Passive Scalar Model Reference

The Passive Scalar model allows you to define variables of arbitrary value and assign them to fluid phases or individual particles.

Passive scalars can be used in physics continua for single phase and Two-Phase Thermodynamic Equilibrium flows. For Mixture Multiphase flows and all other multiphase flows, passive scalars can be used for each Eulerian phase or Lagrangian phase. Passive scalars can also flow through porous media, where they can exhibit anisotropic diffusion.

Provided By	Single phase or mixture multiphase simulation: [physics continuum] > (and then)Models > (and then)Optional Models Multiphase simulation: [phase] > (and then)Models > (and then)Optional Models
Example Node Path	Single phase simulation: Continua > (and then)Physics 1 > (and then)Models > (and then)Passive Scalar Multiphase simulation: Continua > (and then)Physics 1 > (and then)Models > (and then)Multiphase > (and then)Phase 1 > (and then)Models > (and then)Phase 1 > (and then)Phase 1 > (and then)Models > (and then)Phase 1 > (and th
Requires	Single phase simulation: Material: one of Gas, Liquid, Multi-Component Gas, Multi-Component Liquid, Flow: any Multiphase simulation: Material: Multiphase Multiphase Model: one of the following: Two-Phase Thermodynamic Equilibrium, any Flow model. The Passive Scalar model is available in the physics continuum only. Mixture Multiphase (MMP). The Passive Scalar model is available in the physics continuum and for each
	 Eulerian phase. Eulerian Multiphase (EMP) or Volume of Fluid (VOF). The Passive Scalar model is available for each Eulerian phase. It is not available for Fluid Film phases.
Properties	Key properties are: Secondary Gradients Convection Flow Boundary Diffusion SUPG See Passive Scalar Properties.
Right-click Actions	On the Passive Scalar > (and then)Passive Scalars node: New.

Activates	Model Controls (child nodes)	Passive Scalars See <u>Passive Scalars Model Control Reference</u> .
	Materials	Under the Material Properties node of a passive scalar:
		Molecular Diffusivity
		Turbulent Schmidt Number (for turbulent flows)
		See <u>Materials and Methods</u> .
	Initial Conditions	Passive Scalar See Initial Conditions.
	Boundary Inputs	See <u>Boundary Settings</u> .
	Region Inputs	Passive Scalar Source Option See Region Settings.
	Solvers	Passive Scalar See <u>Passive Scalar Solver Properties</u> .
	Monitors	One residual monitor per passive scalar.
	Field Functions	See <u>Field Functions</u> .

Passive Scalar Properties

The properties **Secondary Gradients** and **Convection** are available with the <u>Segregated Flow</u> and <u>Coupled Flow</u> models. The property **SUPG** is available only with the <u>Viscous Flow</u> model.

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 <u>Convective Flux</u>.

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

Flow Boundary Diffusion

When On, enables diffusion of the passive scalar along flow boundaries. Disables diffusion when Off. The default is On.

SUPG

The Streamline-Upwind-Petrov-Galerkin advection stabilization term β_{SUPG} in Eqn. (1042). The default value is 1.0.

Materials and Methods

Molecular Diffusivity

Specifies the molecular diffusivity of the passive scalar.

Passive scalars use the Schmidt number function by default, which is useful for when you want the passive scalar to diffuse at a different rate from the fluid. Alternatively, you can specify a field function.

Method	Corresponding Method Node
Schmidt Number	Schmidt Number
	Provides the molecular Schmidt number σ in Eqn. (1919) and Eqn. (1920).

Turbulent Schmidt Number (for turbulent flows)

Specifies the turbulent Schmidt number σ_t in Eqn. (1919) and Eqn. (1920).

Initial Conditions

Passive Scalar

Sets the passive scalar initial condition. The amount of passive scalar can be set as a constant array profile or a composite array profile.

For single phase and Eulerian Multiphase Mixture Two-Phase Thermodynamic Equilibrium flows, initial values of passive scalars are set for physics continua. For Segregated Multiphase, VOF Multiphase, and Eulerian Multiphase Mixture N-Phase Mixture flows, initial values of passive scalars are set for each phase.

These values can also be set on a region when custom initial conditions are specified for the region (that is, the **Initial Condition Option** is set to **Specify Region Values**).

Boundary Settings

For flow boundaries, you can set the amount of passive scalar crossing the boundary as a simple value. For wall boundaries, a choice is presented between a simple value, zero flux, specified flux, and flux derivative.

Inflow and Outflow Boundaries

Passive Scalar

Sets the passive scalar profile.

For single phase flows, passive scalar profiles can be set for physics continua. For multiphase flows, passive scalar profiles can be set for each Eulerian phase and Lagrangian phase.

Wall Boundaries

Wall Passive Scalar Option

Defines whether you want to enter a scalar value or a flux for this condition.

Method	Corresponding Physics Value Nodes
Zero Flux Do not specify a value.	None.
Specified Value Specify a scalar value term.	Passive Scalar Specifies the passive scalar value for the boundary.
Specified Flux Specify a flux. Selecting this option adds the condition node <i>Wall Passive</i> Scalar Flux Derivative Option.	Passive Scalar Flux Specifies the passive scalar flux value for the boundary. The passive scalar flux value is the mass flux, not the volumetric flux.

Wall Passive Scalar Flux Derivative Option

This condition is available when the **Specified Flux** option is selected and allows you to specify a passive scalar flux derivative.

Specifying the derivative speeds up convergence. When the derivative is deactivated, oscillations occur in the passive scalar values near the wall and the solution does not converge fully.

Method	Corresponding Physics Value Nodes	
None	None.	
Specified	Passive Scalar Flux Derivative	
	Specifies the passive scalar flux derivative value for the boundary.	
	 If a field function which depends on the passive scalar value at the wall defines the passive scalar flux at the wall, define the passive scalar flux derivative using a field function. 	
	If a constant passive scalar flux, or a flux which is independent of the passive scalar value is defined at the wall, the passive scalar flux derivative is unnecessary.	

Region Settings

For single phase flows, region sources of passive scalars are set at the region level. For multiphase flows, region sources of passive scalars are set for each phase in the region.

Applies to fluid and porous regions.

Passive Scalar Source Option

Defines a passive scalar source within a region.

Method	Corresponding Physics Value Nodes
No Sources Active	None.
Mass Flux	Passive Scalar Source
	Source term setting for the passive scalar, specified as a mass flux.
	This value is S_ϕ in Eqn. (1918). It is entered as a scalar array profile. Include the phase volume fraction explicitly for an Eulerian or Lagrangian phase.
	Passive Scalar Source Derivative
	Specifies the derivative of each component of the passive scalar source regarding the corresponding passive scalar component. This value is S_{ϕ_j} in Eqn. (1918).
	The derivative of the user source term is used to linearize <u>Eqn. (1918)</u> . Its value is set to zero by default. Providing a value for the derivative helps stabilize the solution, assuming that the source is set by a differentiable equation. It is entered as a scalar array profile.
Scalar Flux with Inferred Density	Passive Scalar Source
	Source term setting for the passive scalar, automatically using the density of the material composing the phase.
	This value is S_ϕ in <u>Eqn. (1918)</u> . It is entered as a scalar array profile. Include the phase volume fraction explicitly for an Eulerian or Lagrangian phase.
	Passive Scalar Source Derivative
	Specifies the derivative of each component of the passive scalar source, as described above.

Passive Scalar Anisotropic Diffusion Option

Applies to fluid regions associated with a porous phase and porous regions.

Enable Anisotropic Diffusion for Passive Scalars	Corresponding Physics Value Nodes
Off	None.
On Allows passive scalars to diffuse anisotropically through porous media.	Passive Scalar Anisotropic Diffusion Allows you to specify the anisotropic diffusion components for each scalar that is defined under [physics continuum] > (and then)Models > (and then)Passive Scalar > (and then)Passive Scalars and has Transport set to Diffusion only or Convection and Diffusion. You use the Anisotropic Diffusion Tensor subnode to specify the diffusion scaling tensor using the standard profile methods. Orthotropic Tensor is the default.

Passive Scalar Solver Properties

The passive scalar solves a transport equation, <u>Eqn. (1918)</u>, for each passive scalar defined in the simulation.

Under-Relaxation Factor

At each iteration, governs the extent to which the new solution replaces the old one. The default value is 0.8. For the theoretical background, see <u>Eqn. (923)</u> in "Implicit Iteration."

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.

Field Functions

Boundary Passive Scalar Flux of <passive scalar>

The rate per unit area at which a passive scalar quantity flows across a boundary.

Diffusion Coefficient of <passive scalar>

Diffusion coefficient of a particular passive scalar material, relating the diffusive transport of the material to the gradient. It has units of mass/length/time.

Diffusivity of <passive scalar>

Diffusivity of a particular passive scalar material, giving the rate at which it diffuses into another material. It has units of length²/time. This field function is activated only when you select the Laminar viscous option. This can use the Schmidt number method or a field function.

<Passive Scalar>

The field function object that corresponds to a particular passive scalar material. This object makes the passive scalar available as a field function.

Turbulent Schmidt Number of <passive scalar>

Turbulent Schmidt Number of a particular passive scalar material. This field function is activated only when you select the turbulent viscous option. This can be a constant or a field function.