots** > **XY Plot 1** > **Data Series** node and select **Add Data**.

   c) In the *Add Data Providers to Plot* dialog, select **Tables** > **[soot sectional particle size distribution table]** and click **OK**.
4. As the solution runs, the plot automatically updates to show the soot sectional particle size distribution on the selected region or boundary.



Emissions Reference

Most of the controls that you can set for emissions modeling are located in the physics continuum or within the Solvers node. Some models require that you set mass fractions on inlet boundaries.

Contents:

NOx Emission Model Reference

The NOx Emission model provides a framework for modeling the NOx transport equation.

NOx Emission Model Reference

Theory	See NOx.

Provided By	**[physics continuum]** > **Models** > *Optional Models*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **NOx Emission**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport** or **Flamelet**	
Properties	Key properties are: Source Enabled Trigger, Begin, Secondary Gradients, Convection. See NOx Emission Model Properties.	
Activates	Initial Conditions	Nitrogen Oxide. See Initial Conditions.
	Boundary Inputs	Wall Combustion Scalar Option. See Boundary Settings.
	Solvers	NOx. See NOx Emission Solvers.
	Monitors	NO
	Field Functions	Mass Fraction of Nitrogen Oxide Emission. See Field Functions.

NOx Emission Model Properties

Source Enabled Trigger

Controls whether Simcenter STAR-CCM+ starts calculating the chemistry at the time-step, iteration, or physical time that you specify in the *Begin* property, or whether this model never contributes any sources.

Begin

Specifies the iteration, time-step, or physical time after which the reactions are activated. Before this iteration, time-step, or physical time, reactions are deactivated. Specifying a physical time [degCA] allows you to activate chemistry sources just before spark ignition. When specifying it as an expression which varies during the simulation, reactions are only active when the current iteration, time-step, or physical time is higher than the value provided by the expression.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.
- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.
- **Boundaries Only**: Solves for the boundary secondary gradients only.

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

Initial Conditions

Nitrogen Oxide

Allows you to set the profile for the mass fraction of the Nitrogen Oxide emission. For example, when simulating exhaust gas recirculation (EGR).

Boundary Settings

Any Boundary Type

Wall Combustion Scalar Option

Selects the scalars for the wall combustion calculation.

Method	**Corresponding Physics Value Nodes**
Zero Flux	None
Specified Value Allows you to specify the composition of species at a boundary.	**Nitrogen Oxide**

NOx Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Field Functions

Mass Fraction of Nitrogen Oxide Emission

Represents the mass fraction of NO. Since it is considered that NOx emissions consist only of NO, this is the transported scalar of the NOx Emission model.

NOx Fuel Model Reference

The NOx Fuel Model contributes the NOx emission arising from the fuel portion.

The NOx Fuel model takes care of the reactions to produce NOx.

NOx Fuel Model Reference

Theory	See NOx Fuel	
Provided By	**[physics continuum]** > **Models** > *Optional Models*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **NOx Fuel**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport** or **Flamelet** *Optional Models*: **NOx Emission**	
Properties	No properties	
Activates	Initial Conditions	Ammonia, Hydrogen Cyanide. See Initial Conditions.
	Boundary Inputs	Wall Combustion Scalar Option. See Boundary Settings.
	Monitors	HCN, NH3
	Field Functions	Ammonia, Hydrogen Cyanide. See Field Functions.

Initial Conditions

Ammonia

Allows you to specify the mass fraction of ammonia that is present initially. For example, as a result of exhaust gas recirculation (EGR).

Hydrogen Cyanide

Allows you to specify the mass fraction of hydrogen cyanide that is present initially. For example, as a result of exhaust gas recirculation (EGR).

Boundary Settings

Any Boundary Type

Wall Combustion Scalar Option

Selects the scalars for the wall combustion calculation.

Method	**Corresponding Physics Value Nodes**
Zero Flux	None
Specified Value Allows you to specify the composition of species at a boundary.	**Ammonia** **Hydrogen Cyanide**

Field Functions

Ammonia

Displays the mass fraction of ammonia.

Hydrogen Cyanide

Displays the mass fraction of hydrogen cyanide.

NOx Prompt Model Reference

If the conditions are fuel-rich, in which you suspect that there are hydrocarbon fragments, then prompt NOx is important. In cases such as gas turbines and staged combustion, you can include the NOx Prompt model to get more accurate NOx predictions.

NOx Prompt Model Reference

Theory	See NOx Prompt.
Provided By	**[physics continuum]** > **Models** > *Optional Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **NOx Prompt**
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport** or **Flamelet** *Optional Models*: **NOx Emission**
Properties	Key properties are: Fuel Component, Pre-Exponent Correction Factor, Activation Energy Ea. See NOx Prompt Model Properties.

NOx Prompt Model Properties

Fuel Component

Allows you to select the fuel component which contributes to the NOx Prompt source.

Pre-exponent Correction Factor

If you have the kinetics data of a particular hydrocarbon, you can adjust this parameter for it, which is cf in Eqn. (3695) and Eqn. (3699).

Activation Energy, Ea

E_A in Eqn. (3695).

NOx Thermal Model Reference

The NOx Thermal Model contributes to the thermal part of the NOx source term using a variant of the extended three-step Zeldovich mechanism.

NOx Thermal Model Reference

Theory	See NOx Thermal.	
Provided By	**[physics continuum]** > **Models** > *Optional Models*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **NOx Thermal**	
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport** or **Flamelet** *Optional Models*: **NOx Emission**	
Properties	None	
Activates	Model Controls (child nodes)	O Concentration, OH Concentration.
	Field Functions	Molar Concentration (O), Molar Concentration (OH). See Field Functions.

O Concentration

Available only with the Reacting Species Transport model. Selects the approximation model for the concentration of oxygen.

Equilibrium

Selects the approach that is used in Eqn. (3684) and Eqn. (3685)].

Partial Equilibrium

Selects the approach that is used in Eqn. (3684) and Eqn. (3686) which considers a third-body reaction.

Species List

This option is recommended if the O species is present in the gas-phase reaction mechanism.

OH Concentration

Selects the approximation model for the concentration of the OH group.

Exclusion

Selects the approach that is used in Eqn. (3687), in which the third reaction in the extended Zeldovich mechanism is assumed to be negligible.

Partial Equilibrium

Selects the approach that is used in Eqn. (3688).

Species List

This option is recommended if the OH species is present in the gas-phase reaction mechanism.

Field Functions

Molar Concentration (O)

The molar concentration of oxygen.

Molar Concentration (OH)

The molar concentration of the OH species.

Soot Emissions Model Reference

There are three soot emission models available to solve combustion problems, the Soot Moments model, Soot Two-Equation model, and Soot Sections model.

The soot emissions models influence the Participating Media Radiation (DOM) and Gray Thermal Radiation models by contributing to the absorption coefficient of the continuous phase (the absorption coefficient describing both absorption and emission). Simcenter STAR-CCM+ models the soot as a gray medium, treating the soot as one component of the continuous phase. The total absorption coefficient of the gas includes the soot absorption coefficient as part of an algebraic sum. You can specify the value of the absorption coefficient as a constant, as a field function, or by the Planck Mean Absorption Coefficient method.

Soot Emission Model Reference

Theory	See Soot.
Provided By	**[physics continuum]** > **Models** > *Optional Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Soot Emissions**

Requires	**STAR-CCM+ In-cylinder** *Combustion Model*: **Complex Chemistry**, **ECFM-3Z**, or **ECFM-CLEH** **Simcenter STAR-CCM+** *Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** or **Reacting Species Transport** Then either: • *Flamelet Models*: **Chemical Equilibrium**, or **Flamelet Generated Manifold**, or **Steady Laminar Flamelet** • *Reacting Species Models*: **Complex Chemistry** or **Eddy Break-Up** *Flow*: **Segregated Flow**
Properties	None

Soot Moments Model Reference

The Soot Moments Model is based on a technique that is called Method of Moments. This method is used to calculate the soot particle size distribution function (PSDF).

Currently, the nucleation model pathway Eqn. (3724) and Eqn. (3725) is used, which is based on the acetylene concentration.

Soot Moments Model Reference

Theory	See Soot Moments.
Provided By	**[physics continuum]** > **Models** > *Soot Emissions Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Soot Moments**
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** or **Reacting Species Transport** Then either: • *Flamelet Models*: **Chemical Equilibrium**, or **Flamelet Generated Manifold**, or **Steady Laminar Flamelet** • *Reacting Species Models*: **Complex Chemistry** or **Eddy Break-Up** *Flow*: **Segregated Flow** Then: *Optional Models*: **Soot Emissions**
Properties	Key properties are: Source Enabled Trigger, Begin, Secondary Gradients, Convection. See Soot Moments Model Properties.

Activates	Model Controls (child nodes)	Soot, Soot Model Properties
	Boundary Inputs	See Boundary Settings.
	Solvers	Soot. See Soot Moments Model Solvers.
	Monitors	SootMoment0, SootMoment1
	Field Functions	Soot Mass Density, Soot Mean Diameter, Soot Moment 0, Soot Moment 1, Soot Moment Source 0, Soot Moment Source 1, Soot Number Density, Soot Surface Density, Soot Volume Fraction. See Field Functions.

Soot Moments Model Properties

Source Enabled Trigger

Controls whether Simcenter STAR-CCM+ starts calculating the chemistry at the time-step, iteration, or physical time that you specify in the *Begin* property, or whether this model never contributes any sources.

Begin

Specifies the iteration, time-step, or physical time after which the reactions are activated. Before this iteration, time-step, or physical time, reactions are deactivated. Specifying a physical time [degCA] allows you to activate chemistry sources just before spark ignition. When specifying it as an expression which varies during the simulation, reactions are only active when the current iteration, time-step, or physical time is higher than the value provided by the expression.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.
- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.
- **Boundaries Only**: Solves for the boundary secondary gradients only.

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

Flow Boundary Diffusion

When activated, this property includes the flow-boundary diffusion fluxes (or viscous fluxes for flow models) as given by Eqn. (908). This property is activated by default.

Boundary Settings

Inlet or Pressure Outlet Boundary

Soot Moment Profile

Density weighted soot moment profile.

Wall Boundary

Wall Combustion Scalar Option

Sets the scalars for the wall combustion calculation.

Method	**Corresponding Physics Value Nodes**
Zero Flux	None
Specified Value	**Soot Moment Profile** Density weighted soot moment profile.
Specified Flux	None

Soot Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during

subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Field Functions

Soot Mass Density

M in Eqn. (3720). The units are $\left[\mathrm{kg/m^3}\right]$.

Soot Mean Diameter

d in Eqn. (3743).

Soot Moment 0

M_0 related to soot number density in Eqn. (3740).

Soot Moment 1

Mean particle diameter of soot particles, M_1 in Eqn. (3741) and Eqn. (3741).

Soot Moment Source 0

$r = 0$ in Eqn. (3738).

Soot Moment Source 1

$r = 1$ in Eqn. (3738).

Soot Number Density

N in Eqn. (3719) and Eqn. (3740). The units are $\left[\mathrm{/m^3}\right]$.

Soot Size Dispersion

Activated when the *Number of Moments* property is set to 4. This value is calculated as follows:

$$D_{soot} = \frac{(M_2 M_0)}{(M_1)^2}$$

Soot Surface Density

S in Eqn. (3744).

Soot Volume Fraction

f_v in Eqn. (3741).

Steric Factor

α in Eqn. (3780).

Soot

The Soot sub-node allows you to specify specific material properties for the soot material.

Density

ρ in Eqn. (3737).

Molecular Diffusivity

σ in Eqn. (3737).

Turbulent Schmidt Number

σ_t in Eqn. (3737).

Soot Model Properties

Number of Moments

Selects the number of moments to solve. Possible values range from 2 to 4.

Solving for 4 moments is more computationally expensive than 2. However, if the problem and mesh size are not too large, and you are interested in soot size dispersion, then run 4 moments.

Steric Factor Option

Allows you to specify the steric factor α in Eqn. (3772), that is, the fraction of reactive sites on the surface of the soot particle that are available for soot growth or oxidation reactions.

Method	Corresponding Sub Node
Constant	**Steric Factor** Allows you to define a constant value for Alpha (the steric factor α) between 0 and 1.
Premixed Temperature Correlation Uses fitted correlation from Appel et al. [799] for α, where α is a function of the local temperature and the average soot particle size, quantified by the reduced soot moment μ_1, see Eqn. (3780).	None
User Defined Profile	**User-Defined Steric Factor** Allows you to define the steric factor using a scalar profile.

Nucleation Option

Only available as a property of the Soot Moments model or Soot Sections model when using the Complex Chemistry, Reactor Network, ECFM-3Z, or ECFM-CLEH combustion model. When using one of the Flamelet combustion models, you specify the nucleation option as a combustion table parameter.

Allows you to specify the *Nucleation Option* as either:

Nucleation Option	Corresponding Sub-Node
Single PAH Species (C16H10): See Eqn. (3745) and Eqn. (3746). The PAH precursor is recognised as any species which includes either A4 or A3R5 in the species name, or has the composition C16H10.	None

Nucleation Option	**Corresponding Sub-Node**
C2H2: See Eqn. (3748).	None
Multi PAH Species Allows you to select multiple PAH precursor species from those that are present in the chemical mechanism. Simcenter STAR-CCM+ recognises the chemical symbols of the PAH precursor species as described within the table for Multi PAH Species Nucleation. Available only when using the Complex Chemistry or Reactor Network combustion models.	**PAH Species Components** Lists the selected PAH precursor species—each displays its *Sticky Coefficient* property.

Soot Surface Chemistry Option

Soot Surface Chemistry Option	**Corresponding Sub-Node**
HACA The soot surface growth is modeled using the Hydrogen-Abstraction-C2H2-Addition (HACA) surface mechanism. Most appropriate when using the Complex Chemistry model. See HACA.	None
HACA RC The soot surface growth is modeled using the Hydrogen-Abstraction-Carbon-Addition-Ring-Closure (HACA-RC) surface mechanism. Most appropriate when using an ECFM model for diesel fuel. See HACA RC.	None

Surface-growth Scale

Scales surface growth (part of W_r in Eqn. (3739)).

Nucleation Scale

Scales nucleation (R_r in Eqn. (3739)).

Oxidation Scale

Scales oxidation (part of W_r in Eqn. (3739)).

Coagulation Scale

Scales coagulation G_r in Eqn. (3739). Increasing this value increases the soot mean diameter.

Two-Way Coupled Species

In soot reactions, gas phase species are transferred to and from the gas phase to the soot particles. When this property is activated, these gas-phase species are added and removed from the gas-phase simulation. Only available when using a reacting species transport model or the Reactor Network model.

Restoring the 11.06 Soot Moments Model

In Simcenter STAR-CCM+ v.12.02, the A3R5 Soot Moments model nucleation option (which was present in Simcenter STAR-CCM+ v.11.06) is removed for all combustion models. Also, the Soot Moments model is no longer available to use with the Chemical Equilibrium model. This section provides details of how to restore v.11.06 simulation files that use the Soot Moments model with the Steady Laminar Flamelet (SLF) model.

Soot moments libraries that are generated in DARS are no longer supported in Simcenter STAR-CCM+ since v.12.02. Instead, the soot moment source terms are calculated in Simcenter STAR-CCM+, wether you generate a flamelet table in Simcenter STAR-CCM+ or import a DARS flamelet library.

When loading a sim file from v.11.06 which uses the SLF combustion model with the Soot Moments model, you must regenerate the flamelet table. Make sure that all of the species (H2, H, H2O, OH, O2, C2H2) that are required for soot calculations are present.

Note: The SLF soot moment library that is calculated in Simcenter STAR-CCM+ v.12.02 does not include a model for condensation. Therefore, soot results will change from v.11.06 to v.12.02.

To restore v.11.06 simulation files that use the Soot Moments model with the SLF model, you can either import a DARS generated SLF library, or generate a SLF library in Simcenter STAR-CCM+. To generate a SLF library in Simcenter STAR-CCM+:

1. Open the v.11.06 simulation file in Simcenter STAR-CCM+ v.12.02 or later.
2. Expand the **Continua** > **[Continuum]** > **SLF Table Generator** node.
3. Make sure that the chemistry definition contains all of the species (H2, H, H2O, OH, O2, C2H2) that are required for soot calculations. If not:
   a) If you do not have a chemical mechanism, or want to use a different chemical mechanism, right-click the **SLF Table Generator** > **Chemistry Definition** node and select **Delete Complex Chemistry Definition**.
   b) Import or create the complex chemistry definition.
   See Importing Species and Reactions.
   c) Redefine any other necessary settings. If necessary, you can compare the previous and current simulation trees to check that the settings are consistent. See Comparing Simulation Trees.
4. Select the **SLF Table Generator** > **Parameters** > **Emissions** node and activate *Soot Moment*.
5. To generate the flamelet library, right-click the **SLF Table** node and select **Generate Flamelet Library and Construct Table**.

Soot Sections Model Reference

The soot sectional method is based on a description of sections containing soot particles of equal volume, allowing a volume-based discretization of particle sizes together with conservation of the soot number density and mass.

Soot Sections Model Reference

<table>
<tr><td>Theory</td><td colspan="2">See Soot Sections.</td></tr>
<tr><td>Provided By</td><td colspan="2">In Simcenter STAR-CCM+: [physics continuum] > Models > Soot Emissions Model</td></tr>
<tr><td>Example Node Path</td><td colspan="2">Continua > Physics 1 > Models > Soot Sections</td></tr>
<tr><td>Requires</td><td colspan="2">STAR-CCM+ In-cylinder
Optional Models: Combustion
Combustion Model: Complex Chemistry, ECFM-3Z, or ECFM-CLEH</td></tr>
<tr><td></td><td colspan="2">Simcenter STAR-CCM+
Material: Multi-Component Gas
Reaction Regime: Reacting
Then either:
<table><tr><td>Reacting Flow Models: Reacting Species Transport
Reacting Species Models: Complex Chemistry</td><td>Reacting Flow Models: Flamelet
Flamelet Models: Flamelet Generated Manifold (FGM) or Steady Laminar Flamelet</td></tr></table>and:
Optional Models: Soot Emissions</td></tr>
<tr><td>Properties</td><td colspan="2">Key properties are: Convection, Source Enabled Trigger, Begin, Secondary Gradients, and Flow Boundary Diffusion. See Soot Sections Properties.</td></tr>
<tr><td>Activates</td><td>Model Controls (child nodes)</td><td>Soot and Soot Model Properties.</td></tr>
<tr><td></td><td>Other nodes</td><td>[physics continuum] > ECFM Soot Table Generator
Appears when using one of the ECFM models.
See Table Generators Reference.
When using the Complex Chemistry model, the soot species are contained within the mechanism.</td></tr>
<tr><td></td><td>Solvers</td><td>Soot. See Solvers.</td></tr>
<tr><td></td><td>Monitors</td><td>SootSection[n]</td></tr>
<tr><td></td><td>Report Options</td><td>Soot PSDF, Soot, Sections Diameters, Soot Plots, Soot Particle Size Distribution. See Reports.</td></tr>
<tr><td></td><td>Field Functions</td><td>Soot Mass Density, Soot Mass Fraction Sec[n], Soot Mean Diameter, Soot Nucleation Rate, Soot Number Density, Soot PSDF Sec[n], Soot Total Mass Fraction, Soot Volume Fraction, Steric Factor. See Field Functions.</td></tr>
<tr><td></td><td>Tables</td><td>Soot Sectional Particle Size Distribution Table - Boundaries, Soot Sectional Particle Size Distribution Table - Regions</td></tr>
</table>

Soot Sections Model Properties

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

Source Enabled Trigger

Controls whether Simcenter STAR-CCM+ starts calculating the chemistry at the time-step, iteration, or physical time that you specify in the *Begin* property, or whether this model never contributes any sources.

Begin

Specifies the iteration, time-step, or physical time after which the reactions are activated. Before this iteration, time-step, or physical time, reactions are deactivated. Specifying a physical time [degCA] allows you to activate chemistry sources just before spark ignition. When specifying it as an expression which varies during the simulation, reactions are only active when the current iteration, time-step, or physical time is higher than the value provided by the expression.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.
- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.
- **Boundaries Only**: Solves for the boundary secondary gradients only.

Flow Boundary Diffusion

When activated, this property includes the flow-boundary diffusion fluxes (or viscous fluxes for flow models) as given by Eqn. (908). This property is activated by default.

Soot Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Reports

Reports	With Complex Chemistry	With ECFM Models	With Flamelet Models	With Reactor Network
Soot PSDF A sum report of the soot particle size distribution function $\frac{dN}{d\log(d_p)}(i)$.	✓	✓	✓	
Soot Sections Diameters Mean diameter of each soot section.	✓	✓	✓	
Reactor Network Soot PSDF A sum report of the soot particle size distribution function $\frac{dN}{d\log(d_p)}(i)$ for the Reactor Network.				✓
Reactor Network Soot Sections Diameters Mid-point diameter of each soot section for the Reactor Network.				✓

For more information about using Soot PSDF reports, see Plotting Soot Sectional Particle Size Distribution.

Field Functions

Soot Mass Density

m_{soot} in Eqn. (3816).

Soot Mass Fraction Sec[n]

$\widetilde{Y}_{i,\ \text{soot}}$ for section i, in Eqn. (3781).

Soot Mean Diameter

d_p in Eqn. (3818).

Soot Nucleation Rate

$\left(\frac{dN}{dt}\right)_{nu}$ in Eqn. (3724).

Soot Number Density

Total soot number density N_{tot} given by Eqn. (3819).

Soot PSDF Sec[n]

Soot particle size distribution function $\frac{dN}{d\log\left(d_p\right)}(i)$ for section i, given by Eqn. (3820).

Soot Total Mass Fraction

Sum of $Y_{i,\ \text{soot}}$ from i to $i_{\max}$.

Soot Volume Fraction

f_v in Eqn. (3817).

Steric Factor

α in Eqn. (3780).

Tables

Soot Sectional Particle Size Distribution Table - Boundaries / Regions

See Tables Reference.

For instructions on plotting the particle size distribution for soot sections, see Plotting Soot Sectional Particle Size Distribution.

Soot Sections > Soot

Allows you to specify specific material properties for the soot material.

Soot Sections > Soot Model Properties

Allows you to set properties to define the soot sections.

When using the Reactor Network model, the **Reactor Network** > **Emissions** > **Soot Options** node provides similar properties. See Soot Options.

Steric Factor Option

Allows you to specify the steric factor α in Eqn. (3772), that is, the fraction of reactive sites on the surface of the soot particle that are available for soot growth or oxidation reactions.

Method	Corresponding Sub Node
Constant	**Steric Factor** Allows you to define a constant value for Alpha (the steric factor α) between 0 and 1.
Premixed Temperature Correlation Uses fitted correlation from Appel et al. [799] for α, where α is a function of the local temperature and the average soot particle size, quantified by the reduced soot moment μ_1, see Eqn. (3780).	None
User Defined Profile	**User-Defined Steric Factor** Allows you to define the steric factor using a scalar profile.

Nucleation Option

Only available as a property of the Soot Moments model or Soot Sections model when using the Complex Chemistry, Reactor Network, ECFM-3Z, or ECFM-CLEH combustion model. When using one of the Flamelet combustion models, you specify the nucleation option as a combustion table parameter.

Allows you to specify the *Nucleation Option* as either:

Nucleation Option	Corresponding Sub-Node
Single PAH Species (C16H10): See Eqn. (3745) and Eqn. (3746). The PAH precursor is recognised as any species which includes either A4 or A3R5 in the species name, or has the composition C16H10.	None
C2H2: See Eqn. (3748).	None
Multi PAH Species Allows you to select multiple PAH precursor species from those that are present in the chemical mechanism. Simcenter STAR-CCM+ recognises the chemical symbols of the PAH precursor species as described within the table for Multi PAH Species Nucleation. Available only when using the Complex Chemistry or Reactor Network combustion models.	**PAH Species Components** Lists the selected PAH precursor species—each displays its *Sticky Coefficient* property.

(Soot) Surface Chemistry Option

(Soot) Surface Chemistry Option	**Corresponding Sub-Node**
HACA The soot surface growth is modeled using the Hydrogen-Abstraction-C2H2-Addition (HACA) surface mechanism. Most appropriate when using the Complex Chemistry model. See HACA.	None
HACA RC The soot surface growth is modeled using the Hydrogen-Abstraction-Carbon-Addition-Ring-Closure (HACA-RC) surface mechanism. Most appropriate when using an ECFM model for diesel fuel. See HACA RC.	None

Surface-growth Scale

Scales surface growth $\widetilde{\Omega}_{i,\,\mathrm{sg}}$ in Eqn. (3783).

Nucleation Scale

Scales nucleation $\widetilde{\Omega}_{i,\,\mathrm{nuc}}$ in Eqn. (3783).

Oxidation Scale

Scales oxidation $\widetilde{\Omega}_{i,\,\mathrm{ox}}$ in Eqn. (3783).

Coagulation Scale

Scales coagulation $\widetilde{\Omega}_{i,\,\mathrm{coag}}$ in Eqn. (3783). Increasing this value increases the soot mean diameter.

Two-Way Coupled Species

In soot reactions, gas phase species are transferred to and from the gas phase to the soot particles. When this property is activated, these gas-phase species are added and removed from the gas-phase simulation. Only available when using a reacting species transport model or the Reactor Network model.

Soot Sections > Soot Model Properties > Sectional Properties

Number of Sections

Number of discrete sections in the particle size distribution function (PSDF).

Maximum Soot Diameter

Maximum diameter to which the soot particle grows.

Small Diameter Fractal Dimension

Surface growth fractal dimension of soot particles with a diameter θ less than 20nm in Eqn. (3808) and Eqn. (3809). You can set this between `2.0` and `3.0`.

Large Diameter Fractal Dimension

Surface growth fractal dimension of soot particles with a diameter θ greater than 60nm in Eqn. (3808) and Eqn. (3809). You can set this between `2.0` and `3.0`.

Soot Sections > Soot Model Properties > Steric Factor

Alpha

The steric factor α for surface reactions in HACA or HACA-RC mechanisms.

Soot Two-Equation Model Reference

The Soot Two-Equation model is based on a technique that is called the Moss-Brookes-Hall (MBH) soot model.

Soot Two-Equation Model Reference

Theory	See Soot Two-Equation.
Provided By	**[physics continuum]** > **Models** > *Soot Emissions Model*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Soot Two-Equation**
Requires	*Material*: **Multi-Component Gas** *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Flamelet** or **Reacting Species Transport** Then either: • *Flamelet Models*: **Chemical Equilibrium**, or **Flamelet Generated Manifold**, or **Steady Laminar Flamelet** • *Reacting Species Models*: **Complex Chemistry** or **Eddy Break-Up** *Flow*: **Segregated Flow** Then: *Optional Models*: **Soot Emissions**
Properties	Key properties are: Source Enabled Trigger, Begin, Secondary Gradients, Convection. See Soot Two-Equation Properties.

Activates	Model Controls (child nodes)	Soot, Soot Species Option, Soot Model Properties
	Boundary Inputs	See Boundary Settings.
	Solvers	Soot. See Solvers.
	Monitors	SootScaledMassDensity, SootScaledNumberDensity
	Field Functions	Soot Coagulation Rate, Soot Growth Rate, Soot Mass Density, Soot Mean Diameter, Soot Nucleation Rate For Scaled Mass Density, Soot Nucleation Rate For Scaled Number Density, Soot Number Density, Soot Oxidation Rate, Soot Scaled Mass Density, Soot Scaled Mass Density Rate, Soot Scaled Number Density, Soot Scaled Number Density Rate, Soot Surface Density, Soot Volume Fraction. See Field Functions.

Soot Two-Equation Model Properties

Source Enabled Trigger

Controls whether Simcenter STAR-CCM+ starts calculating the chemistry at the time-step, iteration, or physical time that you specify in the *Begin* property, or whether this model never contributes any sources.

Begin

Specifies the iteration, time-step, or physical time after which the reactions are activated. Before this iteration, time-step, or physical time, reactions are deactivated. Specifying a physical time [degCA] allows you to activate chemistry sources just before spark ignition. When specifying it as an expression which varies during the simulation, reactions are only active when the current iteration, time-step, or physical time is higher than the value provided by the expression.

Secondary Gradients

Neglect or include the boundary secondary gradients for diffusion and/or the interior secondary gradients at mesh faces.

- **On**: Default value. Solves for interior and boundary types of secondary gradient.
- **Off**: Does not solve for either type of secondary gradient.
- **Interior Only**: Solves for the interior secondary gradients only.
- **Boundaries Only**: Solves for the boundary secondary gradients only.

Convection

In transport equations, you can choose from a range of schemes that calculate the convection term at a cell face. This calculation requires Simcenter STAR-CCM+ to compute the face value of a quantity from the surrounding cell values. The method used for computing this face value has a profound effect on the stability and accuracy of the numerical scheme. For guidance on selecting a convection scheme, see Convective Flux.

- **1st-order**: First-order convection scheme.
- **2nd-order**: Second-order convection scheme.

Boundary Settings

Inlet or Pressure Outlet Boundary

Soot Scaled Mass Density Profile

Specifies a scalar profile for the soot scaled mass density ϕ_M in Eqn. (3720).

Soot Scaled Number Density Profile

Specifies a scalar profile for the soot scaled number density ϕ_N in Eqn. (3719).

Wall Boundary

Wall Combustion Scalar Option

Sets the scalars for the wall combustion calculation.

Method	**Corresponding Physics Value Nodes**
Zero Flux	None
Specified Value	**Soot Scaled Mass Density Profile** Specifies a scalar profile for the soot scaled mass density ϕ_M in Eqn. (3720). **Soot Scaled Number Density Profile** Specifies a scalar profile for the soot scaled number density ϕ_N in Eqn. (3719).
Specified Flux	**Mass Flux** Specifies a species flux at the boundary. The energy that is associated with the wall species influx or outflux is appropriately added.

Soot Solver Properties

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

Reconstruction Frozen

When **On**, Simcenter STAR-CCM+ does not update reconstruction gradients with each iteration, but rather uses gradients from the last iteration in which they were updated. Activate **Temporary Storage Retained** in conjunction with this property. This property is **Off** by default.

Reconstruction Zeroed

When **On**, the solver sets reconstruction gradients to zero at the next iteration. This action means that face values used for upwinding (Eqn. (914)) and for computing cell gradients (Eqn. (926) and Eqn. (927)) become first-order estimates. This property is **Off** by default. If you turn this property **Off** after having it **On**, the solver recomputes the gradients on the next iteration.

Temporary Storage Retained

When **On**, Simcenter STAR-CCM+ retains additional field data that the solver generates during an iteration. The particular data retained depends on the solver, and becomes available as field functions during subsequent iterations. **Off** by default. For a complete list of these field functions, see Common Solvers Field Functions.

Field Functions

Mixture Fraction (Bilger)

Represents the local mixture fraction that is determined using Bilger's mixture fraction definition Eqn. (3735).

Molar Concentration for Emissions (C2H2)

Displays the molar concentration of acetylene in the soot emissions.

Molar Concentration for Emissions (O)

Displays the molar concentration of oxygen radicals in the soot emissions.

Molar Concentration for Emissions (OH)

Displays the molar concentration of hydroxyl radicals in the soot emissions.

Soot Coagulation Rate

$\left(\frac{dN}{dt}\right)_{co}$ in Eqn. (3726).

Soot Growth Rate

$\left(\frac{dM}{dt}\right)_{sg}$ in Eqn. (3729).

Soot Mass Density

M in Eqn. (3720). The units are $\left[\mathrm{kg/m^3}\right]$.

Soot Mean Diameter

The diameter d of a soot particle.

Soot Nucleation Rate For Scaled Mass Density

$\left(\frac{dM}{dt}\right)_{\mathrm{nu}}$ in Eqn. (3725).

Soot Nucleation Rate For Scaled Number Density

$\left(\frac{dN}{dt}\right)_{nu}$ in Eqn. (3723) for PAH nucleation, or in Eqn. (3724) for C2H2 nucleation.

Soot Number Density

N in Eqn. (3719). The units are $\left[\mathrm{/m^3}\right]$.

Soot Oxidation Rate

$\left(\frac{dM}{dt}\right)_{ox}$ in Eqn. (3731).

Soot Scaled Mass Density

$\emptyset_M$ obtained from Eqn. (3720).

Soot Scaled Mass Density Rate

$\dot{\omega}_{\emptyset M}$ computed from Eqn. (3722).

Soot Scaled Number Density

$\emptyset_N$ obtained from Eqn. (3719).

Soot Scaled Number Density Rate

$\dot{\omega}_{\emptyset N}$ computed from Eqn. (3721).

Soot Surface Density

The surface area of soot particles per unit volume.

Soot Volume Fraction

The volume of soot particles per unit volume.

Soot

The Soot sub-node allows you to specify specific material properties for the soot material.

Soot Species Option

Property	Using a Reacting Species Transport Model	Using a Flamelet Model
O Concentration Required when the OH Concentration is specified using the Partial Equilibrium approach. However, the O Concentration is not used when the OH Concentration is specified by the Species List approximation model.	Uses the **Species List** approximation model for the concentration of oxygen.	**Equilibrium** Selects the approach that is used in Eqn. (3684) and Eqn. (3685). **Partial Equilibrium** Selects the approach that is used in Eqn. (3684) and Eqn. (3686) which considers a third-body reaction. **Species List** Uses the Species List approximation model for the concentration of oxygen. This option is recommended if the O species is present in the gas-phase reaction mechanism.
OH Concentration	Uses the **Species List** approximation model for the concentration of the OH species.	**Exclusion** Selects the approach that is used in Eqn. (3687), in which the third reaction in the extended Zeldovich mechanism is assumed to be negligible. **Partial Equilibrium** Selects the approach that is used in Eqn. (3688). This option uses the O Concentration that is specified. **Species List** Uses the Species List approximation model for the concentration of OH. This option is recommended if the OH species is present in the gas-phase reaction mechanism.

Property	Using a Reacting Species Transport Model	Using a Flamelet Model
C2H2 Concentration	Uses the **Species List** approximation model for the concentration of the C2H2 species.	**Empirical** The concentration of the C2H2 species is calculated empirically. **Species List** Uses the Species List approximation model for the concentration of C2H2. This option is recommended if the C2H2 species is present in the gas-phase reaction mechanism.

Soot Model Properties

Nucleation Option

Allows you to select one of two nucleation options.

- **PAH-based**: This nucleation model pathway, Eqn. (3723), is based on polycyclic aromatic hydrocarbons (PAH). This option is only available when the gas-phase mechanism contains the species: C6H6, C6H5, C2H2, and H2.
  PAH nucleation requires more species than acetylene nucleation, and is therefore more computationally expensive due to the large chemical mechanisms involved.
- **Acetylene-based**: This nucleation model pathway, Eqn. (3724) and Eqn. (3725), is based on the acetylene concentration.

Surface-growth Scale

Scales the surface growth rate for soot mass density $\left(\frac{dM}{dt}\right)_{sg}$ in Eqn. (3729) which contributes to the overall soot scaled mass density rate in Eqn. (3722). Setting this value to zero omits the contribution to the surface-growth source that is calculated by Simcenter STAR-CCM+—in which scenario, you can define the surface-growth source entirely with the user rates.

Coagulation Scale

Scales the coagulation rate for soot number density $\left(\frac{dN}{dt}\right)_{co}$ in Eqn. (3726) which contributes to the overall soot scaled number density rate in Eqn. (3721). Setting this value to zero omits the contribution to the coagulation source that is calculated by Simcenter STAR-CCM+—in which scenario, you can define the coagulation source entirely with the user rates.

Nucleation Scale

Scales the nucleation rate for:

- Soot number density $\left(\frac{dN}{dt}\right)_{nu}$ (in Eqn. (3723) for PAH-based nucleation / in Eqn. (3724) for Acetylene-based nucleation) which contributes to the overall soot scaled number density rate in Eqn. (3721).

- Soot mass density $\left(\frac{dM}{dt}\right)_{nu}$ in Eqn. (3725) which contributes to the overall soot scaled mass density rate in Eqn. (3722).

Setting this value to zero omits the contribution to the nucleation source that is calculated by Simcenter STAR-CCM+—in which scenario, you can define the nucleation source entirely with the user rates.

Oxidation Scale

Scales the oxidation rate for soot mass density $\left(\frac{dM}{dt}\right)_{ox}$ in Eqn. (3731) which contributes to the overall soot scaled mass density rate in Eqn. (3722). Setting this value to zero omits the contribution to the oxidation source that is calculated by Simcenter STAR-CCM+—in which scenario, you can define the oxidation source entirely with the user rates.

Cold Temperature Limit

If the temperature in the cell is lower than this number, then cold flow is assumed—no soot source calculations are performed in that cell.

Soot User Rates

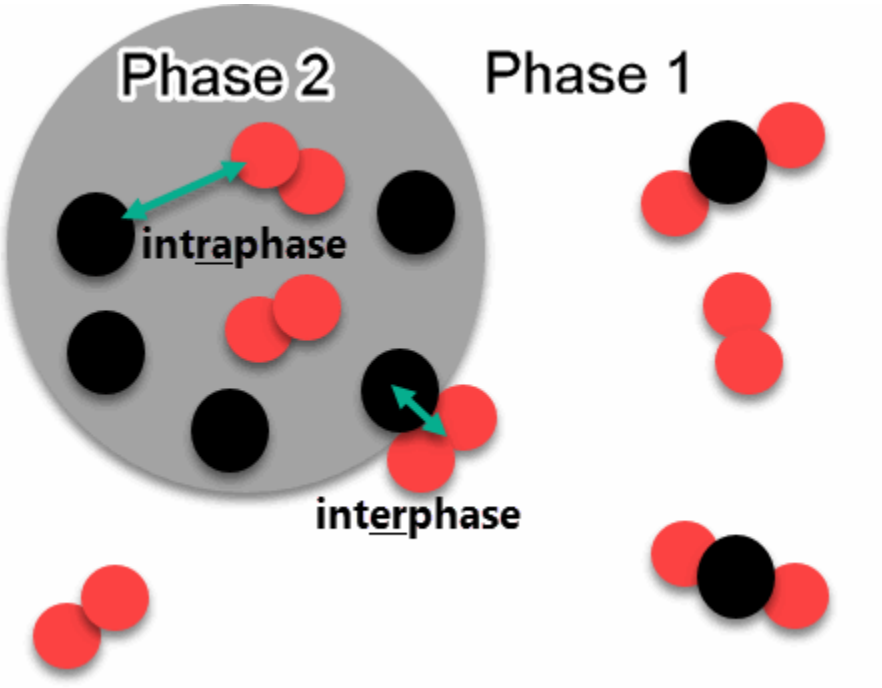
When activated, provides sub-nodes which allow you to include custom rates, and optionally Jacobians (for better numerical stability), for each of the four physical processes—nucleation, coagulation, surface growth, and oxidation.

Each of the custom rates are used to calculate A_1 in Eqn. (3734).

Interphase

There are many applications that involve the transport of reacting particles, such as calcination and char oxidation. You can simulate the process of interphase reactions using Lagrangian Multiphase, Multiphase or Fluid Film models.

The following diagram explains the difference between interphase and intraphase reactions between species.



- Intraphase reactions occur between atoms/molecules in the same phase.
- Interphase reactions occur between atoms/molecules in different phases at the interface between the different phases.

Lagrangian Multiphase Interphase Reactions

You can simulate the process of reacting particles (liquid or solid) using one of the Lagrangian Multiphase models. The particles (liquid or solid) can interact with the continuous phase using the Two-Way Coupling model.

When simulating applications such as coal or biomass combustors, you can use the Lagrangian Particles model to simulate small solid particles that are traveling in a flow. Larger clumps are simulated as Discreet Element Method (DEM) particles. Simcenter STAR-CCM+ also provides the Particle Porosity model which you can use to specify a factor by which solid particles shrink due to reactions.

Particle components can devolatilize or react with a material in a gas phase to form products in gas, liquid, or solid phases.

To model the transport of reacting particles, the Material Particles model is required in the Lagrangian phase. Material particles have mass and volume, obey the physical conservation laws of mass and momentum, and are assumed to be internally homogenous, without internal motion. The type of Material model that is selected influences the type of mass transfer model that is made available:

- When Multi-Component Particle is selected, you can select **Mass Transfer**.
  You can then model the following types of particle reaction (use these models together or separately):
  - **Particle Reaction**
  - **Particle Devolatilization**
- When Multi-Component Coal is selected, you can select **Coal Combustion**. You can use the Coal Combustion model to simulate coal furnaces and gasification.

Particle Reaction

You can use the Particle Reaction model to simulate various particle reactions such as char oxidation, biomass particle oxidation, and ferric oxide reduction. It is possible to simulate multiple reactions between solid particles or liquid droplets reacting with a gas-phase or liquid-phase species to form solid, liquid, and/or gas-phase products.

Particle Devolatilization

The Particle Devolatilization model can simulate various particle mass transfer processes, such as gasification, sublimation, phase transformation, and biomass/coal devolatilization. Particle devolatilization is a gasification process where one or more solid or liquid particles are converted to volatile matter and/or a residue.

Coal Combustion

Coal is an important fuel that is used in electricity generation worldwide. It is pulverized to a fine powder before being blown into the combustion chambers of high-temperature furnaces.

The Coal Combustion model in Simcenter STAR-CCM+ has pre-defined species and reactions that are designed specifically for simulating coal combustion. You can use this model to simulate the transport, gasification, and combustion of coal particles as they pass through such furnaces. This model also allows you to simulate coal fuel NOx emissions.

Coal is a composite material consisting of organic and inorganic substances that can also be moist. The coal particle is assumed to be initially coated with moisture so that a single-component evaporation treatment is appropriate. The driving force for evaporation of this layer is the departure from equilibrium of the liquid-vapor system. In coal combustion, the moisture evaporation is usually heat-transfer limited and takes place rapidly. The devolatilization and char oxidation reactions occur after the moisture has evaporated. In addition to an appropriate combustion model in the continuous phase, coal combustion requires the following Lagrangian phase submodels:

- **Coal Moisture Evaporation**
  Represents the Quasi-Steady Evaporation model for the moisture component (H2O) of the coal particle. This model allows the H2O component of the coal particle to lose its mass through a quasi-steady evaporation process.
- **Raw Coal Devolatilization**
  Defines how the combustible substances are made available for combustion, using either the Two-Step Devolatilization model or the User-Defined Devolatilization model. The Volatile Vapor Component property allows you to select the species to which the raw coal devolatilizes. If no species is selected, an error message (`Error: no CoalVolatile vapor selected for Devolatilization model in coal`) is issued when the solution field is initialized. The benefit of this property is that it allows you to model two different coal types with two different types of CoalVolatiles.

- **Two-Step Devolatilization**

  Controls the process by which raw coal is converted to gaseous combustible material (volatile matter) and solid char residue. Experimental studies have shown that, under certain heating conditions, the volatile matter yield is higher than the value that is obtained from standard proximate analysis. This effect is accounted for by allowing the coal material to devolatilize by two temperature-dependent competing reactions—the Two-Step Devolatilization model [769].

- **User-Defined Devolatilization**

  This model allows you to define the devolatilization rate for the raw coal component of the coal. In addition, you can set the volatile yield in the properties of this model.

- **Char Oxidation**:

  There are three types of char oxidation models available. Each specific char oxidation model node contains three reaction nodes, one for each of the possible char oxidation processes.

  - Char Reaction With O2
  - Char Reaction With H2O
  - Char Reaction With CO2

  Only the first reaction, Char Reaction With O2, is active by default. If you require a more accurate simulation and have reaction rates for the other two reactions, you can activate the two further optional reactions.

  - **First-Order Char Oxidation**

    This model is used to predict the rate at which the char content of the coal burns. The time that is required for this char burnout is a significant part of the coal combustion process. The First-Order Char Oxidation model consists of one or more First-Order Combined Rate reactions that account for gas phase diffusion of the oxidizer as well as the first-order surface reaction kinetics.

  - **Half-Order Char Oxidation**

    The Half-Order Char Oxidation model consists of one or more Half-Order Combined Rate reactions that account for gas phase diffusion of the oxidizer as well as the half-order surface reaction kinetics.

  - **User-Defined Char Oxidation**

    This model provides an alternative to the two other char oxidation rates which you can use to set custom rates as a profile or as a constant.

When these Lagrangian phase models are used with a combustion model in the continuous phase—and if the Two-Way Coupling phase model is also active—the complete coal combustion process can be realized. It is also possible to model a non-reacting Lagrangian phase containing the multi-component coal material model only, without activating coal combustion.

Particle Porosity

Simcenter STAR-CCM+ also provides the optional Lagrangian model, Particle Porosity, which allows you to define how the porosity of particles which burn internally changes through the course of a coal combustion reaction. The porosity of a particle determines how the diameter and surface area of the particle changes throughout a reaction. When the surface area of a particle changes, the overall reaction rate is affected.

Multiphase Interphase Reactions

You can simulate reactions between two different Eulerian phases using the Interphase Reaction model. For example, between fluid and solid particles in a fluidized bed reactor.

Interphase Reaction

The Interphase Reaction model is available to use with the Eulerian Multiphase (EMP) , Volume of Fluid (VOF), or Mixture Multiphase (MMP) variants of the Multiphase model.

The Interphase Reaction model allows you to specify the reactant and product species from either of the phases that are defined within a phase interaction. Phase interactions can define reactions between two phases of the same or different material types—Multi-component Gas, Multi-component Liquid, or Multi-component Particle. You can define specific species which are involved in the interphase reaction from either phase and also specify to which phase each product belongs.

Fluid Film Interphase Reactions

You can simulate reactions between a fluid film phase and its neighbouring gas phase using the Interphase Reaction model in conjunction with the Fluid Film model.

Similar to Multiphase Interphase Reactions, the Interphase Reaction model for fluid film allows you to model reactions between two phases, where the fluid film phase is defined as a multi-component liquid and the gas phase is defined as a multi-component gas.

Contents:

Interphase Reactions Workflow: Lagrangian Multiphase

You can simulate reacting particles using the Lagrangian Multiphase Particle Reaction or Coal Combustion models. Liquid multi-component droplets are supported along with multi-component particles and coal particles.

The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow.

1. For the Physics Continuum that represents the background phase in which the particle reactions occur (the continuous phase), select the following models—in addition to the models that are previously selected, with **Auto-Select recommended models** activated:

Group Box	Model
Optional Models	**Lagrangian Multiphase**

2. Select any further Optional models as necessary.
   For example, if you are simulating reacting flow of solid granular particles such as powders or slurries, select the **Discrete Element Model (DEM)**. See Discrete Element Model Reference.
3. Define the gas or liquid components in the continuous phase.
   a) Expand the **Continua** > **Continuum** > **Models** > **[Multi-Component Gas]** node.
   b) Define the species and corresponding material properties.

4. Add at least one Lagrangian phase. Right-click the **Continuum** > **Models** > **Lagrangian Multiphase** > **Lagrangian Phases** node and select **New**.

   If you are simulating only one type of reacting particle, only one Lagrangian phase is required. See Lagrangian Phases.

5. For each Lagrangian Phase, select the following models, with **Auto-Select recommended models** activated:

Group Box	Model
Particle Type	◦ **Material Particles** ◦ **DEM Particles** (when using DEM)
Material	◦ **Multi-Component Coal**: Designed specifically for simulating coal combustion. ◦ **Multi-Component Particle**: For example, when modeling combustion or devolatilization of a multi-component solid. ◦ **Multi-Component Liquid**: For reactions between a droplet and the surrounding fluid, with or without droplet devolatilization.
Mass Transfer	◦ When **Multi-Component Particle** or **Multi-Component Liquid** are selected, select **Chemical Reactions** ◦ When Multi-Component Coal is selected, select **Coal Combustion**
Char Oxidation (when **Coal Combustion** is selected)	◦ **First-Order Char Oxidation** ◦ **Half-Order Char Oxidation** ◦ **User-Defined Char Oxidation**
Raw Coal Devolitilization (when **Coal Combustion** is selected)	◦ **Two-Step Devolitilization** ◦ **User-Defined Devolitilization**
Particle Reaction Type (when **Chemical Reactions** is selected)	Select one or both: ◦ **Particle Reaction** ◦ **Particle Devolitilization**
Particle Shape (when **DEM Particles** is selected)	any (See DEM Particle Types)
Equation of State	◦ **Constant Density** ◦ **Polynomial Density**

When **Auto-select recommended models** is activated, the following additional phase models are included:

- **Pressure Gradient Force**
- **Spherical Particles** (except with DEM)
- **Energy**
- **Species**
- **Two-Way Coupling**—when the reaction includes interaction with the continuous phase.

6. Select any additional Lagrangian phase models that are required. See: Lagrangian Phase Models.
   For example:
   - **Track File**
   - **Coal Fuel NOx**
   - **Particle Radiation**
7. Define the components in the Lagrangian phases.
   a) Expand the **[Continuum]** > **Models** > **Lagrangian Multiphase** > **Lagrangian Phases** > **[Phase]** > **Models** node.
   b) Set the components as described below.
      - For the **Multi-Component Particle** model:
        Right-click the **Multi-Component Particle** > **Particle Components** node and import species or select mixture components from the material database.
      - For the **Multi-Component Liquid** model:
        Right-click the **Multi-Component Liquid** > **Droplet Components** node and import species or select mixture components from the material database.
      - For the **Multi-Component Coal** model:
        The appropriate species which represent the composition of coal particles are already defined under the **Multi-Component Coal** > **Coal Components** node:
        - **RawCoal**
        - **Char**
        - **Ash**
        - **H20**
   c) If necessary, you can adjust the **[Component]** > **Material Properties**.
      For each component (other than **RawCoal**, **Char**, and **Ash**—which are pre-defined specifically for coal combustion), the Molecular Weight material property method is set to **Elemental Composition** by default. The molecular weight depends on the settings within the Elemental Composition material property node—elemental composition is vital for checking the stoichiometry for a particle reaction.
   d) For DEM particle types, select the **[Particle Type]** node and specify the required settings.
      For more information on particle types, see:
      - The Spherical Particles Model
      - Coarse Grain Particle Models
      - The Composite Particles Model
      - The Particle Clumps Model
      - Working with Individually Composed Shapes
      - Working with Sphere-Filled Parts
      - The Cylindrical Particles Model
      - The Polyhedral Particle Model
8. Define the Particle Reactions.
   - For the **Multi-Component Particle** or **Multi-Component Liquid** models:
     a. Right-click the **Particle Reaction** > **Particle Reactions** or **Particle Devolatilization** > **Particle Reactions** node and select **New Particle Reaction**.
     b. Expand the **Particle Reactions** > **Reaction** node and define the **Reactants** and **Products**.

For Particle Devolatiliziation, reactants can only come from the Lagrangian phase. For Particle Reactions, reactants can come from the Lagrangian phase or the background Fluid. In both cases products can come from either the Lagrangian phase or the background Fluid.

c. Select the **Reaction** > **Reaction Rate** node and select the method that is required for calculating the reaction rate.

- For the **Multi-Component Coal** model, the necessary coal combustion reactions are already defined under the **[Char Oxidation]** node.

9. Set the parameters of other Lagrangian phase models as required.

   See: Lagrangian Phase Models.

10. Collapse the **Lagrangian Multiphase** model node.
11. Set the parameters of the remaining **[Continuum]** > **Models**, as required.
12. For the continuum, define any necessary parameters for the **Reference Values** and **Initial Conditons**.
    - For combustion/devolatilization reactions, make sure that particles reach a high enough temperature to devolatilize and form combustible gaseous fuel. Either set a high initial temperature (around 800K), or temporarily raise the inlet gas temperature or the injection temperature of the coal particles.
    - Make sure that you specify the species mass fraction or species mole fraction for the initial reaction components (in the continuous phase).
13. Define any necessary Physics Conditions and Values for the Region and Boundaries.

    See: Lagrangian Phase Boundary Conditions.

14. If necessary, set up Injectors. The injectors allow you to define where, in what direction, and with what frequency, the Lagrangian particles enter the continuous phase.

    See: Working With Injectors.

15. Return to the Reacting Flow General Workflow.

Interphase Reactions Workflow: Multiphase

When defining reactions within an Eulerian phase, you can include species from the Particle or Gas models within a different Eulerian phase that is specified within the same phase interaction.

The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow.

1. For the Physics Continuum that represents the background phase in which the Eulerian phase reactions occur (the continuous phase), select the following models. Maintain the existing model selections and make sure that **Auto-Select recommended models** is activated.

Group Box	Model
Multiphase Model	Select either: - **Eulerian Multiphase (EMP)** - **Volume of Fluid (VOF)** - **Mixture Multiphase (MMP)**

Group Box	Model
Optional Models	**Phase Coupled Fluid Energy** (available when **Eulerian Multiphase (EMP)** is selected) **Segregated Multiphase Temperature** (available when **Volume of Fluid (VOF)** or **Mixture Multiphase (MMP)** is selected)

2. Select any further optional models as necessary.
3. Under the **Multiphase** model node, create and define the Eulerian phases using the following guidance on model selection (along with any other models that are required).

   For interphase combustion simulations, create at least two phases.

Group Box	Model
Material	For Eulerian phases which participate in reactions, select one of: ◦ **Multi-Component Gas** ◦ **Multi-Component Liquid** (required for multiphase polymerization) ◦ **Multi-Component Particle**
Energy	**Segregated Fluid Enthalpy** or **Segregated Fluid Temperature** (available for Eulerian Multiphase (EMP) Eulerian phases only)
Reaction Regime	◦ For phases in which intraphase reactions occur, select **Reacting** (required for multiphase polymerization) ◦ For any other phases, select **Non-Reacting**
Reacting Flow Models	**Reacting Species Transport**
Reacting Species Models	◦ When using large reaction mechanisms that are imported in the standard format, select **Complex Chemistry** ◦ When using small mechanisms that are defined in the GUI with four steps or less, select **Eddy Break-Up** ◦ For multiphase polymerization, select **Polymerization**
Equation of State (except when the Complex Chemistry model is selected)	any
Turbulence Chemistry Interactions (when the Complex Chemistry model is selected)	Select either: ◦ **Eddy Dissipation Concept** ◦ **Laminar Flame Concept**

For more information, see Defining Eulerian Phases.

Phase interactions can define reactions between any two phases of Multi-Component Gas, Multi-Component Liquid, or Multi-Component Particle. You can specify any number of phase interactions—each with any number of reactions. However, each phase interaction can only contain two phases. Depending on the multiphase model that you select, the following phase interaction models are available:

- Continuous Dispersed Phase Interaction (for Eulerian Multiphase (EMP) only)
  Define the phase interaction between the continuous and the dispersed phase. When you create a phase interaction, you select the *Continuous Phase* first, and then the *Dispersed Phase*. When you select the dispersed phase, you also choose the phase interaction type.
- Multiple Flow Regime Phase Interaction (for Eulerian Multiphase (EMP) only)
- VOF-VOF Phase Interaction (for Volume of Fluid (VOF) only)
- MMP-MMP Phase Interaction (for Mixture Multiphase (MMP) only)
  Define the phase interaction between the primary phase and the secondary phase. You select the *Primary Phase* first, and then the *Secondary Phase*. When you select the secondary phase, you also choose the phase interaction type.

Create and define the phase interactions.

4. Right-click the **Models** > **Multiphase Interaction** > **Phase Interactions** node and set the appropriate phase interactions.

Phase Interaction	Model
Continuous Dispersed	**New** > **[continuous Phase]** > **[dispersed Phase] (Continuous-Dispersed)**
Multiple Flow Regime	**New** > **[primary phase]** > **[secondary phase] (Multiple Flow Regime)**
VOF-VOF or MMP-MMP	**New** > **[primary phase]** > **[secondary phase]**

   The **Phase Interaction 1** node is added under **Phase Interactions**.

5. Right-click the **[phase interaction]** > **Models** node and click **Select Models**.
   ► For Eulerian Multiphase (EMP), in the *Phase Interaction Model Selection* dialog, select the following phase interaction models, with **Auto-Select recommended models** activated:

Group Box	Model
Optional Models	**Interphase Mass Transfer**
Interphase Mass Transfer Ratel Interphase Mass Transfer Models	**Interphase Reaction**

   ► For Volume of Fluid (VOF) or Mixture Multiphase (MMP), in the *Phase Interaction Model Selection* dialog select **Interphase Reaction**.

6. Create and define the interphase reactions within each phase interaction. Right-click the **Interphase Reaction** > **Reactions** node and select **New Reaction**.
   You can specify reactant and product species from either of the two phases that are specified for a phase interaction.
   See Modeling Interphase Reactions.

7. For each component that you want to include in the reaction, right-click the **Reactions** > **[reaction]** > **Reactants** node, click **Add Reactant**, and then select the component.
8. For each product of the reaction, right-click the **Reactions** > **Reaction 1** > **Products** node, click **Add Product**, and then select the product.
9. For each reaction component and product, select the component node and, in the *Properties* window, specify the appropriate values:

Stoich. Coeff.	The stoichiometric coefficient that is appropriate to the reaction.
Rate Exponent	The rate exponent that is appropriate to the reaction.

10. Select the **Properties** > **Reaction Coefficient** node and specify the appropriate reaction rate properties. See, Interphase Reaction Model Reference.
11. If you are simulating multiphase polymerization, proceed to the Polymerization Workflow.
12. Return to the Reacting Flow General Workflow.

Interphase Reactions Workflow: Fluid Film

You can simulate chemical reactions between a fluid film phase and the surrounding gas phase using the Interphase Reaction model.

The Interphase Reaction model requires the **Multi-Component Liquid** model for the fluid film phase. The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow and after the steps in Setting Up a Fluid Film Simulation.

1. Maintain the existing model selections and make sure that **Auto-Select recommended models** is activated. Right-click **Continua** > **Physics 1** > **Models** and select the following model:

Group Box	Model
Optional Models	**Multiphase Interaction**

2. Select the gas components.
   a) Right-click **Continua** > **Physics 1** > **Models** > **Multi-Component Gas** > **Gas Components** and select **Select Mixture Components**.
   b) In *Select Mixture Components* window select components from the Material Databases.
3. Select the liquid components.
   a) Right-click **Continua** > **Physics 1** > **Models** > **Fluid Film** > **Fluid Film Phases** > **Phase 1** > **Models** > **Multi-Component Liquid** > **Liquid Components** and select **Select Mixture Components**.
   b) In *Select Mixture Components* window select components from the Material Databases.
4. Right-click **Continua** > **[physics continuum]** > **Models** > **Multiphase Interaction** > **Phase Interactions** and create a new phase interaction.
5. Right-click the **Phase Interactions** > **[phase interaction]** > **Models** node and select the following model:

Group Box	Model
Phase Interaction Topology	**Film-Physics Continuum Interaction**

Select any further optional models as necessary.

6. Select the **Film-Physics Continuum Interaction** node and set **Fluid Film Phase** to **[fluid film phase]**.
7. Right-click the node **Phase Interactions** > **Phase Interaction 1** > **Models** and select the following model:

Group Box	Model
Optional Models	**Interphase Reaction** See Fluid Film Interphase Reaction Model Reference

8. Define the interphase reactions between the fluid film phase and the neighbouring gas phase:
   a) Right-click the **Models** > **Interphase Reaction** > **Reactions** node and select **New Reaction**.
   b) Right-click the **[reaction]** > **Reactants** node, select **Add Reactant** and select the liquid and gas mixture components that participate in the reactions.
   c) Right-click the **[reaction]** > **Products** node, select **Add Products** and select the liquid and gas mixture components that form the products of the reactions.
9. Specify the user reaction coefficient (k_i in Eqn link). Depending on how you want to specify the coefficient, do one of the following:

User Reaction Coefficient Method	Steps
To use constant, table, or field functions from the gas phase:	a. Select the **[reaction]** > **Properties** > **Reaction Coefficient** > **User reaction coefficient** node and specify the user reaction coefficient using the selected method.
To use field functions from the fluid film phase, for example, the fluid film thickness `$FluidFilmThickness`:	Map the fluid film phase field function from the fluid film side of the interface to the gas phase side of the interface: a. Right-click the **Tools** > **Data Mappers** node and select **New Data Mapper** > **Surface Data Mapper**. b. Select the **[surface data mapper]** node and set the following properties:

Property	Setting
Source Surfaces	Click (**Custom Editor**) and select the fluid film side of the interface between the fluid film and the gas.
Scalar Field Functions	Select the fluid film phase field function that you want to use in your user reaction coefficient definition, for example, **FluidFilmThickness**.

c. Select the **Target Specifications** > **[surface]** node and set *Target Entities* to the gas phase side of the interface between the fluid film and the gas.

d. Select the **[surface data mapper]** > **Update** node and activate *Enabled*.

e. To specify the user reaction coefficient using the mapped fluid film phase field function, select the **Reactions** > **[reaction]** > **Properties** > **Reaction Coefficient** > **User Reaction Coefficient** node and set the following properties:

Property	Setting
Method	**Field Function**
Scalar Function	Select the mapped fluid film phase field function with the pre-fix **MappedVertex**. For example, for the fluid film thickness, select **MappedVertexFluidFilmThickness**

For more information on data mappers, see Data Mappers.

10. Return to the Reacting Flow General Workflow.

Interphase Reference

This section provides reference material, including properties, sub-nodes, field functions, and other model-specific settings, for the specific reacting flow interphase models.

You can find more information about using Lagrangian Multiphase and Multiphase models in the following sections of the User Guide:

- Using the Lagrangian Multiphase Model
- Using the Multiphase Model

Contents:

Particle Reaction Model Reference

The Particle Reaction model allows you to simulate processes in which one or more solid components react with one or more gas-phase and/or liquid-phase components to form solid, liquid, and/or gas-phase products.

Particle Reaction Model Reference

Theory	See Particle Reaction.	
Provided By	**[Lagrangian Phase]** > **Models** > *Particle Reaction Type*	
Example Node Path	**[physics continuum]** > **Models** > **Lagrangian Multiphase** > **Lagrangian Phases** > **[Phase 1]** > **Models** > **Particle Reaction**	
Requires	Either:	
	Material: **Gas** or **Liquid** *Flow*: any *Optional Models*: **Lagrangian Multiphase**	*Material*: **Multi-Component Gas** or **Multi-Component Liquid** *Flow*: any *Optional Models*: **Lagrangian Multiphase**
	Then, in a Lagrangian phase: *Particle Type*: **Material Particles** *Material*: **Multi-Component Particle** *Mass Transfer*: **Mass Transfer** *Particle Reaction Type*: **Particle Reaction**	
Specific Right-Click Actions	New Particle Reactions. See Right-Click Actions.	
Activates	Model Controls (child nodes)	Particle Reactions. See Particle Reactions Reference.

Right-Click Actions

New Particle Reactions

Creates a **Particle Reactions** sub-node. This new object contains sub-nodes for specifying reactants, products, and the reaction rate.

Particle Devolatilization Model Reference

The Particle Devolatilization model controls the process by which one or more solid reactants (such as raw coal) are converted to gaseous combustible material (volatile matter) and solid char residue.

This model supplies the rate of devolatilization for the raw coal component of the coal.

Particle Devolatilization Model Reference

Theory	See Particle Devolatilization.
Provided By	**[Lagrangian Phase]** > **Models** > *Particle Reaction Type*
Example Node Path	**[physics continuum]** > **Models** > **Lagrangian Multiphase** > **Lagrangian Phases** > **[Phase 1]** > **Models** > **Particle Devolatilization**

Requires	Either:		
	Material: **Gas** or **Liquid** *Flow*: any *Optional Models*: **Lagrangian Multiphase**		*Material*: **Multi-Component Gas** or **Multi-Component Liquid** *Flow*: any *Optional Models*: **Lagrangian Multiphase**
	Then, in a Lagrangian phase: *Particle Type*: **Material Particles** *Material*: **Multi-Component Particle** or **Multi-Component Liquid** *Mass Transfer*: **Chemical Reactions** *Particle Reaction Type*: **Particle Devolatilization**		
Specific Right-Click Actions	New Particle Reactions. See Right-Click Actions.		
Activates	Model Controls (child nodes)	Particle Reactions. See Particle Reactions Reference.	

Right-Click Actions

New Particle Reactions

Creates a **Particle Reactions** sub-node. This new object contains sub-nodes for specifying reactants, products, and the reaction rate.

Particle Reactions Reference

You can define Particle Reactions under the Particle Reaction or Particle Devolatilization nodes.

Components from the continuous gas or liquid phase can be used as both reactants and as products in the particle reactions within the Lagrangian phase. Therefore, these components need to be defined in the multi-component gas or liquid phase mixture in the continuous phase.

Particle Reactions

The Particle Reactions node has no properties, however, the context menu has the following options:

New Particle Reaction

Creates a particle reaction. This new object contains sub-nodes for reactants, products, and the reaction rate.

Reactants / Products

The **Reactants** and **Products** sub-nodes both have a context menu with the following options:

Add Solid Reactant

Add Fluid Reactant

Add Solid Product

Add Fluid Product

Selecting one of these options opens a submenu of all materials of the same phase in the material database. When you select a material, a **[Reaction Component]** sub-node is created for that material. You can add as many reactant or product components as required.

[Reaction Component]

Each **[Reaction Component]** node has the following Properties:

Stoich. Coeff.

Allows you to set the stoichiometric coefficient for that reaction component in the reaction definition.

Reaction Rate

The **Reaction Rate** node, which controls the rate of the particle devolatilization or particle combustion reaction, has the following *Properties*:

Method

- **Diffusion Limited User Reaction Rate**: Activates the **Diffusion Limited User Reaction Rate** node.
- **First-Order Combined Rate**: When using the Particle Reaction model, activates the **First Order Combined Rate** node.
- **Half-Order Combined Rate**: When using the Particle Reaction model, activates the **Half-Order Combined Rate** node.
- **First-Order Rate**: When using the Particle Devolitilization model, activates the **First-Order Rate** node.
- **User Reaction Rate**: Activates the **User Reaction Rate** node.
  If you have specified multiple solids and/or multiple gas/liquids as reactants, this is the only method that is available.

[Reaction Rate Method] Properties

The **First-Order Combined Rate**, **Half-Order Combined Rate**, and **First-Order Rate** sub-nodes have the following Properties:

Temperature Exponent, Beta

Sets the temperature exponent β for this reaction. See Eqn. (3822), Eqn. (3826), and Eqn. (3431).

Activation Energy, Ea

Sets the temperature exponent E_a for this reaction. See Eqn. (3822), Eqn. (3826), and Eqn. (3431).

First-Order Combined Rate

The first-order combined rate, available for the Particle Reaction model, calculates the effective particle reaction rate by accounting for both chemical kinetics at the particle surface and diffusion of gas-phase reactant species. The term first-order means that the kinetics reaction rate is first-order with respect to gas-phase reactant species concentration. The First-Order Combined Rate node uses its properties to control part of

this calculation method, while its sub-nodes Pre-exponent and Diffusion Coefficient provide inputs as scalar profiles. See Eqn. (3826) and Eqn. (3827).

Half-Order Combined Rate

The half-order combined rate, available for the Particle Reaction model, calculates the effective particle reaction rate by accounting for both chemical kinetics at the particle surface and diffusion of gas-phase reactant species. The term half-order means that the kinetics reaction rate is half-order with respect to gas-phase reactant species concentration. The Half-Order Combined Rate node uses its properties to control part of this calculation method, while its sub-nodes Pre-exponent and Diffusion Coefficient provide inputs as scalar profiles. See Eqn. (3431) and Eqn. (3829).

First-Order Rate

The first-order rate, available for the Particle Devolatilization model, calculates the particle reaction rate where the chemical kinetics is first-order with respect to solid-particle reactant concentration. The First-Order Rate node uses its properties to control part of this calculation method, while its sub-node Pre-exponent provides inputs as a scalar profile. See Eqn. (3822) and Eqn. (3823).

User Reaction Rate

Use this method when you have multiple solids and/or multiple gas/liquids as reactants.

The user-reaction rate, available for both Particle Reaction and Particle Devolatilization models, allows you to specify custom reaction rates. The User Reaction Rate node functions as a scalar profile (see Eqn. (3824)).

Pre-exponent

The Pre-exponent node, which is a sub-node of reaction rate nodes other than the User Reaction Rate node, functions as a scalar profile. It lets you use the Arrhenius form. See Eqn. (3822), Eqn. (3826), and Eqn. (3431).

Diffusion Coefficient

The Diffusion Coefficient node is included in the First-Order Combined Rate and Half-Order Combined Rate nodes (Particle Reaction only). It is needed because this reaction includes a gas oxidizer, and you have to know the rate at which it diffuses. It represents D_m in Eqn. (3828), and functions as a scalar profile.

Coal Combustion Model Reference

There are several Lagrangian phase models available to select alongside the Coal Combustion model for simulating coal combustion in Simcenter STAR-CCM+.

Coal Combustion Model Reference

Theory	See Coal Combustion.
Provided By	**[Lagrangian Phase]** > **Models** > *Mass Transfer*
Example Node Path	**[physics continuum]** > **Models** > **Lagrangian Multiphase** > **Lagrangian Phases** > **[Phase 1]** > **Models** > **Coal Combustion**

Requires	In the continuous phase, either:		
	Material: **Gas** *Flow*: any *Optional Models*: **Lagrangian Multiphase**		*Material*: **Multi-Component Gas** *Reaction Regime*: **Non-reacting** *Flow*: any *Optional Models*: **Lagrangian Multiphase**
	Then, in a Lagrangian phase: *Particle Type*: **Material Particles** *Material*: **Multi-Component Coal**		
Activates	Physics Models	*Two-Way Coupling*: **Two-Way Coupling** *Energy*: **Energy** *Moisture Evaporation*: **Coal Moisture Evaporation**	

Coal Moisture Evaporation Model Reference

The Coal Moisture Evaporation model allows the H2O component of the coal particle to lose its mass through a quasi-steady evaporation process.

The coal particle is assumed to be initially coated with moisture so that a single-component evaporation treatment is appropriate. The driving force for evaporation of this layer is the departure from equilibrium of the liquid-vapor system. In coal combustion, the moisture evaporation is usually heat-transfer limited and takes place rapidly. The devolatilization and char oxidation reactions occur after the moisture has evaporated.

The formulation is that of the Quasi-Steady Single-Component Droplet Evaporation model as applied to a water droplet, and the associated Sherwood and Nusselt numbers are calculated using the Ranz-Marshall correlation.

Coal Moisture Evaporation Model Reference

Theory	See Droplet Evaporation		
Provided By	**[Lagrangian Phase]** > **Models** > *Moisture Evaporation*		
Example Node Path	**[physics continuum]** > **Models** > **Lagrangian Multiphase** > **Lagrangian Phases** > **[Phase 1]** > **Models** > **Coal Moisture Evaporation**		
Requires	In the continuous phase, either:		
	Material: **Gas** *Flow*: any *Optional Models*: **Lagrangian Multiphase**		*Material*: **Multi-Component Gas** *Reaction Regime*: **Non-reacting** *Flow*: any *Optional Models*: **Lagrangian Multiphase**
	Then, in a Lagrangian phase: *Particle Type*: **Material Particles** *Material*: **Multi-Component Coal** *Mass Transfer*: **Coal Combustion**		
Activates	Field Functions	Coal Moisture Latent Heat of Vaporization (H2O), Coal Moisture Saturation Pressure (H2O). See Field Functions.	

Field Functions

Coal Moisture Latent Heat of Vaporization (H2O)

Coal Moisture Saturation Pressure (H2O)

Interphase Reaction Model Reference - Eulerian Phases

You can use the Interphase Reaction model to define reactions that result in mass transfer between different Eulerian phases.

Interphase Reaction Model Reference (Eulerian Phases)

Theory	Interphase Reactions for Multiphase Models	
Provided By	**Continua** > **[physics continuum]** > **Models** > **Multiphase Interaction** > **Phase Interactions** > **[phase interaction]** > **Models** > **Optional Models** > *Interphase Mass Transfer Rate* (for Eulerian Multiphase (EMP) only) **Continua** > **[physics continuum]** > **Models** > **Multiphase Interaction** > **Phase Interactions** > **[phase interaction]** > **Models** > *Optional Models* (for Volume of Fluid (VOF) and Mixture Multiphase (MMP))	
Example Node Path	**Continua** > **Physics** > **Models** > **Multiphase Interaction** > **Phase Interactions** > **Phase Interaction 1** > **Models** > **Interphase Reaction**	
Requires	Physics continuum selection: *Material*: **Multiphase** *Multiphase Model*: **Eulerian Multiphase (EMP)**, **Volume of Fluid (VOF)**,**Mixture Multiphase (MMP)** *Energy*: **Phase Coupled Energy**, **Segregated Multiphase Temperature** *Optional Models*: **Multiphase Interaction** Eulerian phase selection: A minimum of two Eulerian phases. For each Eulerian phase, select: *Material*: **Multi-Component Gas**, **Multi-Component Liquid**, or **Multi-Component Particle** For Eulerian Multiphase (EMP) Eulerian phases only, select one of: *Energy*: **Segregated Fluid Enthalpy**, **Segregated Fluid Temperature** Phase interaction selections: VOF-VOF phase interaction (for Volume of Fluid (VOF) only) MMP-MMP phase interaction (for Mixture Multiphase (MMP) only) Continuous-Dispersed Topology phase interaction or Multiple Flow Regime topology (for Eulerian Multiphase (EMP) only)	
Activates	Model Controls (child nodes)	Reactions. See Interphase Reaction: Reactions.

Interphase Reaction > Reactions

Details the reactions taking place between two different Eulerian phases.

[reaction]

The defined reaction *Type* can only be **Interphase**.

Reactants

Defines the reactant components of the interphase reaction.

Products

Defines the product components of the interphase reaction.

Properties > Reaction Coefficient

Defines the reaction rate method for the interphase reaction. Following are the methods that can be applied:

Method	Corresponding Method Node
Diffusion Limited User Reaction Rate (for Eulerian Multiphase (EMP) only) Use this method when you have Eulerian particle, gas, or liquid phase components as reactants. The Diffusion Limited User Reaction Rate method limits the reaction rate by the rate of species diffusion. The interphase reaction rate is the minimum of user reaction rate and species diffusion rate to the interface. See Diffusion Limited Reaction Rate.	**Diffusion Limited User Reaction Rate** Specifies the diffusion limited user *Reaction Coefficient* in equation Eqn. (3653). With the *Diffusion Multiplier*, you can scale the diffusion rates in the net reaction rate Eqn. (3658).
First-Order Combined Rate (for Eulerian Multiphase (EMP) only) The first-order combined rate, available when a Eulerian particle phase reacts with a Eulerian gas phase, calculates the effective reaction rate by accounting for both chemical kinetics at the particle surface and diffusion of gas-phase reactant species. The term first-order means that the kinetics reaction rate is first-order with respect to gas-phase reactant species concentration.	**First-Order Combined Rate** The **First-Order Combined Rate** node uses its properties to control part of this calculation method, while its sub-nodes **Pre-exponent** and **Diffusion Coefficient** provide inputs as scalar profiles. See Eqn. (3826) and Eqn. (3827).

Method	Corresponding Method Node
Half-Order Combined Rate (for Eulerian Multiphase (EMP) only) The half-order combined rate, available when a Eulerian particle phase reacts with a Eulerian gas phase, calculates the effective reaction rate by accounting for both chemical kinetics at the particle surface and diffusion of gas-phase reactant species. The term half-order means that the kinetics reaction rate is half-order with respect to gas-phase reactant species concentration.	**Half-Order Combined Rate** The **Half-Order Combined Rate** node uses its properties to control part of this calculation method, while its sub-nodes **Pre-exponent** and **Diffusion Coefficient** provide inputs as scalar profiles. See Eqn. (3431) and Eqn. (3829).
Second-Order Combined Rate (for Eulerian Multiphase (EMP) only) The second-order combined rate, available when a Eulerian particle phase reacts with a Eulerian gas phase calculates the effective reaction rate by accounting for both chemical kinetics at the particle surface and diffusion of gas-phase reactant species. The term second-order means that the kinetics reaction rate is second-order with respect to gas-phase reactant species concentration.	**Second-Order Combined Rate** The **Second-Order Combined Rate** node uses its properties to control part of this calculation method, while its sub-nodes **Pre-exponent** and **Diffusion Coefficient** provide inputs as scalar profiles.
User Reaction Coefficient Use this method when you have multiple solids and/or multiple gas/liquids as reactants. The user reaction coefficient allows you to specify custom reaction coefficients.	**User Reaction Coefficient** The **User Reaction Coefficient** node functions as a scalar profile. See Eqn. (3653).

Interphase Reaction Model Reference - Fluid Film

You can use the Interphase Reaction model to define reactions between multi-component fluid film phases and neighbouring multi-component gas phases.

Interphase Reaction Model (Fluid Film) Reference

Theory	Fluid-Fluid Interphase Reactions
Provided By	**Continua** > **[physics continuum]** > **Models** > **Multiphase Interaction** > **Phase Interactions** > **[phase interaction]** > **Models**>*Optional Models*
Example Node Path	**Continua** > **[physics continuum]** > **Models** > **Multiphase Interaction** > **Phase Interactions** > **[phase interaction]** > **Models** > **Interphase Reaction**

<table>
<tr><td>Requires</td><td colspan="2">• Main physics continuum (background fluid):
Time: any
Material: **Multi-Component Gas**
Reaction Regime: any
Flow: any
Equation of state: any
Viscous Regime: **Laminar** or **Turbulent**
Optional Models: **Fluid Film**
Optional Models: **Multiphase Interaction**
• **Fluid Film** > **Fluid Film Phases** > **[fluid film phase]**
For each fluid film phase, select:
Space: **Three Dimensional**
Material: **Multi-Component Liquid**
Equation of State: Any
Reaction Regime: Any. Reacting regime requires additional models.
Define the multi-component materials.
• **Multiphase Interaction** > **Phase Interactions** > **[phase interaction]**
For each phase interaction, select:
Phase Interaction Topology: **Film-Physics Continuum Interaction**
Select fluid film phase.</td></tr>
<tr><td rowspan="2">Activates</td><td>Model Controls (child nodes)</td><td>Reactions. See Interphase Reaction > Reactions</td></tr>
<tr><td>Field Functions</td><td>Interphase Transfer Species Source of Reaction Component of Phase Interaction.
Interphase Transfer Species Source Jacobian of Reaction Component of Phase Interaction.
See Field Functions</td></tr>
</table>

Interphase Reaction > Reactions

Details the reactions that take place between a fluid film phase and a neighbouring gas phase.

[reaction]

For fluid film interphase reactions, the defined reaction *Type* can only be **Interphase**.

Reactants

Reactant components of the reaction at the interphase between the fluid film and the gas phase.

Products

Product components of the reaction at the interphase between the fluid film and the gas phase.

Properties

Reaction rate for the reaction at the interphase between the fluid film and the gas phase Eqn. (3653).

Reaction Coefficient

Specifies the reaction coefficient k_i for the reaction rate Eqn. (3653). For reactions at the interphase between the fluid film and gas phase, only a user-defined reaction coefficient is available.

Field Functions

Interphase Transfer Species Source of [reaction component] of [phase interaction]

Refers to the net source term S_{Y_i} for species Y_i due to the interphase reactions.

See equations Eqn. (3417) and Eqn. (3418).

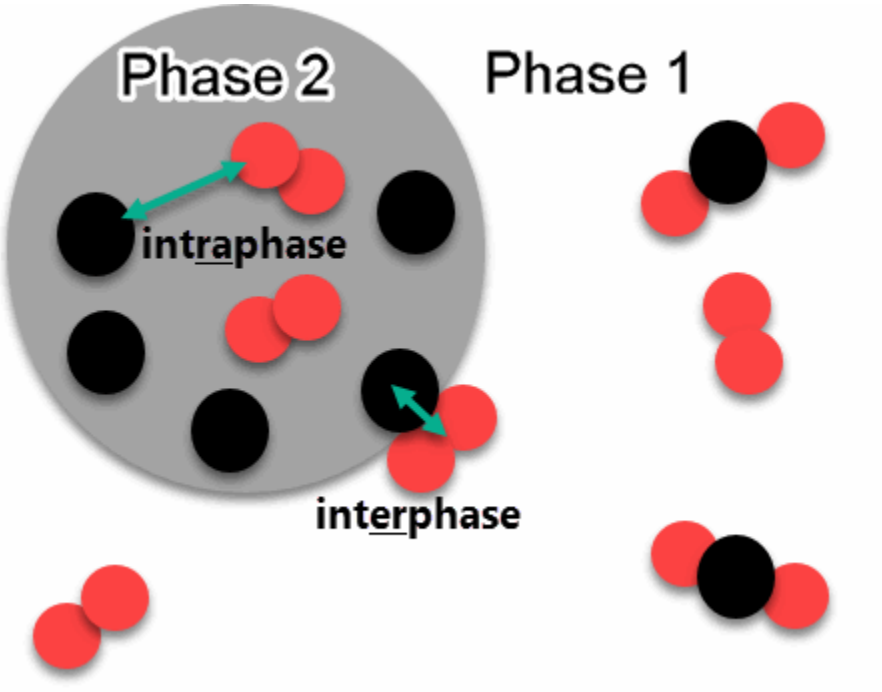
Interphase Transfer Species Source Jacobian of [reaction component] of [phase interaction]

Refers to the net Jacobian of the source term S_{Y_i} for species Y_i, defined as $\frac{\partial S_{Y_i}}{\partial Y_i}$, which represents the derivative of source term S_{Y_i} with respect to the mass fraction of species Y_i.

Intraphase

You can simulate reactions that occur within one Eulerian phase using Flamelet or Reacting Species Transport combustion models in that phase.

The following diagram explains the difference between interphase and intraphase reactions between species.



- Intraphase reactions occur between atoms/molecules in the same phase.
- Interphase reactions occur between atoms/molecules in different phases at the interface between the different phases.

Volume of Fluid (VOF) Multiphase Intraphase Reactions

You can simulate reactions that occur within one Eulerian phase (VOF) using Flamelet or Reacting Species Transport combustion models in that phase. This feature is useful for simulating a reacting phase within a flow of several immiscible fluid phases between which the interfaces can be resolved.

The ability to model reactions within a phase is particularly useful for applications such as glass production, and manufacturing insulation materials.

To simulate intraphase reactions, follow the Reacting Flow General Workflow with one of the following workflows for the reacting phase:

- When using a Flamelet model, follow the Flamelet Workflow.
- When using a Reacting Species Transport model, follow the Reacting Species Transport Workflow.

See also, Volume of Fluid (VOF) Workflow.

Eulerian Multiphase (EMP)

You can simulate reactions that occur within one Eulerian phase (EMP) using Reacting Species Transport combustion models in that phase. You cannot use a Flamelet model in an Eulerian Multiphase (EMP) phase.

Follow the Reacting Flow General Workflow with the Reacting Species Transport Workflow.

See also, Modeling Eulerian Multiphase Flow.

Mixture Multiphase (MMP)

You can simulate reactions that occur within one Eulerian phase (MMP) using Reacting Species Transport combustion models in that phase. You cannot use a Flamelet model in a Mixture Multiphase (MMP) phase.

Follow the Reacting Flow General Workflow with the Reacting Species Transport Workflow.

See also, Modeling a Eulerian Multiphase Mixture.

Surface Chemistry

The Surface Chemistry model is used to represent surface reaction mechanisms on interfaces, boundaries, or surfaces in porous regions. You can use this model to simulate applications such as monolithic catalysts, chemical vapor deposition (CVD), and packed bed reactors.

Surface Chemistry Model

There are two options available for simulating surface chemistry reactions.

- If the simulation involves reacting flow reactions other than the surface reactions, you can: follow another reacting flow workflow, select **Surface Chemistry** as an optional model, and then follow the surface chemistry workflow.
- If the simulation only involves surface reactions and does not involve any other reacting flow reactions, you can follow the surface chemistry workflow.

You can simulate surface chemistry reactions on fluid or porous regions (or porous phases) with reacting surfaces when using the following models:

- The Complex Chemistry model.
- The Eddy Break-Up (EBU) model.
- The Non-Reacting and Segregated Species models.

You can simulate surface chemistry reactions and electrochemical surface reactions within the same region, using both the **Surface Chemistry** model and the **Electrochemical Reactions** model. See Modeling Electrochemical Surface Reactions.

The **Surface Chemistry** model provides the **Surface Mechanism Manager** node which contains details of the bulk species, site species, and reactions within the **Reacting Surface** and **Solid Composition** model nodes.

Note: You can import surface mechanisms which contain multiple sites or bulk mixtures within the same surface mechanism.

The way in which the ODEs (Ordinary Differential Equations) that arise from the reaction mechanism are solved depends on the other physics models that are selected.

- When **Surface Chemistry** is selected with the **Complex Chemistry** model, the CVODE solver resolves the reaction system.
- When **Surface Chemistry** is selected with the **Eddy-Break Up** model, or with the **Non-Reacting** and **Segregated Species** models, the **Surface-Gas Interaction** model resolves the reaction system.

The Reacting Surface Model

The **Reacting Surface** model defines chemical reactions for the surface mechanism in the same manner that the **Reacting** model defines reactions for the continuum gas or liquid phase. See Reacting Model Reference.

The Solid Composition Model

The **Solid Composition** model is a multi-component material model that allows you to specify two distinct types of surface species:

- **Solid Composition** > **Site Solid Mixture** (surface species that occupy a surface site that is next to the gas or liquid)

- **Solid Composition** > **Bulk Solid Mixture** (species that are underneath the site layer)

  When the **Complex Chemistry** model uses the CVODE solver to resolve surface chemistry reaction mechanisms, the **Site Solid Mixture** and **Bulk Solid Mixture** managers cannot be manipulated explicitly. No adding, removing, or renaming species is possible. However, when a complex chemistry definition is imported, these nodes are populated with the mechanisms and surface species that are involved in surface-gas or surface-liquid reactions.

  When the **Surface-Gas Interaction** model is used, you can define the surface chemistry by importing the Chemkin-formatted surface chemistry definition.

The Surface-Gas Interaction Model

The **Surface-Gas Interaction** model is activated when the **Surface Chemistry** model is chosen together with either, the **EBU** model, or the **Non-Reacting** and **Segregated Species** models. The **Surface-Gas Interaction** model solves the ODEs that arise from the surface reaction system using the CVODE solver from the Sundials kit. If you are using the **Surface-Gas Interaction** model with the **Surface Chemistry** model, first import a chemical library for the **Surface Chemistry** model.

Limitations Modeling Surface Chemistry

- No energy equations are solved for the reactive surface. Fixed temperature boundary conditions apply.
- Surface growth and shrinking are not taken into account.

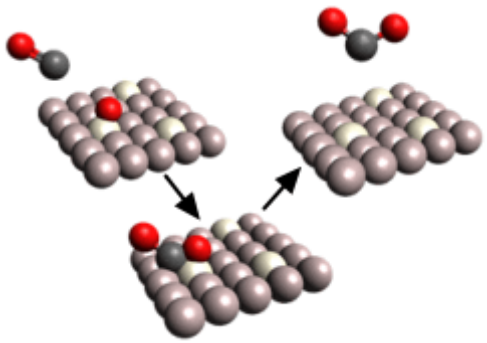
You specify the surface reaction mechanism, which you can import (see Reaction Mechanism Formats). The surface reaction rate is defined per unit surface area—different from fluid-phase reactions, which are based on unit volume.

Contents:

Surface Chemistry Workflow

Use the following procedure to simulate surface reactions which occur when a gaseous or liquid mixture contacts a reacting surface in a fluid or porous region.

The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow.



1. For the physics continuum which contains the reacting surface, select the following models in order—in addition to the models that are previously selected, with **Auto-select recommended models** activated.

Group Box	Model
Reacting Flow Models (when Reacting is selected)	**Reacting Species Transport**
Reacting Species Models (when Reacting is selected)	◦ For detailed mechanisms, select **Complex Chemistry**. ◦ For simple mechanisms, select **Eddy Break-Up**.
Turbulence Chemistry Interactions (when Complex Chemistry is selected)	◦ For steady-state diffusion flames, select **Eddy Dissipation Concept** ◦ For premixed, partially-premixed, and unsteady flames, **Laminar Flame Concept**
Optional Models	**Surface Chemistry**
Enabled Models	**Surface-Gas Interaction**: Selected automatically when Non-Reacting is selected, or when Reacting and Eddy Break-Up are selected.

2. Select any Optional models that are necessary. For example:
   - **NOx Emission** or **Soot Emissions**—to model the formation of these pollutants.
   - **Porous Media**—to model surface reactions on porous phases. See Porous Media Models.
   - The **Radiation** model is useful for modeling applications in which radiative heat transfer is important, such as in glass furnaces. The soot emission models influence the **Participating Media Radiation (DOM)** and **Gray Thermal Radiation** models by contributing to the absorption coefficient of the continuous phase (the absorption coefficient describing both absorption and emission).
3. Import the surface mechanism as follows:
   a) Right-click the **Complex Chemistry** node (or **Surface-Gas Interaction** node) and select **Import Chemistry Definition (Chemkin format)**.
   b) In the *Import Chemkin Files* dialog, select appropriate files as shown below, then click **OK**.
      - *Chemical Mechanism File*
        If multiple surface mechanisms are required, you define them all within this file.
      - *Thermodynamic Properties File*
      - *Transport Properties File* (optional)
      - *Surface Chemical Mechanism File*
      - *Surface Thermodynamic Properties File*

      Upon import, the **Surface Chemistry** > **Surface Mechanism Manager** node becomes populated with the surface mechanism.

   See Importing Species and Reactions.

   The Chemkin mechanism must contain, at a minimum, the description of the NASA polynomials for all the species that are involved in the mechanism. Put this information into the mechanism file itself or in separate files.

Note: You can use open site formalism for surface chemistry mechanisms in Simcenter STAR-CCM+. For the surface site species to be defined as open (have no elemental composition and molecular mass of 0), the open site species name must include `OPEN` in its name. For more details, please refer to the Chemkin manuals.

4. Define the surface for each reacting surface mechanism:

On a Boundary Not Associated With an Interface	When the reacting surface is represented by a boundary that is not associated with an interface, you define the mechanism at the boundary. a. Select the **Boundaries** > **[boundary]** > **Physics Conditions** > **Surface Mechanism Option** node and set *Mechanism* to one of the available mechanisms for your simulation. b. Expand the **[boundary]** > **Physics Values** node and define the properties.
On a Baffle Interface	When different surface mechanisms are required on either side of a baffle interface, you define a mechanism at each specific boundary—instead of at the interface. a. Select the **Boundaries** > **[boundary]** > **Physics Conditions** > **Surface Mechanism Option** node and set *Mechanism* to one of the available mechanisms for your simulation. b. Expand the **[boundary]** > **Physics Values** node and define the properties. Surface Chemistry Model Reference: Boundary Settings.
On Any Other Interface	For an interface other than a baffle interface, you define a surface mechanism at the interface for the reacting surface. a. Select the **Interfaces** > **[interface]** > **Physics Conditions** > **Surface Mechanism Option** node and set *Mechanism* to one of the available mechanisms for your simulation. b. Expand the **[interface]** > **Physics Values** node and define the properties. See Surface Chemistry Model Reference: Interface Settings.
On Surfaces in a Porous Region	To allow the internal surfaces within a porous region to become reactive surfaces, you define a surface mechanism for the porous region. a. Select the **Regions** > **[region]** > **Physics Conditions** > **Surface Mechanism Option** node and set *Mechanism* to one of the available mechanisms for your simulation. b. Expand the **[region]** > **Physics Values** node and define the properties. Surface Chemistry Model Reference: Region Settings.

5. If the Eddy Break-Up model or Complex Chemistry model is selected, define the parameters of the Reacting Species physics model:
   - For the Complex Chemistry model, define the Properties of the Complex Chemistry model and its sub-nodes.
     a. Select the **Models** > **Complex Chemistry** node and set the required *Properties*.
     b. Select the **Complex Chemistry** > **Chemistry Acceleration** node and if necessary, you can activate *ISAT*, *Clustering*, or *Dynamic Mechanism Clustering*. Then define the Properties.

For more information, see Complex Chemistry Model Reference.

- For the EBU model, define the EBU Properties.

  The EBU property, *Reaction Control*, is set to **Hybrid** by default—which is appropriate for most simulations. Hybrid specifies the reaction rate as the minimum of the rate predicted by turbulent mixing and the rate predicted by finite-rate chemical kinetics. However, if the turbulent mixing scale solely defines the rate, select **Standard EBU** instead.

  See Eddy Break-Up Model Reference.

6. Set the parameters of any other **[Continuum]** > **Models**, as required.

   When using the Eddy Dissipation Concept model or the Laminar Flame Concept model, you can adjust the flame position by changing the **Multi-Component Gas** > **Material Properties** > **Turbulent Schmidt Number**.

7. For the continuum, define any necessary parameters for the **Reference Values** and **Initial Conditons**.
8. Define any necessary Physics Conditions and Values for the Region and Boundaries.
   - If you are modeling surface reactions on porous phases, make sure that you set the porosity within the fluid region, and the volume fraction within the porous phase. See Porous Media Model Region Settings and Porous Media Model Phase Settings.
   - To limit the surface reaction rate to the minimum of the reaction rate and the diffusive flux, activate the physics condition *Enable Reaction-Diffusion Flux Limiting*. See Surface-Gas Interaction Model Reference: Region Inputs.
9. Return to the Reacting Flow General Workflow.

Surface Chemistry Reference

This section provides reference material, including properties, sub-nodes, field functions, and other model-specific settings, for the Surface Chemistry models.

Contents:

Surface Chemistry Model Reference

You use the Surface Chemistry model to define surface reaction mechanisms and surface species on the reacting walls of solid regions, or surfaces in porous regions.

Surface Chemistry Model Reference

Theory	See Chemical Kinetics: Surface Chemistry Surface Chemistry
Provided By	**[physics continuum]** > **Models** > **Optional Models**
Example Node Path	• **Continua** > **Physics 1** > **Models** > **Surface Chemistry** • **Porous Media** > **Porous Phases** > **Phase 1** > **Models** > **Surface Chemistry**

<table>
<tr><td>Requires</td><td colspan="2">One of the following combinations of model selections:</td></tr>
<tr><td></td><td>Material: Multi-Component Gas or Multi-Component Liquid
Reaction Regime: Reacting
Reacting Flow Models: Reacting Species Transport
Reacting Species Models: Complex Chemistry or Eddy Break-Up
Flow: Segregated Flow or Coupled Flow</td><td>Material: Multi-Component Gas or Multi-Component Liquid
Reaction Regime: Non-Reacting
Flow: Segregated Flow</td></tr>
<tr><td rowspan="9">Activates</td><td>Physics Models</td><td colspan="2">After selecting the Surface Chemistry model when the Eddy Break-Up model or Non-Reacting model is selected, the Surface-Gas Interaction model is also selected. See Surface-Gas Interaction Model Reference.</td></tr>
<tr><td>Model Controls (child nodes)</td><td colspan="2">Surface Mechanism Manager. See Surface Mechanism Manager Right-Click Actions.</td></tr>
<tr><td>Materials</td><td colspan="2">Specify or review the imported species:
gases under the Multi-Component Gas node
liquids under the Multi-Component Liquid node
site and bulk species under the Surface Chemistry > [SurfaceMechanism] > Solid Composition node
See Materials and Methods.</td></tr>
<tr><td>Interface Inputs</td><td colspan="2">See Interface Settings.</td></tr>
<tr><td>Boundary Inputs</td><td colspan="2">See Boundary Settings.</td></tr>
<tr><td>Region Inputs</td><td colspan="2">See Region Settings.</td></tr>
<tr><td>Phase Inputs</td><td colspan="2">See Porous Phase Settings.</td></tr>
<tr><td>Solvers</td><td colspan="2">See Porous Mass Phase.</td></tr>
<tr><td>Field Functions</td><td colspan="2">See Field Functions.</td></tr>
</table>

Surface Mechanism Manager Right-Click Actions

New Surface Mechanism

Creates a new **SurfaceMechanism** with the **Reacting Surface** subnode, which allows you to create chemical reactions. See Reacting Surface Model Reference.

Right-clicking the **SurfaceMechanism** node opens the *Dependencies* dialog that lets you find out which interfaces, regions, or boundaries use the surface mechanism. This option is useful, for example, if you want to delete the **SurfaceMechanism** node. Before you can delete the **SurfaceMechanism** node, you must deselect the mechanism from the location where it is applied.

Remove Invalid Surface Mechanism

Removes incorrectly defined surface mechanisms.

Materials and Methods

Specify or review the imported gas or liquid components using the **Continua** > **Physics 1** > **Models** > **Multi-Component Gas/Multi-Component Liquid** node. See Defining Species Manually.

Specify the reacting surface using the **Models** > **Surface Chemistry** > **Surface Mechanism Manager** > **[Mechanism]** > **Solid Composition** node. See Solid Composition Model Reference.

Site Occupancy

Allows you to specify the number of surface sites, σ_j (in Eqn. (3467), Eqn. (3468), and Eqn. (3469)), that each of the adsorbed molecules (species) occupies. Available to set as a material property for each [Site Species] that is specified within the Solid Composition model.

Site Density

Allows you to specify the number of active sites, ρ_{site} (in Eqn. (3661)), that exist on the surface (kmol/m^2). Available to set as a material property for the **Site Solid Mixture** within the **Solid Composition** model.

Bulk Density

Allows you to specify the number of surface sites on the solid surface that are occupied by bulk species, N_b in Eqn. (3459), (kg/m^3). Available to set as a material property for each **[Bulk Species]** that is specified within the **Solid Composition** model.

Interface Settings

All Except Baffle

For baffle interfaces, you define mechanisms at the baffle interface boundaries.

Surface Mechanism Option

To allow the interface to become a reactive surface, select the **Physics Conditions** > **Surface Mechanism Option** sub-node of that interface. Change the *Mechanism* property to one of the available mechanisms for your simulation. Mechanisms are available only after you import the chemistry definition.

Mechanism	**Corresponding Physics Value Nodes**
[Surface Mechanism] Defines the interface as a reacting surface.	**Surface Initial Bulk Activity Profiles** Allows you to set the surface molar fraction for species of the given mechanism on the interface as a scalar array profile, B_i in Eqn. (3459). **Surface Initial Site Fraction Profiles** Allows you to set (as a scalar profile) the fraction of the total number of sites that a given species occupies, z_i in Eqn. (3661). This fraction only applies to species of the given mechanism between the interface and the fluid phase.

	Surface Washcoat Factor Allows you to account for a porous washcoat layer which increases the active surface area of a solid catalyst surface. For example, on interface surfaces that are covered by a porous washcoat, you can specify a surface washcoat factor, γ_w in Eqn. (3659) and Eqn. (3660), greater than 1.0. A value of 1.0 represents the surface area before a washcoat is applied.
NONE Defines the interface as a non-reacting surface.	

Boundary Settings

Baffle Interface Boundary

Wall Boundary (for boundaries not associated with an interface)

Surface Mechanism Option

To allow a boundary to become a reactive surface, select the **Physics Conditions** > **Surface Mechanism Option** sub-node of that boundary. Change the *Mechanism* property to one of the available mechanisms for your simulation. Mechanisms are available only after you import the chemistry definition. You can define different mechanisms for boundaries on opposite sides of a baffle interface.

Mechanism	**Corresponding Physics Value Nodes**
[Surface Mechanism] Defines the boundary as a reacting surface.	**Surface Initial Bulk Activity Profiles** Allows you to set the surface molar fraction for species of the given mechanism on the interface as a scalar array profile, B_i in Eqn. (3459). **Surface Initial Site Fraction Profiles** Allows you to set (as a scalar profile) the fraction of the total number of sites that a given species occupies, z_i in Eqn. (3661). This fraction only applies to species of the given mechanism between the reactive wall and the fluid phase. **Surface Washcoat Factor** Allows you to account for a porous washcoat layer which increases the active surface area of a solid catalyst surface. For example, on surfaces that are covered by a porous washcoat, you can specify a surface washcoat factor, γ_w in Eqn. (3659) and Eqn. (3660), greater than 1.0. A value of 1.0 represents the surface area before a washcoat is applied.

NONE Defines the boundary as a non-reacting surface.	

Region Settings

Porous

Surface Mechanism Option

To allow the internal surfaces within a porous region to become reactive surfaces, select the **Physics Conditions** > **Surface Mechanism Option** sub-node of that porous region. Change the *Mechanism* property to one of the available mechanisms for your simulation. Mechanisms are available only after you import the chemistry definition.

Mechanism	**Corresponding Physics Value Nodes**
[Surface Mechanism] Defines the porous region as a reacting surface.	**Area to Volume Ratio** Specifies the surface area of the reacting/catalytic solid per unit volume. **Surface Initial Bulk Activity Profiles** The **Surface Initial Bulk Activity Profiles** > **[Bulk] Solid Mixture Activity** node allows you to set the surface molar fraction for species of the given mechanism on the reactive region as a scalar array profile. **Surface Initial Site Fraction Profiles** The **Surface Initial Site Fraction Profiles** > **[Site] Solid Mixture Fraction** node allows you to set (as a scalar profile) the fraction of the total number of sites that a given species occupies. This fraction only applies to species of the given mechanism on the interface between the reactive region and the fluid phase.
NONE Defines the porous region as non-reacting.	

Field Functions

Surface Bulk Fraction of [Species]

Surface Bulk Growth Rate of [Species]

Surface Bulk Source of [Species]

Surface Chemistry Energy Source

Surface Site Fraction of [Species]

$Z_{S_i,n}$ in Eqn. (3461).

Surface Site Source of [Species]

Surface-Gas Interaction Model Reference

Surface-Gas Interaction Model Reference

Theory	See Surface Chemistry.	
Provided By	**[physics continuum]** > **Models** > *Surface Chemistry Reaction*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Surface-Gas Interaction**	
Requires	One of the following combinations:	
	Material: **Multi-Component Gas** *Flow*: any *Reaction Regime*: **Reacting** *Reacting Flow Models*: **Reacting Species Transport** *Reacting Species Models*: **Eddy Break-Up** *Flow*: any *Optional Models*: **Surface Chemistry**	*Material*: **Multi-Component Gas** *Reaction Regime*: **Non-Reacting** *Flow*: any *Optional Models*: **Surface Chemistry**
Properties	See Surface-Gas Interaction Model Properties.	
Specific Right-Click Actions	See Right-Click Actions.	
Region Inputs	See Region InputsRegion Inputs.	

Surface-Gas Interaction Model Properties

Source Enabled Trigger

Controls whether Simcenter STAR-CCM+ starts calculating the chemistry at the time-step, iteration, or physical time that you specify in the *Begin* property, or whether this model never contributes any sources.

Begin

Specifies the iteration, time-step, or physical time after which the reactions are activated. Before this iteration, time-step, or physical time, reactions are deactivated. Specifying a physical time [degCA] allows you to activate chemistry sources just before spark ignition. When specifying it as an expression which varies during the simulation, reactions are only active when the current iteration, time-step, or physical time is higher than the value provided by the expression.

Verbose on Error

Provides details about solver errors.

Activated: During iterations, this option generates maximum details in the *Output* window about solver errors.

Deactivated: Uses standard iteration output.

Absolute Tolerance

Absolute tolerance for the CVODE ODE solver.

Relative Tolerance

Relative tolerance for the CVODE ODE solver.

Right-Click Actions

Import Chemistry Definition (Chemkin format)

Activates a standard *Open* dialog that imports files for the chemistry definition in Chemkin™ format. Upon importing a chemistry definition, the reactions for the definition appear as sub-nodes of the Chemistry Definition node.

If you import transport data along with the chemical mechanism and thermal data, Simcenter STAR-CCM+ tabulates the molecular transport properties for the Dynamic Viscosity, Molecular Diffusivity, and Thermal Conductivity material properties. You can then choose to use these tabulated molecular transport properties after table generation, in the Multi-Component Gas node, by selecting the `Flamelet Table` option for each of the Material Properties.

Delete Chemistry Definition

Removes all the species and their reactions in the chemistry definition.

Region Inputs

Porous

Enable Reaction-Diffusion Flux Limiting

Accounts for situations where the diffusion flux is small relative to reaction, reactants/products diffuse slowly to/from the surface, and the reaction rate is limited by the diffusion rate. Available when a surface mechanism is specified for the porous region.

Enable Reaction-Diffusion Flux Limiting Option	**Corresponding Physics Value Nodes**
When activated, limits the reaction rate based on the rate of diffusion of individual species to the porous surface.	**Reaction-Diffusion Flux Multiplier** Specifies the scaling factor F in Eqn. (3667).

Reacting Surface Model Reference

Simcenter STAR-CCM+ automatically activates the **Reacting Surface** model when the **Surface Chemistry** model is active and contains a surface mechanism. This model cannot be deselected.

Reacting Surface Model Reference

Theory	See Chemical Kinetics: Surface Chemistry and Surface Chemistry	
Provided By	*Surface Mechanism Model Selection* dialog, *Enabled Models*	
Example Node Path	**Surface Chemistry** > **Surface Mechanism Manager** > **SurfaceMechanism** > **Reacting Surface**	
Requires	• Follow the instructions to select the Surface Chemistry Model. See Surface Chemistry Model Reference • Create a surface mechanism within the Surface Chemistry model.	
Activates	Model Controls (child nodes)	• Reactions • Reacting System Properties

Reactions

Contains three further sub-nodes that allow you to specify **Reactants**, **Products**, and **Properties** for the reactions. See Importing Species and Reactions or Defining Chemical Reactions Manually.

The following properties are available for the **Properties** > **Reaction Coefficient** > **Arrhenius Coefficients** node.

Temperature Exponent, Beta

Sets the temperature exponent, β, for this reaction in Eqn. (3431).

Activation Energy, Ea

Sets the activation energy, E_a, for this reaction in Eqn. (3431).

Pre-Exponent Unit System

Units for the pre-exponential factor.

Pre-exponent A

Defines the pre-exponential factor, A, in Eqn. (3431).

Reversible

When activated, the reaction is specified as reversible. In a reversible reaction, you specify the forward rate coefficients and select how the backward rate is calculated using the **Properties** > **Reverse Reaction Coefficient** node. When reversible reactions are read from a Chemkin mechanism, this property is activated and the reaction properties are set automatically. If you define a reversible reaction, make sure that you specify values for the enthalpy, entropy, and specific heat for each component of the mixture. For the specific heat, you choose either the thermodynamic polynomial or polynomial in T option.

Motz-Wise Correction

When activated, modifies the sticking coefficient rate expression as in Eqn. (3468).

Bohm Correction

When activated, modifies the rate constant to include a Bohm velocity correction as in Eqn. (3469).

Sticky

The sticking coefficient S_c in Eqn. (3466) describes the probability for a species to stick to a surface.

Langmuir-Hinshelwood

When activated, allows you to specify a global Langmuir-Hinshelwood surface reaction that incorporates species adsorption, surface reactions, and desorption into a single step.

Provides a **Langmuir-Hinshelwood Coefficients** sub-node with the properties:

Langmuir-Hinshelwood Exponent

(superscript m in Eqn. (3474))

Equilibrium Constant Units

Allows specification of the equilibrium constant in Concentration, Atmosphere, Bar, Torr, Pascal or Dyne units.

Each of the Langmuir-Hinshelwood components are listed under the **Langmuir-Hinshelwood Coefficients** node, and allow you to specify the *Langmuir-Hinshelwood Data*:

Pre-exponential Factor

A in Eqn. (3475).

Temperature Exponent

β in Eqn. (3475).

Equilibrium Enthalpy (J/kmol)

H in Eqn. (3475).

Reaction Order

Activating *Equilibrium Constant in Numerator* includes the equilibrium constants in the numerator of the Langmuir-Hinshelwood rate Eqn. (3474).

The **Properties** > **Reaction Coefficient** > **Arrhenius Coefficients** > **Surface Coverage Factors** sub-node also provides the right-click option to **Add Surface Coverage Factors** > **[species]**. A sub-node appears for the selected species which allows you to specify the following properties:

Eta

$\eta_{i,j}$ in Eqn. (3465).

Mu

$\mu_{i,j}$ in Eqn. (3465).

Epsilon

$\varepsilon_{i,j}$ in Eqn. (3465).

Reacting System Properties

Species Reaction Source Jacobian

When using user-coded reaction rates, it is strongly recommended to use the Numerical option for the Jacobian calculation. However, if you require the additional computational speed of an analytical Jacobian, Simcenter STAR-CCM+ does allow the option of a user-code analytical Jacobian.

Method	**Corresponding Sub-Nodes**
`Analytical` An analytical Jacobian is used in the CVODE solver.	**Analytical** • When the *Species Reaction Sources* method is set to `Internal`, Simcenter STAR-CCM+ calculates the Jacobian analytically. • When the *Species Reaction Sources* method is set to `User-Defined`, you specify a user function that defines the analytical Jacobian. See Working With User Functions.
`Numerical Jacobian` The Jacobian is calculated numerically.	**Numerical**

A Jacobian is a square matrix of derivatives of the reaction rate with respect to the species specific mole fractions (mass fraction divided by molecular weight), surface site coverage fractions, bulk fractions, and temperature. For surface chemistry reactions, the Jacobian J_ω in Eqn. (3491) and Eqn. (3492) also adds the surface site species and bulk species in addition to the gas-phase species.

Species Reaction Sources

Method	**Corresponding Sub-Nodes**
Internal The Simcenter STAR-CCM+ CVODE solver provides the reaction rate source terms for reacting species.	None.

Method	**Corresponding Sub-Nodes**

User-Defined
Provides the **User-Defined Species Sources Specification** node which allows you to specify whether you are modifying the internally calculated reaction rate source terms, defining entirely new reaction rate source terms, or modifying the rates of single reactions.
	User-Defined
	Allows you to specify a previously imported user function that defines the species reaction rate source terms. See Working With User Functions.
	Field Functions
	Specifies the scalar field function to be used in corresponding user function for modifying the calculated reaction rates or defining reaction rate source terms.
	The following text is an example of how to access field functions in the user code:
	`struct UserAccessibleData *udata = (struct UserAccessibleData *)data;`
	`if (udata->_fieldFunctionsData._nFF > 1) { double ff0 = udata->_fieldFunctionsData._ffVal[0]; double ff1 = udata->_fieldFunctionsData._ffVal[1]; ... }`
	If you are using clustering in your simulation, these field functions will appear automatically under the **Clustering** > **Components** node.

User-Defined Species Sources Specification

Available when the Species Reaction Sources method is set to User-Defined.

Method	**Corresponding Sub-Nodes**
Calculate Species Sources	**Calculate Species Sources** Specifies that entirely new reaction rate source terms are to be defined with a previously imported user function. In this case, the internal reaction rate sources are not calculated. Displays the following property: *Internal Reaction Energy Source* When activated, the source term of the ODE energy equation is calculated internally, assuming a constant pressure reactor. See Eqn. (3488). When deactivated, the ODE energy source term must be calculated and stored in the (N+1)'th element of the reaction rate $\dot{\omega}$ vector.
Modify Internal Species Sources	**Modify Internal Species Sources** Specifies that the existing reaction rate source terms are to be modified with a previously imported user function —typically by multiplying the existing values with a constant.
Modify Internal Reaction Rates	**Modify Internal Reaction Rates** Specifies that existing rates of individual reactions are to be modified. Forward and reverse reaction rates are provided. Internal reaction rates can be modified with a previously imported user function.

You use the **Species Reaction Sources** > **User-Defined** node to select the appropriate user function. For further details, see User-Defined Reaction Rate Source Terms. For more information on how to create user functions, see Working With User Functions.

Solid Composition Model Reference

Solid Composition Model Reference

Theory	See Surface Chemistry Surface Chemistry
Provided By	*Surface Mechanism Model Selection* dialog, *Enabled Models*
Example Node Path	**Surface Chemistry** > **Surface Mechanism Manager** > **Surface Mechanism** > **Solid Composition**

Requires	• Follow the instructions to select the Surface Chemistry Model. See Surface Chemistry Model Reference • Create a surface mechanism within the **Surface Chemistry** model.	
Activates	Model Controls (child nodes)	**Site Solid Mixture** and **Bulk Solid Mixture**

Site Solid Mixture

Provides the **Site Species** sub-node which allows you to specify surface species that occupy a surface site that is next to the gas. See Managing Mixture Components. You can also specify material properties that are specific to the Site Solid Mixture under the **Material Properties** sub-node.

Bulk Solid Mixture

Provides the **Bulk Species** node which allows you to specify species that are underneath the site layer. See Managing Mixture Components.

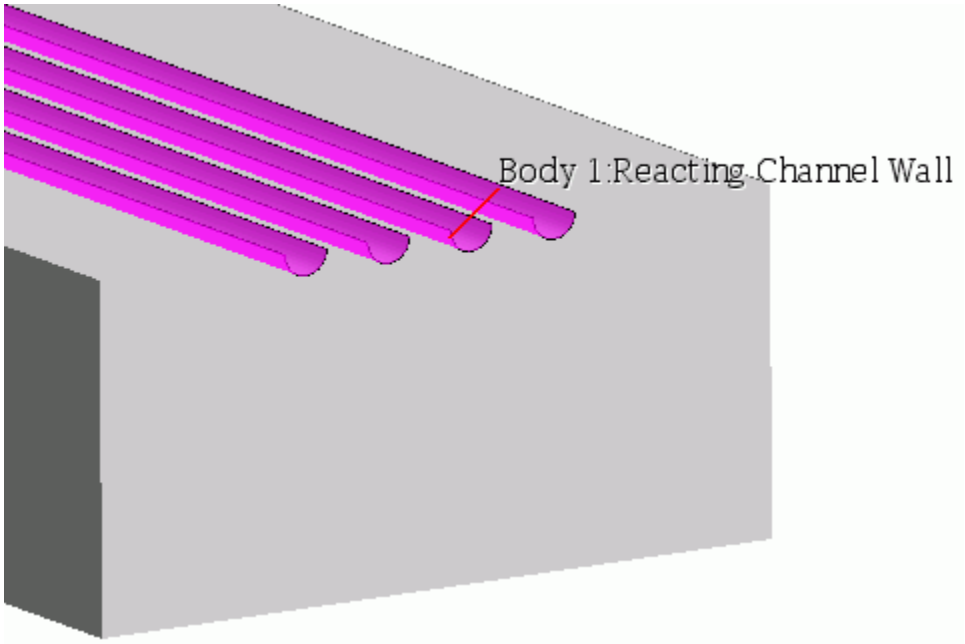
Reacting Channels

The Reacting Channel Coupling feature provides the ability to exchange data between a three-dimensional Simcenter STAR-CCM+ simulation and a one-dimensional Plug Flow Reactor (PFR) simulation which uses the CVODE solver. You can use the **Reacting Channel** co-simulation model in Simcenter STAR-CCM+ to solve reacting flow simulations in tubular heat exchangers with channels that are long and thin.

When simulating Reacting Channels, you simulate combustion in the three-dimensional background phase which surrounds the reacting channels. The Flamelet Generated Manifold model is often the most appropriate model for simulating combustion in a firebox surrounding the reacting channels. This functionality is useful for simulating chemical processes such as methane steam reforming and cracking.

When the **Reacting Channel** model is selected along with the **Co-Simulation** model, an **External Links** > **Reacting Channel Co-Simulation** node appears.

Several geometrical channels can represent one reacting channel zone—as long as all of the geometrical channels have identical geometries of the same orientation. For geometrical channels that differ in length, diameter, or orientation, define each different group of geometrical channels as a separate reacting channel zone. It is possible to model a reacting channel simulation in which a reacting flow exits channels in one zone and re-enters channels in another zone. The geometry of the reacting channels does not need to represent reacting channels that are physically connected by a U-bend, as long as the reacting channel boundaries are defined in Simcenter STAR-CCM+.

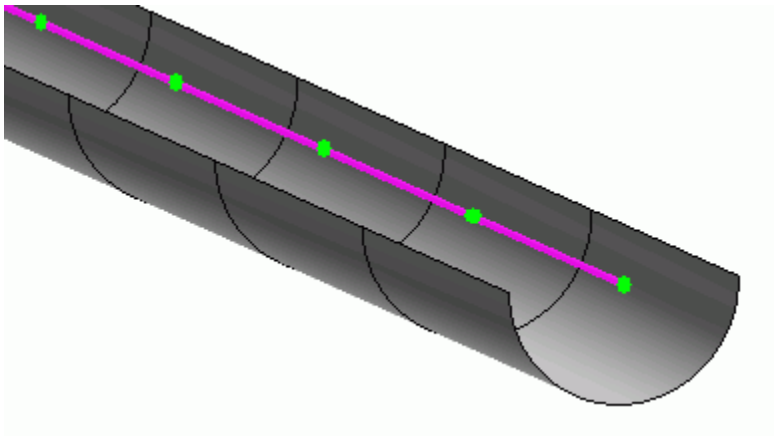


Simcenter STAR-CCM+ meshes and solves the volume of the outer flow. The reacting channels are solved using a Plug Flow Reactor (PFR) approximation. The reacting channels are not meshed and are considered 1D. However, the outer flow volume must account for the presence of the reacting channels in its geometry.

The coupling happens on the reacting channel wall boundary between the outer flow in Simcenter STAR-CCM+ and the reacting channel in the PFR. The temperature is exchanged from the outer flow to the reacting channel and heat flux is returned back from the reacting channel to the outer flow. Although reacting channels appear

as 3D features in a geometry, they become 1D representations when defined as reacting channels in the Reacting Channel Coupling model.

Since the reacting channels are one-dimensional and have no mesh, data is exchanged between axial points, whose frequency you specify, along a vector through the centre of the reacting channel and the surface boundary of the outer flow, as represented by the diagram below:



Note: It is imperative that all geometrical channels that are defined within a single reacting channel zone, are the same length and diameter with the same properties.

Reactions that occur in a reacting channel can be endothermic (absorbing heat) or exothermic (releasing heat). At specified time intervals, Simcenter STAR-CCM+ sends the temperature along the geometrical channel wall to the Plug Flow Reactor (PFR). The PFR then solves for the reacting flow, determines the temperature within the reacting flow, and calculates the heat flux at each axial point in the reacting flow channel. The PFR then sends this data back to the outer flow in Simcenter STAR-CCM+. See Eqn. (3892).

Contents:

Reacting Channels Workflow

The **Reacting Channel** co-simulation model in Simcenter STAR-CCM+ allows you to exchange data between reacting channels that use a one-dimensional Plug Flow Reactor (PFR) and three-dimensional Simcenter STAR-CCM+ simulations.

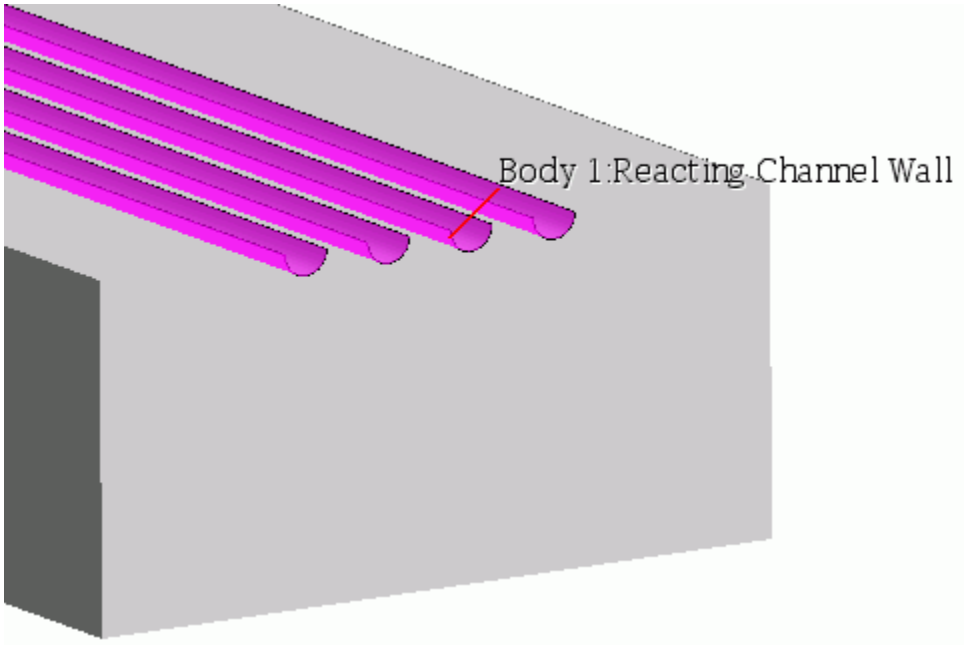
Before setting up reacting channels, make sure that:

- you have a fluid domain with a three-dimensional mesh that contains unmeshed voids that represent the reacting channels.
- the **Steady** model is previously selected.

The steps in this workflow are intended to follow on from the initial steps in the Reacting Flow General Workflow.

Note: For an example of how to use the Reacting Channel Co-Simulation model, see the Reacting Channels: Steam Methane Reforming tutorial. The tutorial demonstrates how you set up firebox and the physics for the reacting channels.

When using the reacting channel coupling model, set up at least one reacting channel co-simulation zone. Each reacting channel zone can represent several geometrical channels. At least two zones are required when simulating a reacting flow which exits channels in one zone (a **Specified Inlet** zone) and re-enters channels in another zone (a **Re-Entry** zone).



1. For the physics continuum that represents the fluid domain that surrounds the reacting channels, select the following models—in addition to the models that are previously selected, with **Auto-Select recommended models** activated:

Group Box	Model
Reacting Flow Models (when the Reacting model is selected)	◦ **Flamelet** Often the most appropriate for firebox combustors. ◦ **Reacting Species Transport** For detailed reaction mechanisms.
Flamelet Models (when the Flamelet model is selected)	Any For example, **Flamelet Generated Manifold (FGM)** is suitable for all premixed or partially premixed flames where the flamelet assumption is valid. Further model selections are necessary.

Group Box	Model
Reacting Species Models (when the Reacting Species Transport model is selected)	Any For example, **Complex Chemistry** is applicable for combustors with multiple fuel streams, and with kinetically dominant processes such as flame quenching. Further model selections are necessary.
Optional Models	**Co-Simulation**
Co-Simulation Models	**Reacting Channel**
Reacting Channel Coupling Models	**Reacting Channel Steady Coupling** (selected automatically)

2. Click **Close**.

   Simcenter STAR-CCM+ adds the **External Links** node and a single **Reacting Channel Co-Simulation** sub-node.

Within one simulation, it is possible to create more than one reacting channel co-simulation. Separate reacting channel co-simulations are necessary if more than one chemical mechanism is required in the simulation. Each reacting channel co-simulation must contain at least one reacting channel zone. You can specify reaction conditions and values for each reacting channel co-simulation and also define further conditions and values that are specific to each reacting channel zone.

3. Create a **Reacting Channel Co-Simulation** node for each reacting channel mechanism that you want to use. To specify more than one reacting channel mechanism, right-click the **External Links** node and select **New** > **Reacting Channel Link**.

   A **Link** node appears, which you can set up as another reacting channel co-simulation.

Specify the Conditions and Values for each Reacting Channel Co-Simulation.

4. Select the **Reacting Channel Co-Simulation** > **Values** > **Coupling Strategy** node and specify the parameters that are required for coupling.
5. Right-click the **Reacting Channel Co-Simulation** > **Values** > **Chemistry Definition** node and select **Import Chemistry Definition (Chemkin format)**.
6. In the *Import Chemkin Files* dialog, browse to and select the appropriate files, then click **OK**. When you intend to use user coding, you select an edited Chemkin file for the *Fluid Chemistry Reaction File* which contains a list of atoms and species only.
7. Select the **Reacting Channel Co-Simulation** > **Values** > **Chemistry Definition** > **Reacting System Properties** > **Species Reaction Sources** node and set *Method* to either:
   - ► To use internally-defined reaction types in the standard Chemkin format, select **Internal** (default).
   - ► To specify reactions with user coding, select **User-Defined**.
8. To import and set up the user coding:
   a) Right-click the **Tools** > **User Code** node and select **New User Library**.
   b) In the *Open* dialog, browse to and select the appropriate library, then click **Open**.
   c) Select the **Species Reaction Sources** > **User-Defined** node and set *User Function* to `[user_function]`.
   d) Select the **Reacting System Properties** > **User-Defined Species Sources Specification** node and set *Method* to one of the following:

- To calculate the species sources from the user code, select *Calculate Species Sources*. Then select the **User-Defined Species Sources Specification** > **Calculate Species Sources** node and make sure that *Internal Reaction Energy Source* is activated.
- To modify the species sources from the internally-defined chemistry, select *Modify Internal Species Sources*.

The **Zones** node contains a **Zone 1** node by default. If you are simulating re-entry from one set of reacting channels to another, you must set up at least two zones.

9. To create more reacting channel zones, right-click the **Reacting Channel Co-Simulation** > **Zones** node and select **New**.

   A **Zone [2]** node appears.

10. To specify the boundaries for a reacting channel zone, group the boundaries for each reacting channel zone.

    a) Right-click the **Regions** > **[Region]** > **Boundaries** node and select **New Group**.

    b) Rename the **New Group** node appropriately.

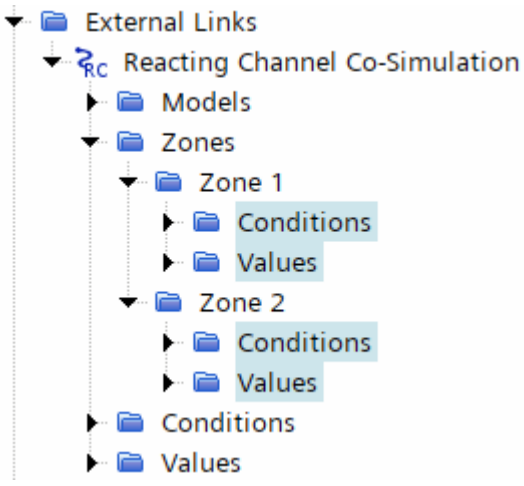
    c) Expand the **Boundaries** node and multi-select the boundaries for one reacting channel zone.

    d) Drag the selected boundaries on to the **[New Group]** node.

    You can use the **[New Group]** node to edit the Properties, Conditions, and Values of all boundaries that it contains.

Each zone represents one reacting channel (a group of geometrical channels) and contains a set of conditions and values which are applied to the boundaries that you specify for that reacting channel zone.

11. Right-click the **[New Group]** node and select **Edit**.
12. In the *Multiple Objects* dialog, expand the **Physics Conditions** > **External Code Coupling Specification** node and set *External Code Coupling Specification* to the Reacting Channel Co-Simulation Zone for the selected boundaries.
13. Group the remaining boundaries as necessary, and select an appropriate zone for the **External Code Coupling Specification** for each group of boundaries.
14. Specify the Conditions and Values for each Zone within each Reacting Channel Co-Simulation.

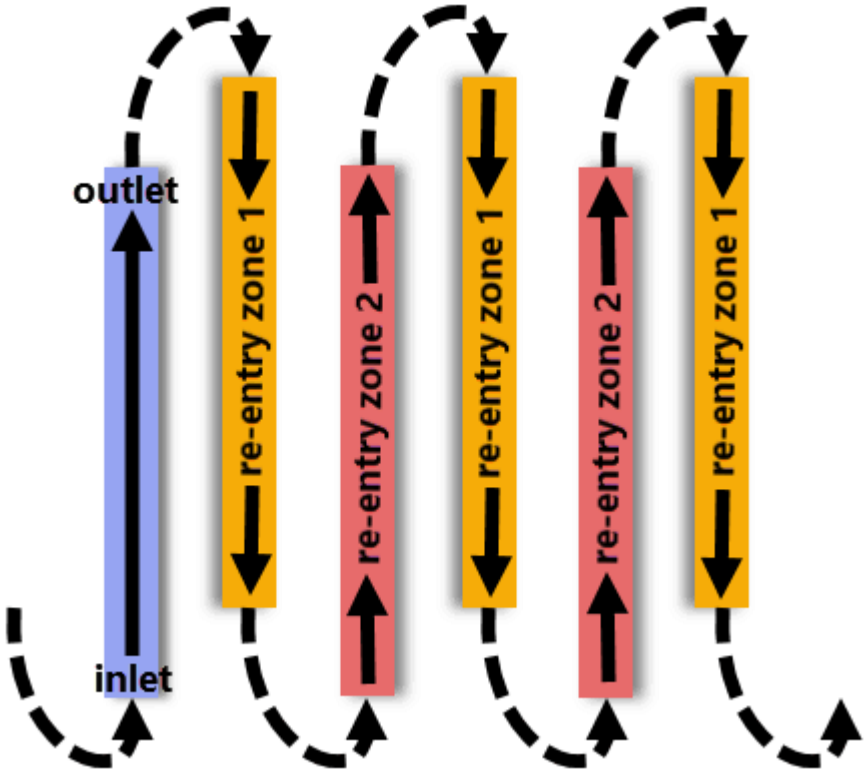


In particular, specify the following conditions and values:

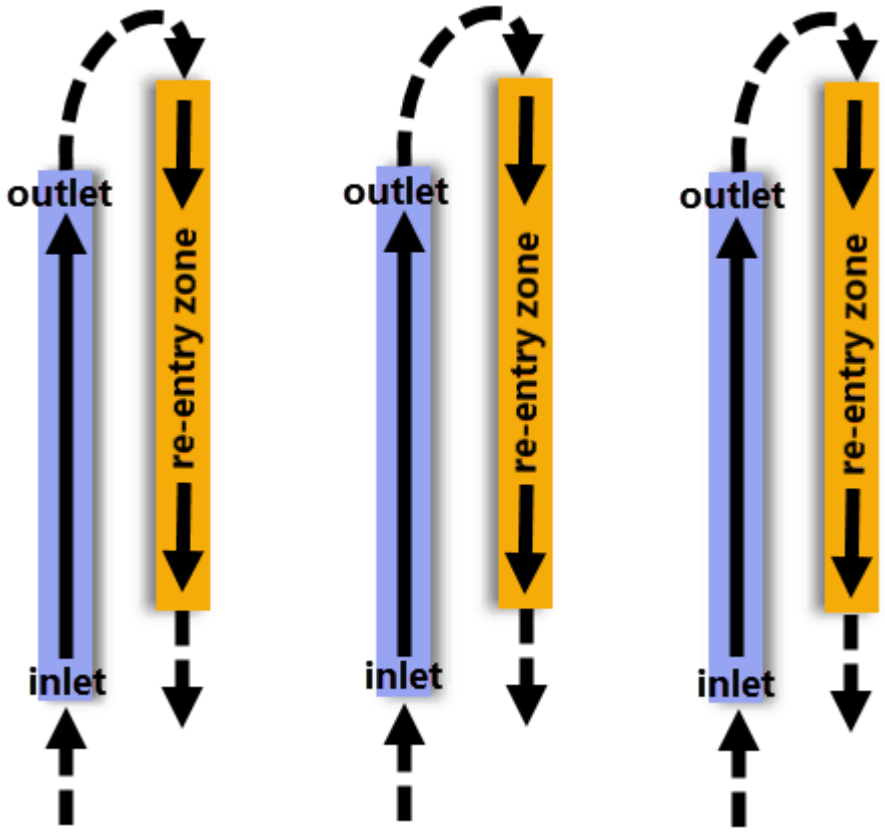
a) **Conditions** > **Reacting Channel Inlet Type**, *Inlet Type*:

- To simulate uninterrupted flow into this zone from another zone, select **Re-Entry**. When you select **Re-Entry** for one zone, make sure that at least one other zone is set to **Specified Inlet**. The conditions and values that are not available to set for the Re-Entry zone are taken from the Specified Inlet zone.
- To simulate flow between the inlet and outlet of reacting channels (from which you can, if required, specify the flow to re-enter reacting channels in a zone that is set as **Re-Entry**), select **Specified Inlet**.

The diagrams below represent two possible scenarios. In the first diagram, the channel on the left must be in a zone that is set to Specified Inlet. The remaining channels are then grouped into zones with the same properties—one re-entry zone in which the flow orientation is downwards, and one re-entry zone in which the flow orientation is upwards.

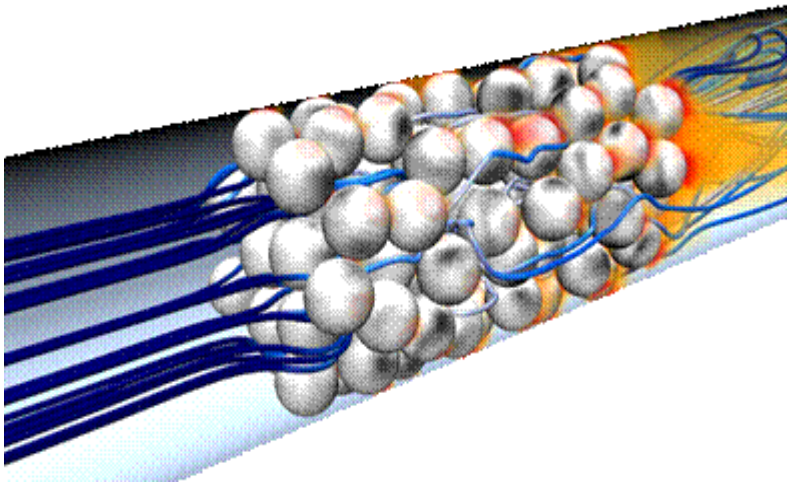


It is also possible to simulate multiple channels in a Specified Inlet zone—as long as these channels are all receiving an external flow that is not from a re-entry channel.



b) **Conditions** > **Reacting Channel Type**, *Correlation Type*:

- To simulate reacting channels that are void of any porous material, through which the reacting material will flow freely, select **Pipe**.
- To simulate reacting channels that are packed with porous material through which the reacting material will pass through, select **Packed Bed**. You can specify the parameters of the porous material.



c) **Conditions** > **Heat Transfer Coefficient Correlation**, *Correlation Type*.

d) If the *Inlet Type* is set to **Re-Entry**, expand the **Values** > **Re-Entry Boundaries** node and specify the *Outlet Boundary* from which each **[re-entry boundary]** receives the flow.

e) **Values** > **Wall Orientation**, *Orientation*.
Make sure that the direction of flow in each zone is correct.
f) Set other **[Zone]** > **Conditions** and **[Zone]** > **Values** as necessary.

15. Set the parameters of any other **[Continuum]** > **Models**, as required.
16. For the continuum that represents the fluid domain which surrounds the reacting channels, define any necessary parameters for the **Reference Values** and **Initial Conditons**.
Make sure that you specify the initial Species Mass Fraction.
17. Define any necessary Physics Conditions and Values for the Region and Boundaries.
    - For the inlet boundaries, specify the Species Mass Fraction and the Mass Flow Rate.
    - For the wall boundaries within the reacting flow region, specify the Surface Emissivity.
18. Return to the Reacting Flow General Workflow.

Contents:

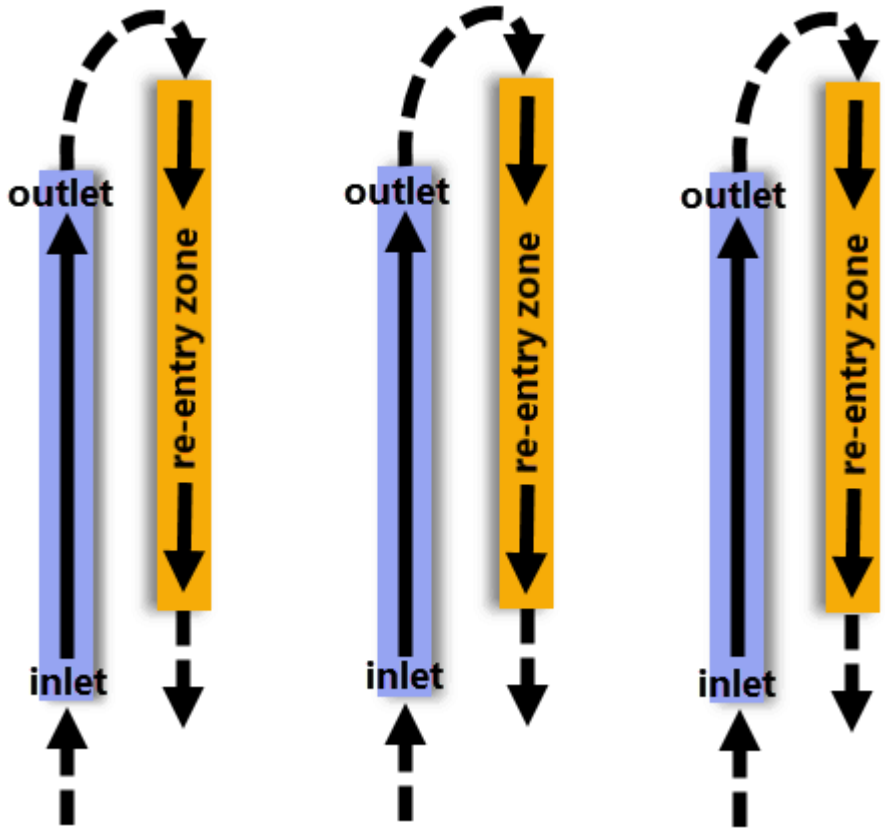
Creating Reacting Channels XY Plots

You can plot, for example, the temperature and heat flux within the reacting channels using Reacting Channel XY plots.

1. Right-click the **Plots** node and select **New Plot** > **Reacting Channel XY Plot**.
2. Select the **Reacting Channel XY Plot** node and set the *Parts* to all of the reacting channel tubes that you want to plot.
3. Multi-select all of the **Plots** > **Reacting Channel XY Plot** > **Data Series** > **[tubes]** nodes and select an option for *Y Variable*.

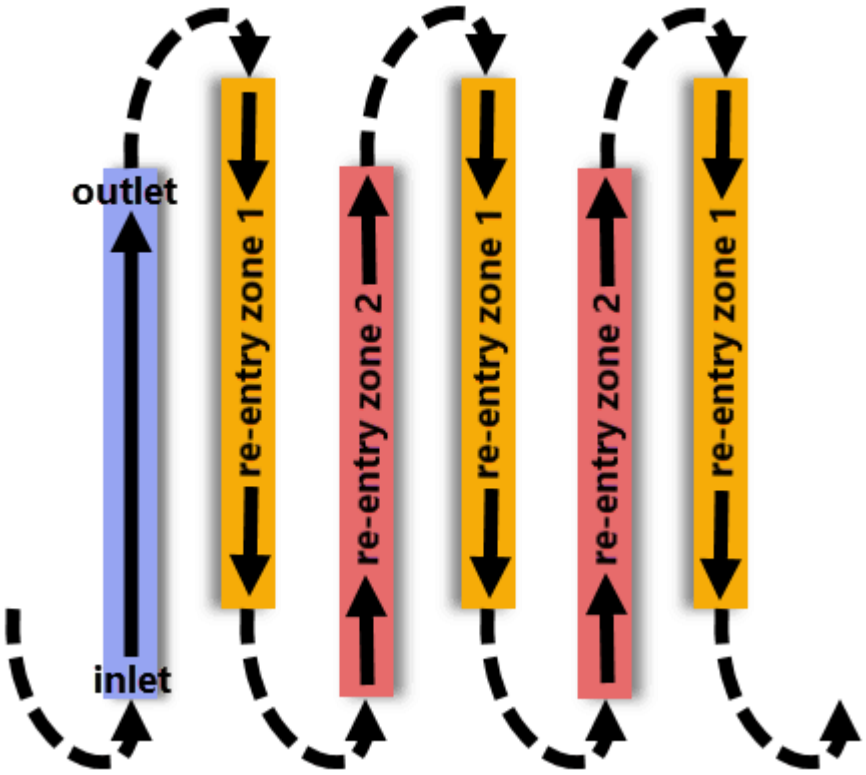
The XY plot is ready. However, if the reacting channels are set up so that the flow from some tubes re-enters other tubes, you can offset the plot for the re-entry tubes and visualise the continuation of the plot along the full length of the flow.

4. For reacting channels with only one re-entry zone—as described in the image:



Multi-select the **Plots** > **Reacting Channel XY Plot** > **Data Series** > **[re-entry tube x]** nodes and set *X Offset* to the length of a single tube in the non-re-entry zone.

5. For reacting channels with more than one re-entry zone—as described in the following image:

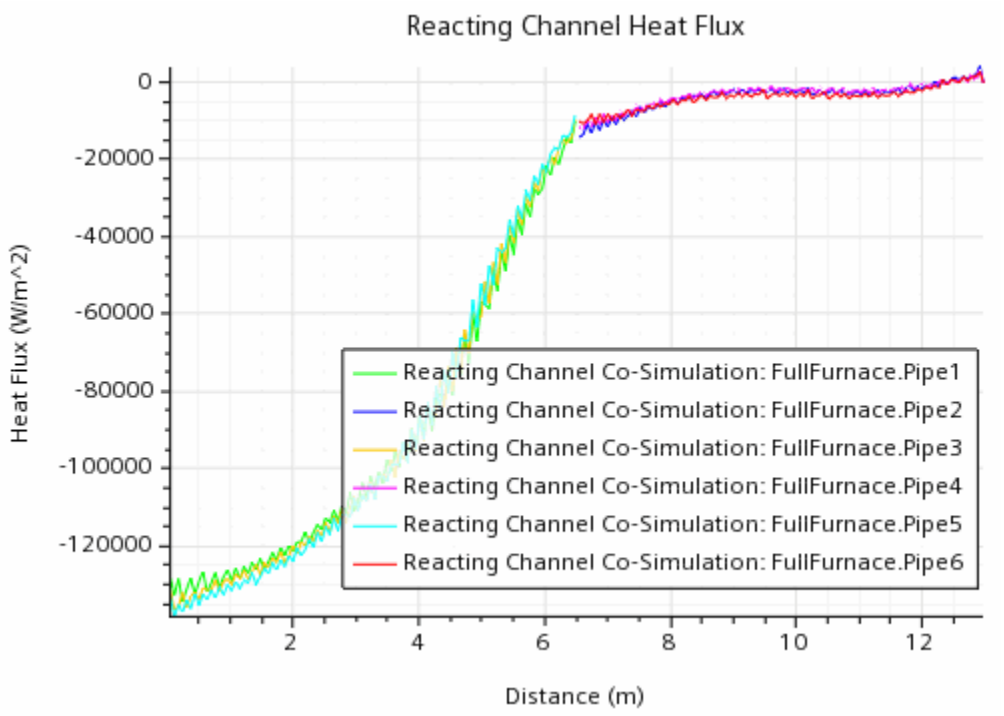


a) Select the **Plots** > **Reacting Channel XY Plot** > **Data Series** > **[first re-entry tube]** node and set *X Offset* to the length of the previous tube.

b) Select the **Plots** > **Reacting Channel XY Plot** > **Data Series** > **[next re-entry tube]** node and set *X Offset* to the length of the previous tubes combined.

c) Repeat step b until all of the required tubes are plotted. Make sure to increase the value for the *X Offset* to account for the combined length of all previous tubes.

Example Heat Flux XY Plot with Re-Entry



In the plot above, reacting channel tubes 1, 3, and 5 are plotted from 0.0–6.5 m, followed by tubes 2, 4, and 6 from 6.5–13.0 m.

Reacting Channel Co-Simulation Reference

Reacting channel co-simulation occurs between a 3D domain in Simcenter STAR-CCM+ and reacting channels that use a 1D Plug Flow Reactor (PFR).

You can use the Reacting Channel co-simulation model in Simcenter STAR-CCM+ to solve reacting flow simulations in tubular heat exchangers with channels that are long and thin.

This functionality is useful for simulating chemical processes such as steam reforming which occurs within narrow tubes surrounded by a firebox that is heated by combustion.

Reacting Channel Model Reference

Theory	See Reacting Channel Coupling.
Provided By	**[physics continuum]** > **Models** > *Co-Simulation Models*
Example Node Path	**Continua** > **Physics 1** > **Models** > **Reacting Channel**
Requires	One of the following combinations of model selections:

	When reactions occur in the fluid that surrounds the reacting channels: *Material*: **Multi-Component Gas** or **Multi-Component Liquid** *Reaction Regime*: **Reacting** *Reacting Flow Models*: any Additional combustion/turbulence models, as required. *Flow*: any *Space*: **Three Dimensional** *Time*: **Steady** *Enthalpy*: any *Optional Models*: **Co-Simulation**	When there are no reactions within the fluid that surrounds the reacting channels: *Material*: **Multi-Component Gas**, **Multi-Component Liquid**, **Gas**, or **Liquid** (when Multi-Component Gas or Multi-Component Liquid are selected: *Reaction Regime*: **Non-Reacting**) *Flow*: any *Space*: **Three Dimensional** *Time*: **Steady** (*Equation of State*: any) *Energy*: any *Optional Models*: **Co-Simulation**

Activates	Physics Models	*Reacting Channel Coupling Models*
	Model Controls	When the Reacting Channel model is selected, an **External Links** > **Reacting Channel Co-Simulation** node is added to the simulation object tree. The **Reacting Channel Co-Simulation** node contains four sub-nodes which allow you to define the reacting channel: Models, Zones, Conditions, and Values.
	Reports	**Combustion** > **Reacting Channel Outlet Quantity**. See Reports.
	Reference Values	Minimum Allowable Temperature, Maximum Allowable Temperature. See Reference Values.
	Boundary Inputs	External Code Coupling Specification. See Boundary Settings.

Models

Link models configure the connection to a partner application or file. The link icon changes based on the application, or file, that Simcenter STAR-CCM+ connects to through the link. The link model must be appropriate for the co-simulation or file export model selected in the physics continuum.

For reacting channel co-simulations, the Reacting Channel model is selected and cannot be modified.

Zones

The Zones node contains a [Zone n] node for each zone that you specify. Each [Zone n] node contains two additional sub-nodes in which you specify the **Conditions** and **Values** of that specific zone.

Zones > [Zone n] > Conditions

Coupled Model Parts

Boundaries

Displays a read only value which contains the boundaries that are specified for that reacting channel zone.

Regions

Displays a read only value which contains the regions that are specified for that reacting channel zone.

Equation of State (EOS) Option

Equation of State (EOS) Type

EOS Type	**Corresponding Values Node**
Ideal Gas The fluid within the reacting channels follows the ideal gas law. This option is intended for modeling gas-filled reacting channels.	
Constant The mixture density in the reacting channels is calculated as a mass fraction weighted sum of the individual species densities, which are specified as constant. This option is intended for modeling liquid-filled reacting channels.	**Component Densities** Allows you to define a constant density value for each species in the fluid. By default, if a species is contained in the material database, the constant densities are set to those of the material database.

Heat Transfer Coefficient Correlation

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet` and *Reacting Channel Type* is set to `Packed Bed`.

Correlation Type

Allows you to specify the correlation type for the heat transfer coefficient:

- **Leva/Grummer**
  Determines the heat transfer coefficient using Eqn. (3883)
- **Beek**
  Determines the heat transfer coefficient using Eqn. (3885)
- **DeWasch/Froment**
  Determines the heat transfer coefficient using Eqn. (3886)

Pipe Friction Correlation

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.

Correlation Type

Allows you to specify the correlation type for the pipe friction coefficient

- **Blasius** (Pipe)
  Determines the pipe friction coefficient using Eqn. (3887)
- **Filonenko** (Pipe)

Determines the pipe friction coefficient using Eqn. (3888)

- **Ergun** (Packed Bed)
  Determines the pipe friction coefficient using Eqn. (3890) which is valid for simulations with low $\frac{\mathrm{Re}}{1-\chi}$ values.
- **Hicks** (Packed Bed)
  Determines the pipe friction coefficient using Eqn. (3889) which is valid for simulations with high $\frac{\mathrm{Re}}{1-\chi}$ values.
- **Ergun/Hicks** (Packed Bed)
  Determines the pipe friction coefficient using Ergun correlation (Eqn. (3890)) when $\frac{\mathrm{Re}}{1-\chi} < 300$, Hicks correlation (Eqn. (3889)) when $\frac{\mathrm{Re}}{1-\chi} > 500$, and linear interpolation in between.

Reacting Channel Area Option

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.
Allows you to specify the cross-sectional area of one geometrical channel in a reacting channel zone (each geometrical channel within a reacting channel zone is expected to be of equivalent dimensions).

Reacting Channel Area Option

Sets the method for defining the channel cross-sectional area which is used to compute the diameter D_C for the convective heat transfer coefficient of the reacting channel, h_f in Eqn. (3879).

- **Constant**
  Allows you to specify the Reacting Channel Area as a constant value.
- **Tabular**
  Adds a **Values** > **Area** node which allows you to specify the channel cross-sectional area as a function of channel distance using imported tabular data.

Reacting Channel Heat Transfer Coefficient Option

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.

Reacting Channel Heat Transfer Coefficient Option

Allows you to specify the method for determining the Heat Transfer Coefficient, h_f which is used to determine the convective heat transfer source $\dot{Q}_C$ in Eqn. (3878).

- **Constant**
  Adds a **Values** > **Heat Transfer Coefficient** node which allows you to specify the Heat Transfer Coefficient, h_f as a constant array value.
- **Uniform**
  Allows you to specify the Heat Transfer Coefficient using values which are taken directly from the reacting channel Inlet values.
- **Non-Uniform**
  Determines the heat transfer coefficient using data from each axial point.
- **Tabular**

Adds a **Values** > **Heat Transfer Coefficient** node which allows you to specify the Heat Transfer Coefficient using tabular data which you can import.

Reacting Channel Inlet Type

Inlet Type

- **Specified Inlet**
  Allows you to specify which boundaries of the reacting channels are the inlet boundaries. The inlet and outlet boundaries are not connected.
- **Re-Entry**
  Simulates uninterrupted flow from one reacting channel into another by allowing Simcenter STAR-CCM+ to account for joined-up channels by means of a virtual U-bend. Provides the **Values** > **Re-Entry Boundaries** which you use to specify the boundaries that are concurrent. Also provides the *Orientation* property under the **Values** > **Wall Discretization** node which you use to specify the orientation of the channels in each zone.

Reacting Channel Inlet Viscosity Option

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.

Option

Allows you to specify how the viscosity, μ, of the components entering the reacting channel is determined at the reacting channel inlet:

- **Constant**
  Adds a **Values** > **Inlet Viscosity** node which allows you to set a value for the gas Viscosity at the inlet.
- **Uniform**
  Allows you to specify the gas Viscosity at the inlet using values which are taken directly from the reacting channel Inlet values.

Reacting Channel Pipe Friction Factor Option

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.

Option

Allows you to specify a multiplying factor for the pipe friction, f which is used to calculate the Nusselt number Eqn. (3881) for cases with turbulent flow. It is also used to calculate pressure drop in Eqn. (3891).

- **Constant**
  Allows you to specify a constant value for the **Values** > **Pipe Friction Factor** node.
- **Tabular**
  Allows you to specify the **Values** > **Pipe Friction Factor** using tabular data that you can import.

Reacting Channel Type

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.

Correlation Type

Allows you to specify the correlation type for the reacting channel:

- **Pipe**
  Specifies the pipes as empty reacting channels – which contain no material other than the gas that is in them.
- **Packed Bed**
  Specifies the pipes as fixed bed / packed bed reacting channels. This option is suitable for modeling applications such as steam cracking and methane steam reforming.

Reacting Channel Wall Temperature Option

Only available when *Reacting Channel Inlet Type* is set to `Specified Inlet`.

Option

Allows you specify how the Reacting Channel Wall Temperature T_W, Eqn. (3878), is determined at the wall boundary:

- **Uniform**
  Determines the temperature using data that is averaged from all axial points throughout the reacting channel zone.
- **Non-Uniform**
  Determines the temperature using data from each axial point throughout the reacting channel zone.

Thermal Conductivity/Dynamic Viscosity Method

Thermal Conductivity/Dynamic Viscosity Method

- **Kinetic Theory**
- **Constant**

Zones > [Zone n] > Values

The following Values are available to specify for each reacting channel zone:

Component Dynamic Viscosities

Available to specify when *Thermal Conductivity/Dynamic Viscosity Method* is set to **Constant**.

Allows you to specify the constant dynamic viscosities, μ in Eqn. (3882), of the components entering the reacting channel inlet.

Component Thermal Conductivities

Available to specify when *Thermal Conductivity/Dynamic Viscosity Method* is set to **Constant**.

Allows you to specify the constant thermal conductivities of the components entering the reacting channel inlet.

Area

Allow you to specify the reacting channel area using the following options:

- As a constant value when **Reacting Channel Area Option** is set to **Constant**
- As tabular data when **Reacting Channel Area Option** is set to **Tabular** .

> **Note:** If you are using additional re-entry zones, ensure that your tabular data cover for the total length of all channels.

This value is used to calculate the channel diameter D_C which is used to determine the convective heat transfer coefficient of the reacting channel, h_f in Eqn. (3879).

Inlet Mass Fractions

Allows you to specify the initial mass fraction profile of the components entering the reacting channel.

Inlet Pressure

Allows you to specify the pressure at the reacting channel inlet.

Inlet Temperature

Allows you to specify the reacting channel bulk temperature, T.

Inlet Velocity

Allows you to specify the velocity of the components entering the reacting channel inlet.

Packed Bed Heat Transfer Factor

Available when the reacting channel correlation type is set to **Packed Bed**. Allows you to specify the heat transfer factor, f_{htg} , which is used to calculate the heat transfer correlation for the packed bed reacting channel in Eqn. (3883) and Eqn. (3885).

Packed Bed Particle Diameter

Available when the reacting channel correlation type is set to **Packed Bed**. Allows you to specify the equivalent packed bed particle diameter, D_p , which is used to calculate the heat transfer correlation for the packed bed reacting channel in Eqn. (3883) and Eqn. (3885).

Packed Bed Porosity

Available when the reacting channel correlation type is set to **Packed Bed**. Allows you to specify the porosity, χ , of the material within the packed bed reacting channel.

Pipe Friction Factor

The pipe friction factor, f, is available to specify as:

- a constant value when **Reacting Channel Pipe Friction Factor** is set to **Constant**.
- tabular data when **Reacting Channel Pipe Friction Factor** is set to **Tabular**.

This value is used to determine the Nusselt number for cases with turbulent flow, in Eqn. (3881), which is used to calculate the convective heat transfer coefficient, h_f, in Eqn. (3879). It is also used to calculate pressure drop in Eqn. (3891).

Pipe Length

Allows you to specify the length of one geometrical channel in the reacting channel zone.

Re-Entry Boundaries

Available when the **Reacting Channel Inlet Type** condition for the reacting channel zone has the *Inlet Type* set to **Re-Entry**.

Provides a list of re-entry boundaries, that is, a list of boundaries which will receive incoming flow from an outlet boundary. You specify an *Outlet Boundary* for each re-entry boundary.

Make sure that the reacting channels are oriented correctly using the *Orientation* property of the **Wall Orientation** value node.

Solver Settings

Allows you to set the reacting channel solver settings for the zone.

ODE Solver Absolute Tolerance

ODE Solver Relative Tolerance

Under-Relaxation Factor

Allows you to set an under-relaxation factor, a, which governs the extent to which the old solution is supplanted by the newly computed solution.

Wall Discretization

Simcenter STAR-CCM+ receives a gradient of different temperature or heat flux values at intervals of this distance along the length of the reacting channel in the specified **Wall Orientation**.

Wall Orientation

Allows you to set the direction of flow in the reacting channels—which is important when simulating re-entry from one zone of reacting channels to another.

Conditions

Reacting Channel Species

PFR Species (read only)

Allows you to see all species that are involved in this mechanism in the reacting channel—reactants and products.

Values

Coupling Strategy

Couple After Step

Specifies the time-step after which data is transferred from the Plug Flow Reactor (PFR) to Simcenter STAR-CCM+. Delaying the data transfer until a specified time step allows the solver to reach a level of stability while receiving data from the PFR, before sending data back to the PFR.

Coupling Frequency

Specifies the interval of time steps that occur between each transfer of data from the PFR to Simcenter STAR-CCM+.

Chemistry Definition

Node	Description / Properties
Chemistry Definition	Provides the right-click options to **Import Chemistry Definition (Chemkin Format)** or **Delete Chemistry Definition**. Properties: *Material Database Path* and *Number of Species* (both read-only).
└ **Reacting System Properties**	
└ **Species Reaction Sources**	Properties: *Method*—`Internal` or `User-Defined`
└ **Internal**	Simcenter STAR-CCM+ defines the reactions from an internal set of standard Chemkin format reactions.
└ **User-Defined**	Allows you to define the reactions with user coding—useful for non-standard reaction types. Properties: *User Function*—when user coding is set up, the `wdot` option (the name of the function in the user code) becomes available. For an example of user coding for reacting channels, see the tutorial: Reacting Channels: Steam Methane Reforming.
└ **User-Defined Species Sources Specification**	Properties: *Method*—`Calculate Species Sources` or `Modify Internal Species Sources`
└ **Calculate Species Sources**	Properties: *Internal Reaction Energy Source*—when activated, calculates the reaction energy source internally for a constant pressure reactor based on user-calculated species reaction sources.
└ **Modify Internal Species Sources**	Existing internal species sources are modified.
└ **Reactions**	Provides the right-click option to create a **New Reaction**. Upon importing a chemistry definition / defining user coding, this node becomes populated with the appropriate reactions.

Reports

Reacting Channel Outlet Quantity

Units

Units for the quantity that is selected.

Reacting Channels

The report runs on the outlets of the reacting channels that are selected.

Quantity

The quantity that is reported at the outlet—such as temperature, velocity, heat flux, or a particular species.

Reference Values

Minimum Allowable Temperature

The smallest temperature value that is permitted anywhere in the continuum.

The Energy models (Coupled Energy, Coupled Solid Energy, Segregated Solid Energy, Segregated Fluid Enthalpy, Segregated Fluid Temperature) limit temperature corrections such that the corrected value does not go below this minimum. If this occurs, a message is printed to the *Output* window.

Maximum Allowable Temperature

The largest temperature value that is permitted anywhere in the continuum.

The Energy models (Coupled Energy, Coupled Solid Energy, Segregated Solid Energy, Segregated Fluid Enthalpy, Segregated Fluid Temperature) limit temperature corrections such that the corrected value does not exceed this maximum. If this occurs, a message is printed to the *Output* window.

Boundary Settings

Domain Boundary

External Code Coupling Specification

Allows you to assign the boundary to a co-simulation zone for coupling. During the co-simulation, the Simcenter STAR-CCM+ boundary exchanges data with the corresponding coupled surface in the partner simulation, according to the co-simulation zone specifications.

Reactor Network

You can reduce the computational cost of solving complex chemistry for each cell in the computational domain of a steady combustor by simulating with an economical combustion model—such as a flamelet model, or the Eddy Break-Up (EBU) model—then clustering cells into a specified number of reactors and solving detailed chemistry on this network of reactors.

The process of clustering CFD cells into reactors consists of three operations. In the first, the clustering algorithm is used to group cells with similar states—temperature and equivalence ratio by default. These cells are typically non-contiguous, and the second operation is to split non-contiguous clusters into separate clusters. The final step is to group clusters with the smallest number of cells to their closest neighbor in composition space until approximately the specified number of reactors are attained.

Contents:

Reactor Network Workflow

Use the Reactor Network Workflow when you want to rapidly simulate detailed chemistry in a steady combustor.

Note: If required, you can automate running the reactor network using the Simulation Operations feature. See Run Reactor Network.

1. Set up and run a steady-state reacting flow simulation until you reach a converged solution using either:
   - ► Any of the flamelet models (see Flamelet Workflow).
   - ► Any of the Reacting Species Transport models (see Reacting Species Transport Workflow).
2. For the physics continuum that represents the reacting flow, from the *Optional Models* group box, select the **Reactor Network** model.
3. Right-click the **[physics continuum]** > **Reactor Network** > **Chemistry Definition** node and import a detailed chemistry mechanism in Chemkin format.
4. To specify the similar states to be used for clustering, select the **Reactor Network** > **Clustering Components** node and set one or more *Clustering Components*—typically, Temperature or Equivalence Ratio. You can also specify user-defined clustering components in the form of field functions.
5. Specify the reactor type to be used by selecting the **Reactor Network** > **Reactor Type** node.
   a) Set the *Reactor Option* to either **Constant Pressure** or **Perfectly Stirred Reactor**.
   b) Set the *Temperature Option* to either **Equation of State**, **Frozen from CFD**, or **Enthalpy**.

   For more information, see Reactor Network Model Reference: Reactor Type.
6. To specify how many reactors are to be created approximately, select the **Numerical Settings** node and set *Target Number of Reactors*. To attain the most accurate solution possible, set this value as high as is feasible—considering the availability of computational resources (serial or parallel), and run-time constraints.

   For more information, see Reactor Network Model Reference: Numerical Settings.

7. Set up any monitors, plots, and scenes that you require. For Reactor Network simulations, you can visualize specifically:
   - RN Index
   - RN Mass Fractions of Individual Species
   - RN Temperature

   For more information, see Reactor Network Model Reference: Field Functions.
8. Right-click the **[physics continuum]** > **Reactor Network** > **Chemistry Definition** node and select **Run Reactor Network**.

Reactor Network Model Reference

You use the Reactor Network model to rapidly simulate detailed chemistry in a steady combustor.

Reactor Network Model Reference

Theory	See Reactor Network.	
Provided By	**[physics continuum]** > **Models** > *Optional*	
Example Node Path	**Continua** > **Physics 1** > **Models** > **Reactor Network**	
Requires	Starting from a completely run steady-state reacting flow simulation. *Material*: either **Multi-Component Gas** or **Multi-Component Liquid** *Time*: **Steady** *Reaction Regime*: **Reacting** either: • *Reacting Flow Models*: **Reacting Species Transport** *Reacting Species Models*: any • *Reacting Flow Models*: **Flamelet** *Flamelet Models*: any and: *Flow*: any	
Activates	Model Controls (child nodes)	**[physics continuum]** > **Reactor Network** See Reactor Network • Chemistry Definition • Clustering • Reactor Type • Numerical Settings • Emissions
	Field Functions	**RN Density**, **RN Index**, **RN Mass Fraction of [species]**, **RN Soot Mass Density**, **RN Soot Mean Diameter**, **RN Soot Moment of [n]**, **RN Soot Number Density**, **RN Soot Size Dispersion**, **RN Soot Volume Fraction**, **RN Temperature**. See Reactor Network Field Functions.
	Simulation Operations	See Run Reactor Network.

You are recommended to use the Reactor Network model with the Steady model since the fluxes, and hence the reactors, are based on the instantaneous solution and not on a time-averaged solution.

[physics continuum] > Reactor Network

Here you specify the detailed chemistry mechanism that the reactor network model solves within the network of reactors. There are also several numerical parameters to set, in particular, the number of reactors that are in the network.

Reactor Network Right-Click Menu

Run Reactor Network

Runs the Reactor Network Solution. You can also run from previous reactor network solutions without clearing the solution first.

Stop Reactor Network Calculations

Stops solving the Reactor Network.

Clear Reactor Network Solution

Clears the existing Reactor Network Solution.

Chemistry Definition

The Chemistry Definition describes the chemical reaction mechanism, which is the collection of all species and their corresponding reactions, as well as the species thermodynamic properties.

Right-Click Actions

Import Complex Chemistry Definition (Chemkin format)

Activates a standard *Open* dialog that imports files for the reactor network chemistry definition in Chemkin™format. Upon importing a chemistry definition, the reactions for the definition appear as sub-nodes of the Chemistry Definition node.

Delete Complex Chemistry Definition

Removes all the species and their reactions in the reactor network chemistry definition.

Chemistry Definition > Reactions

See Complex Chemistry

Clustering

See Chemistry Acceleration Properties: Clustering

Reactor Type

Reactor Option

Constant Pressure Reactor

The mass fractions in a reactor are calculated as the output of a 0D constant pressure reactor (CPR), where the input is the mass flux weighted average mass fractions from neighbor reactors (Eqn. (3894)). The integration time is the residence time in the reactor.

Perfectly Stirred Reactor

The mass fractions in a reactor are calculated as the output of a perfectly stirred reactor (PSR), which is a 0D steady-state equation system (Eqn. (3898)). The input mass fluxes into each PSR are the mass fluxes from neighbour reactors.

Temperature Option

Equation of State

The temperature is calculated by Eqn. (679).

Frozen from CFD

The reactors use the temperature from the CFD solution.

Enthalpy

The temperature is calculated from the CFD enthalpy field and the reactor network species.

Numerical Settings

Target Number of Reactors

The approximate number of reactors into which the computational domain is split by the Reactor Network model. Contiguous cells of similar composition are clustered into approximately this number of reactors. The accuracy of reactor network predictions, as well as the computational cost, increase with the specified Target Number of Reactors. Set this value to the largest value that you can afford with the available computational resources (serial or parallel) and run-time constraints.

Max Iterations

Maximum number of iterations for which the reactor network is solved. You can continue to run the reactor network solution from previous solutions by increasing this value—without clearing the solution first.

Residual Tolerance

The constant pressure reactor (CPR) or perfectly-stirred reactor (PSR) set of equations is iteratively solved until the residual is less than this value, or the maximum number of iterations are exceeded.

Absolute ODE Tolerance

Allows you to specify an absolute tolerance for the solver.

Relative ODE Tolerance

Allows you to specify a relative tolerance for the solver.

Under-Relaxation Factor

In order to promote convergence, this property is used to under-relax changes of the solution during the iterative process. If residuals show solution divergence or do not decrease, reduce the under-relaxation factor.

Diffusion Flux Multiplier

The scaling factor for the internally calculated diffusion flux. The reactor network convective and diffusive fluxes are calculated from the steady reacting flow solution. Since there are usually far fewer reactors than cells, the predicted reactor network species fields can be overly diffusive. For example, combustion products in the flame zone can un-realistically diffuse upstream to the combustor inlets. This effect can be mitigated by reducing the Diffusion Flux Multiplier from 1 towards 0.

Emissions

Soot

When activated, provides the **Soot Options** sub-node with which you choose to account for soot emissions within the reactor network using either the soot moments method or the soot sections method.

Soot Options

Discretization Option

Discretization Option	**Corresponding Sub-Node**
Moments Accounts for soot emissions within the reactor network using the soot moments method, where the soot moment source term ω_{M_r} is given by Eqn. (3738).	None.

Discretization Option	**Corresponding Sub-Node**
Sections Accounts for soot emissions within the reactor network using the soot sections method.	**Soot Sections** *Number of Sections* Number of discrete sections in the particle size distribution function (PSDF). *Maximum Soot Diameter* Maximum diameter to which the soot particle grows. *Small Diameter Fractal Dimension* Surface growth fractal dimension of soot particles with a diameter θ less than 20nm in Eqn. (3808) and Eqn. (3809). You can set this between `2.0` and `3.0`. *Large Diameter Fractal Dimension* Surface growth fractal dimension of soot particles with a diameter θ greater than 60nm in Eqn. (3808) and Eqn. (3809). You can set this between `2.0` and `3.0`.

Nucleation Option

Only available as a property of the Soot Moments model or Soot Sections model when using the Complex Chemistry, Reactor Network, ECFM-3Z, or ECFM-CLEH combustion model. When using one of the Flamelet combustion models, you specify the nucleation option as a combustion table parameter.

Allows you to specify the *Nucleation Option* as either:

Nucleation Option	**Corresponding Sub-Node**
Single PAH Species (C16H10): See Eqn. (3745) and Eqn. (3746). The PAH precursor is recognised as any species which includes either A4 or A3R5 in the species name, or has the composition C16H10.	None
C2H2: See Eqn. (3748).	None

Nucleation Option	**Corresponding Sub-Node**
Multi PAH Species Allows you to select multiple PAH precursor species from those that are present in the chemical mechanism. Simcenter STAR-CCM+ recognises the chemical symbols of the PAH precursor species as described within the table for Multi PAH Species Nucleation. Available only when using the Complex Chemistry or Reactor Network combustion models.	**PAH Species Components** Lists the selected PAH precursor species—each displays its *Sticky Coefficient* property.

(Soot) Surface Chemistry Option

(Soot) Surface Chemistry Option	**Corresponding Sub-Node**
HACA The soot surface growth is modeled using the Hydrogen-Abstraction-C2H2-Addition (HACA) surface mechanism. Most appropriate when using the Complex Chemistry model. See HACA.	None
HACA RC The soot surface growth is modeled using the Hydrogen-Abstraction-Carbon-Addition-Ring-Closure (HACA-RC) surface mechanism. Most appropriate when using an ECFM model for diesel fuel. See HACA RC.	None

Steric Factor

Allows you to define a constant value for the steric factor α in Eqn. (3772).

Surface-growth Scale

Scales surface growth (part of W_r in Eqn. (3739)).

Nucleation Scale

Scales nucleation (R_r in Eqn. (3739)).

Oxidation Scale

Scales oxidation (part of W_r in Eqn. (3739)).

Two-Way Coupled Species

In soot reactions, gas phase species are transferred to and from the gas phase to the soot particles. When this property is activated, these gas-phase species are added and removed from the gas-phase simulation. Only available when using a reacting species transport model or the Reactor Network model.

Field Functions

RN Density

Density in the reactor.

RN Index

The index values of the reactors that the Reactor Network model creates.

RN Mass Fraction of [species]

The mass fraction of the [species] in the reactor.

RN Soot Mass Density

M in [eqnlink] within the reactor.

RN Soot Mean Diameter

$d = \left(\frac{6M}{\pi N \rho_{soot}}\right)^{\frac{1}{3}}$ in the reactor.

RN Soot Moment of [n]

For the ith reactor, M_r^i in Eqn. (3897) for constant pressure reactors, and in Eqn. (3900) for perfectly stirred reactors.

RN Soot Number Density

N in Eqn. (3740) within the reactor.

RN Soot Size Dispersion

$D_{soot} = \frac{(M_2 M_0)}{(M_1)^2}$ in the reactor.

RN Soot Volume Fraction

f_v in Eqn. (3741) within the reactor.

RN Temperature

The temperature in the reactor.

Common Reacting Flow Actions

This section contains short sets of instructions that describe how to perform some of the actions which are common to several of the reacting flow detailed workflows.

Contents:

Importing Species and Reactions

Simcenter STAR-CCM+ allows you to import mechanisms in Chemkin format. You can also import species separately in Chemkin format.

To import species or mechanisms, do one of the following:

Objective	Steps
Species: Importing Mixture Components from a Chemkin-formatted (`.chm`) File	1. Right-click the **[continuum]** > **Models** > **Multi-Component [gas]** > **[gas] Components** node and select **Import Species**. 2. In the *Select file and material database* dialog that appears, click **Browse**. 3. In the *Open* dialog, navigate to and select the required file. Click **Open**. 4. In the *Select file and material database* dialog, click **OK**. The **[Gas] Components** node is populated with species data.

Objective	Steps
Mechanisms: Importing Mechanisms from a Chemkin-Formatted File	When importing kinetic mechanisms in Chemkin format, it is necessary to import the Chemkin reaction mechanism file along with the corresponding NASA thermodynamic file. Importing the associated transport file is optional. See Using Thermodynamic Polynomial Data. For laminar flame simulations, the molecular transport properties are important and therefore a transport file is generally imported. However, for turbulent flames where turbulent transport dominates over molecular transport, it is not necessary to import the molecular transport properties—constant laminar transport properties are sufficient. 1. Right-click the **Complex Chemistry** or **Surface-Gas Interaction** node and select **Import Chemistry Definition (Chemkin Format)** 2. In the *Import Chemkin Files* dialog that appears: a. Select the *Fluid Chemistry Reaction File* and the *Fluid Thermodynamic Properties File* to import. b. If you are simulating a laminar flame and the molecular transport properties are important: ▪ Make sure that the *Import Fluid Transport Properties File* option is activated. ▪ Select the *Fluid Transport Properties File* to import. c. If you are simulating turbulent flames, deactivate the *Import Fluid Transport Properties File* option. d. If you are importing a surface mechanism, also select the *Surface Chemistry Reaction File* and the *Surface Thermodynamic Properties File* to import—you can select more than one of each. e. Click **OK**. **Note:** The thermodynamic properties files provide the specific heat polynomial coefficients, as well as the heat of formation, standard state entropy, and elemental composition for all species in the mechanism. The transport properties files provide the Lennard Jones properties: dipole, rotation, polarization, molecule type, characteristic energy, and characteristic length. 3. Expand the **[continuum]** > **Models** node. ◦ The gas components appear under the **Multi-Component Gas** > **Gas Components** node. ◦ The reactions appear under the **Reacting** > **Reactions** node—or for surface chemistry mechanisms, under the **Reacting Surface** > **Reactions** node. ◦ The polynomial data appears under the **Material Properties** > **Specific Heat** > **Thermodynamic Polynomial Data** node for each species. **Note:** If species are imported without properties, the missing properties are copied from the standard material database—if available.

Restrictions on Importing Reactions (Within a Mechanism)

There should be no space between the stoichiometric coefficient and reactant/product.

For example, this format is invalid:

CH4 + 2 O2 => CO2 + 2 H2O

The correct format is:

CH4 + 2O2 => CO2 + 2H2O

Restrictions on Importing Species

- Thermodynamical polynomials and molecular data also must be present for the imported species, either in the supplied files or in the user-defined files.
- You can import either 7-coefficient or 9-coefficient thermodynamic polynomial data, however, you cannot use a mixture of these formats within the same file.
- The species names that are used in the thermodynamic polynomial data must match the species names that are used in the chemical mechanism.
- The species phase in the user-defined Chemkin database file must be G(gas), L(liquid), or S(solid).

Restrictions on Importing Surface Mechanisms

- Species in the site phase must have the suffix (S).
- Species in the bulk phase must have the suffix (B).

Defining Species Manually

Before you can select a species as a component in a chemical reaction, the species must be defined as a component under the material model.

The Standard Material Database is provided in Simcenter STAR-CCM+ by default. This database contains a wide selection of species components. However, if necessary, you can create and save custom material databases. See Using Material Databases.

1. Right-click the material model node, for example, the **[Physics 1]** > **Models** > **Multi-Component Gas** node, and choose **Select Mixture Components**.
2. In the *Select Mixture Components* dialog, expand the **Material Databases** > **Standard** > **[Gases]** node.
   a) Select all of the species components that are present in the reactions.
   b) Click **Apply**, then click **Close**.

   The Gas or Liquid species components appear under the Material model node, for example, the **Multi-Component Gas** > **Gas Components** node.
3. If necessary, you can replace a species component. Right-click the **Multi-Component Gas** > **Gas Components** > **[Component]** node.
   a) Select **Replace with**.
   b) In the *Replace Mixture Component* dialog, select the component that is required.
   c) Click **OK**.
4. The order in which the mixture components are added is not important as all species are solved for. However, if you wish, you can reorder species components. Right-click the **Multi-Component Gas** > **Gas Components** node.
   a) Select **Reorder Mixture Components**.

b) In the *Reorder Mixture Components* dialog, drag and drop the species into the order that is required.

c) Click **OK**.

5. For each species component, set the Material Properties.

a) For a species component, expand the **[Gas Components]** > **[Component]** > **Material Properties** node.

b) Select a Material Property node and set the Method that is required. See Material Property Node Properties.

c) Select the Material Property sub-node and set any properties that are required.

d) Repeat these steps until all of the necessary properties are set for all species components.

Defining Chemical Reactions Manually

The **Models** > **Reacting** > **Reactions** node and the **Reacting Surface** > **Reactions** node allow you to define reactions which occur within the reacting flow.

Before defining chemical reactions manually, make sure that species are defined under the relevant materials node. See Defining Species Manually or Importing Species and Reactions.

In Simcenter STAR-CCM+, you can define simple reacting flow chemistry definitions manually. You can define reaction components as reactants or products, however, it is not possible to define any intermediate reaction components manually. If it is important to define specific intermediate reaction components in the chemistry definition, you can import an externally compiled reaction mechanism. See Importing Species and Reactions.

1. To set up a new reacting flow chemistry definition, right-click the **Reactions** node and select **New Reaction**.

   A **[Reaction n]** sub-node appears.

2. Define the reaction components:

a) Right-click the **[Reaction n]** > **Reactants** node and select **Add Reactant**.

b) Select a reactant from the submenu.

   The menu displays components that are already defined as part of the mixture and not already selected as a reactant in this reaction.

c) Select any further reactants for the reaction.

d) Right-click the **[Reaction n]** > **Products** node and select **Add Product**.

e) Select products from the submenu in the same manner as for the reactants.

3. Specify the properties of each reaction component.

a) Set stoichiometric coefficients, ν_{ij}, that are appropriate to the reaction.

   Make sure that the stoichiometric coefficients represent the correct ratio of reactants and products as are defined in the balanced chemical equation.

b) For the EBU model and surface chemistry reactions, specify a rate exponent, p_{ij}.

   This parameter is used to calculate chemical reaction rates from finite-rate kinetics—not required if the **Standard EBU** model is used for **Eddy Break-up**.

4. Repeat the steps above until all reactions that are required to describe the reacting flow chemistry definition are fully defined.

5. If necessary, define the overall properties for the reacting flow chemistry definition. Expand the **[Reaction n]** > **Properties** node.

- When using the Eddy Break-Up (EBU) model, expand the **Properties** > **EBU Coefficients** node and specify the EBU rate coefficients.
- When using other reacting flow models, expand the **Properties** > **Reaction Coefficient** node and specify the Arrhenius coefficients or User-defined reaction coefficient.