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. (3698) and Eqn. (3699) is used, which is based on the acetylene concentration.

oot Moments Model Reference

Theory	See Soot Moments.	
Provided By	**[physics continuum]** > (and then)**Models** > (and then)*Soot Emissions Models*	
Example Node Path	**Continua** > (and then)**Physics 1** > (and then)**Models** > (and then)**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. (902). 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. (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

Soot Mass Density

M in Eqn. (3694). The units are $\left[\mathbf{kg/m^3}\right]$.

Soot Mean Diameter

d in Eqn. (3717).

Soot Moment 0

M_0 related to soot number density in Eqn. (3714).

Soot Moment 1

Mean particle diameter of soot particles, M_1 in Eqn. (3715) and Eqn. (3715).

Soot Moment Source 0

$r = 0$ in Eqn. (3712).

Soot Moment Source 1

$r = 1$ in Eqn. (3712).

Soot Number Density

N in Eqn. (3693) and Eqn. (3714). The units are $\left[\mathbf{/m^3}\right]$.

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. (3718).

Soot Volume Fraction

f_v in Eqn. (3715).

Steric Factor

α in Eqn. (3754).

Soot

The Soot sub-node allows you to specify specific material properties for the soot material.

Density

ρ in Eqn. (3711).

Molecular Diffusivity

σ in Eqn. (3711).

Turbulent Schmidt Number

σ_t in Eqn. (3711).

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. (3746), 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. [788] 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. (3754).	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. (3719) and Eqn. (3720). 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. (3722).	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. (3713)).

Nucleation Scale

Scales nucleation (R_r in Eqn. (3713)).

Oxidation Scale

Scales oxidation (part of W_r in Eqn. (3713)).

Coagulation Scale

Scales coagulation G_r in Eqn. (3713). 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.