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.

oot 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] > (and then)Models > (and then)Soot Emissions Model</td></tr>
<tr><td>Example Node Path</td><td colspan="2">Continua > (and then)Physics 1 > (and then)Models > (and then)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

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 rowspan="6">Activates</td><td>Model Controls (child nodes)</td><td>Soot and Soot Model Properties.</td></tr>
<tr><td>Other nodes</td><td>[physics continuum] > (and then)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>Solvers</td><td>Soot. See Solvers.</td></tr>
<tr><td>Monitors</td><td>SootSection[n]</td></tr>
<tr><td>Report Options</td><td>Soot PSDF, Soot, Sections Diameters, Soot Plots, Soot Particle Size Distribution. See Reports.</td></tr>
<tr><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>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. (902). 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. (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.

Reports

Reports	With Complex Chemistry	With ECFM Models	With Flamelet Models	With Reactor Network

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. (3790).

Soot Mass Fraction Sec[n]

$\widetilde{Y}_{i,\text{soot}}$ for section i , in Eqn. (3755).

Soot Mean Diameter

d_p in Eqn. (3792).

Soot Nucleation Rate

$\left(\frac{dN}{dt}\right)_{nu}$ in Eqn. (3698).

Soot Number Density

Total soot number density N_{tot} given by Eqn. (3793).

Soot PSDF Sec[n]

Soot particle size distribution function $\frac{dN}{d\log(d_p)}(i)$ for section i , given by Eqn. (3794).

Soot Total Mass Fraction

Sum of $Y_{i,\text{soot}}$ from i to i_{max} .

Soot Volume Fraction

f_v in Eqn. (3791).

Steric Factor

α in Eqn. (3754).

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** > (and then)**Emissions** > (and then)**Soot Options** node provides similar properties. See Soot Options.

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 $\widetilde{\Omega}_{i,\mathrm{sg}}$ in Eqn. (3757).

Nucleation Scale

Scales nucleation $\widetilde{\Omega}_{i,\mathrm{nuc}}$ in Eqn. (3757).

Oxidation Scale

Scales oxidation $\widetilde{\Omega}_{i,\mathrm{ox}}$ in Eqn. (3757).

Coagulation Scale

Scales coagulation $\widetilde{\Omega}_{i,\mathrm{coag}}$ in Eqn. (3757). 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 > (and then)Soot Model Properties > (and then)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. (3782) and Eqn. (3783). 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. (3782) and Eqn. (3783). You can set this between 2.0 and 3.0.

Soot Sections > (and then)Soot Model Properties > (and then)Steric Factor

Alpha

The steric factor α for surface reactions in HACA or HACA-RC mechanisms.