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.

oot Two-Equation Model Reference

Theory	See Soot Two-Equation.	
Provided By	**[physics continuum]** > (and then)**Models** > (and then)*Soot Emissions Model*	
Example Node Path	**Continua** > (and then)**Physics 1** > (and then)**Models** > (and then)**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 $\varnothing_M$ in Eqn. (3694).

Soot Scaled Number Density Profile

Specifies a scalar profile for the soot scaled number density $\varnothing_N$ in Eqn. (3693).

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 $\varnothing_M$ in Eqn. (3694). **Soot Scaled Number Density Profile** Specifies a scalar profile for the soot scaled number density $\varnothing_N$ in Eqn. (3693).
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. (908)) and for computing cell gradients (Eqn. (920) and Eqn. (921)) 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. (3709).

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. (3700).

Soot Growth Rate

$\left(\frac{dM}{dt}\right)_{sg}$ in Eqn. (3703).

Soot Mass Density

M in Eqn. (3694). 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. (3699).

Soot Nucleation Rate For Scaled Number Density

$\left(\frac{dN}{dt}\right)_{nu}$ in Eqn. (3697) for PAH nucleation, or in Eqn. (3698) for C2H2 nucleation.

Soot Number Density

N in Eqn. (3693). The units are $\left[/\mathrm{m^3}\right]$.

Soot Oxidation Rate

$\left(\frac{dM}{dt}\right)_{ox}$ in Eqn. (3705).

Soot Scaled Mass Density

$\varnothing_M$ obtained from Eqn. (3694).

Soot Scaled Mass Density Rate

$\dot{\omega}_{\varnothing M}$ computed from Eqn. (3696).

Soot Scaled Number Density

$\varnothing_N$ obtained from Eqn. (3693).

Soot Scaled Number Density Rate

$\dot{\omega}_{\emptyset N}$ computed from Eqn. (3695).

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. (3658) and Eqn. (3659). Partial Equilibrium Selects the approach that is used in Eqn. (3658) and Eqn. (3660) 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. (3661), 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. (3662). 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. (3697), 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. (3698) and Eqn. (3699), 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. (3703) which contributes to the overall soot scaled mass density rate in Eqn. (3696). 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. (3700) which contributes to the overall soot scaled number density rate in Eqn. (3695). 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. (3697) for PAH-based nucleation / in Eqn. (3698) for Acetylene-based nucleation) which contributes to the overall soot scaled number density rate in Eqn. (3695).
- Soot mass density $\left(\frac{dM}{dt}\right)_{nu}$ in Eqn. (3699) which contributes to the overall soot scaled mass density rate in Eqn. (3696).

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. (3705) which contributes to the overall soot scaled mass density rate in Eqn. (3696). 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. (3708).