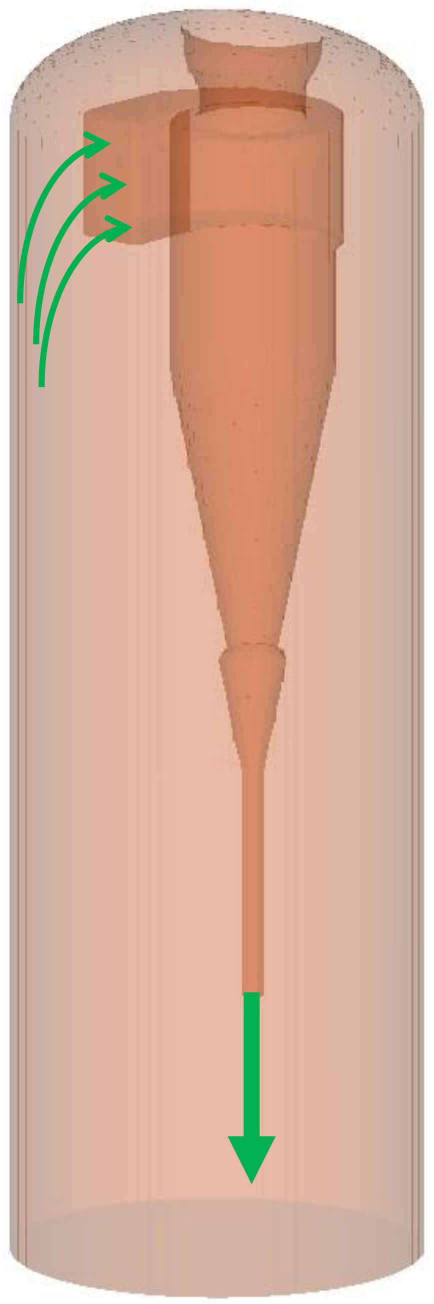
New Features in Barracuda

Overview and Selected Examples

Selected New Features

- **Boundary Condition (BC) Connections**
- **Drag models: user-defined expressions, drag multiplier tables**
- **Baffles**
- **Chemistry: distribution of heat of reaction**, **age factor,** catalyst deactivation, table-based rate coefficients
- **Solver options (run window)**
- **Save Case As**
- Area specification for injection BCs

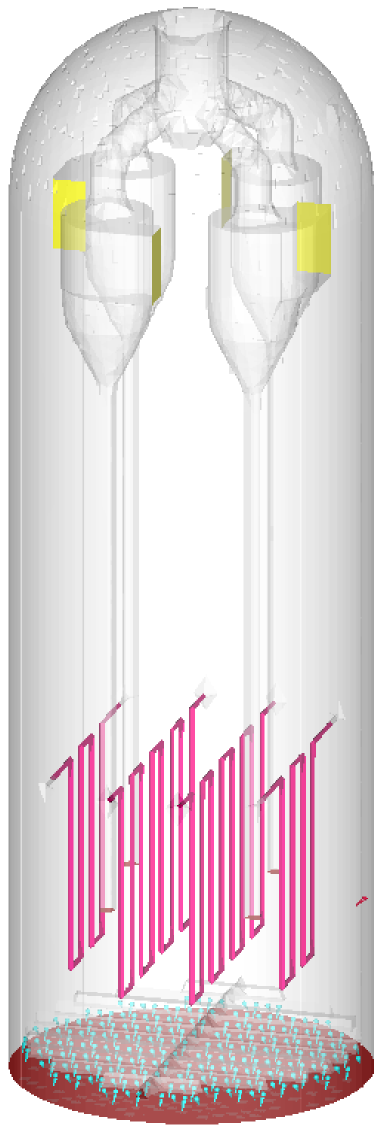
BC Connections



BC Connections

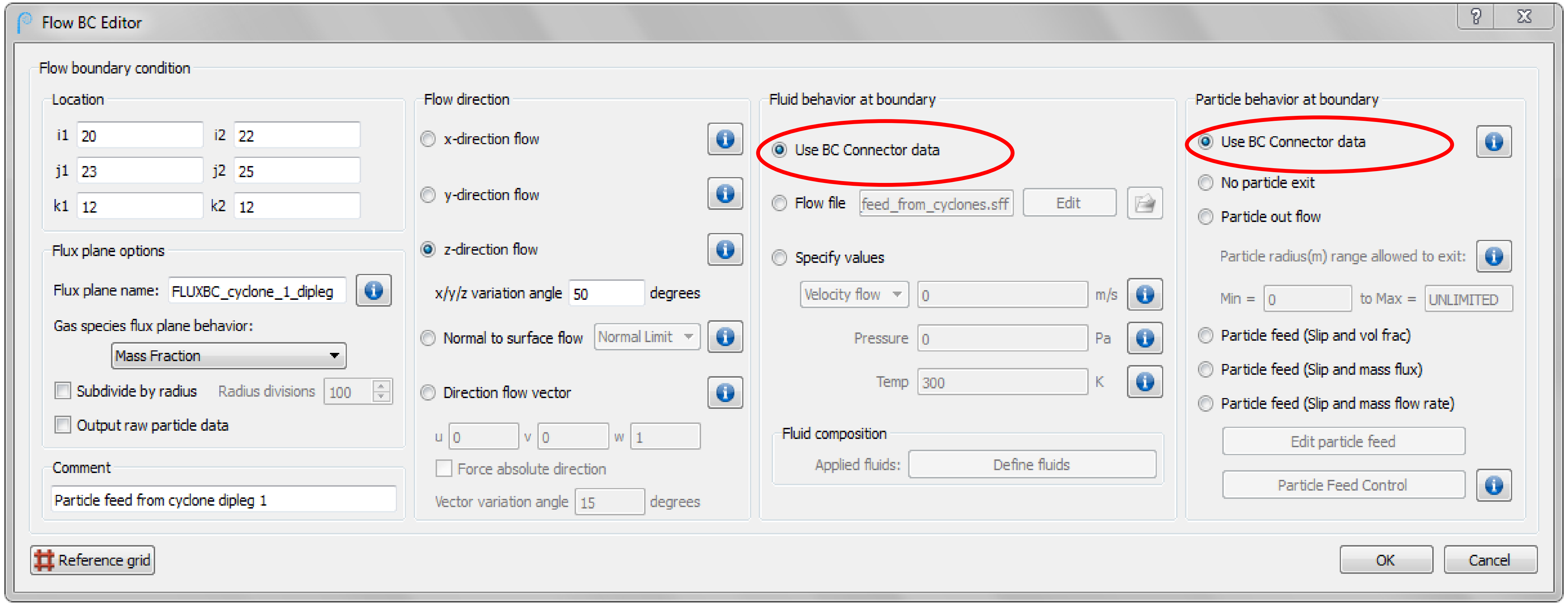
- Used to recycle materials (fluid and/or particles) from an **outlet** BC to an **inlet** BC.
- **Internal recycle** – cyclone/dipleg combinations
- **External recycle**
- **Submodels** – ability to maintain material within the computational domain
- Capability to combine with an exterior input (i.e. carrier gas, solids makeup)
- Many different options for particle and fluid control

BC Connections – Example Setup



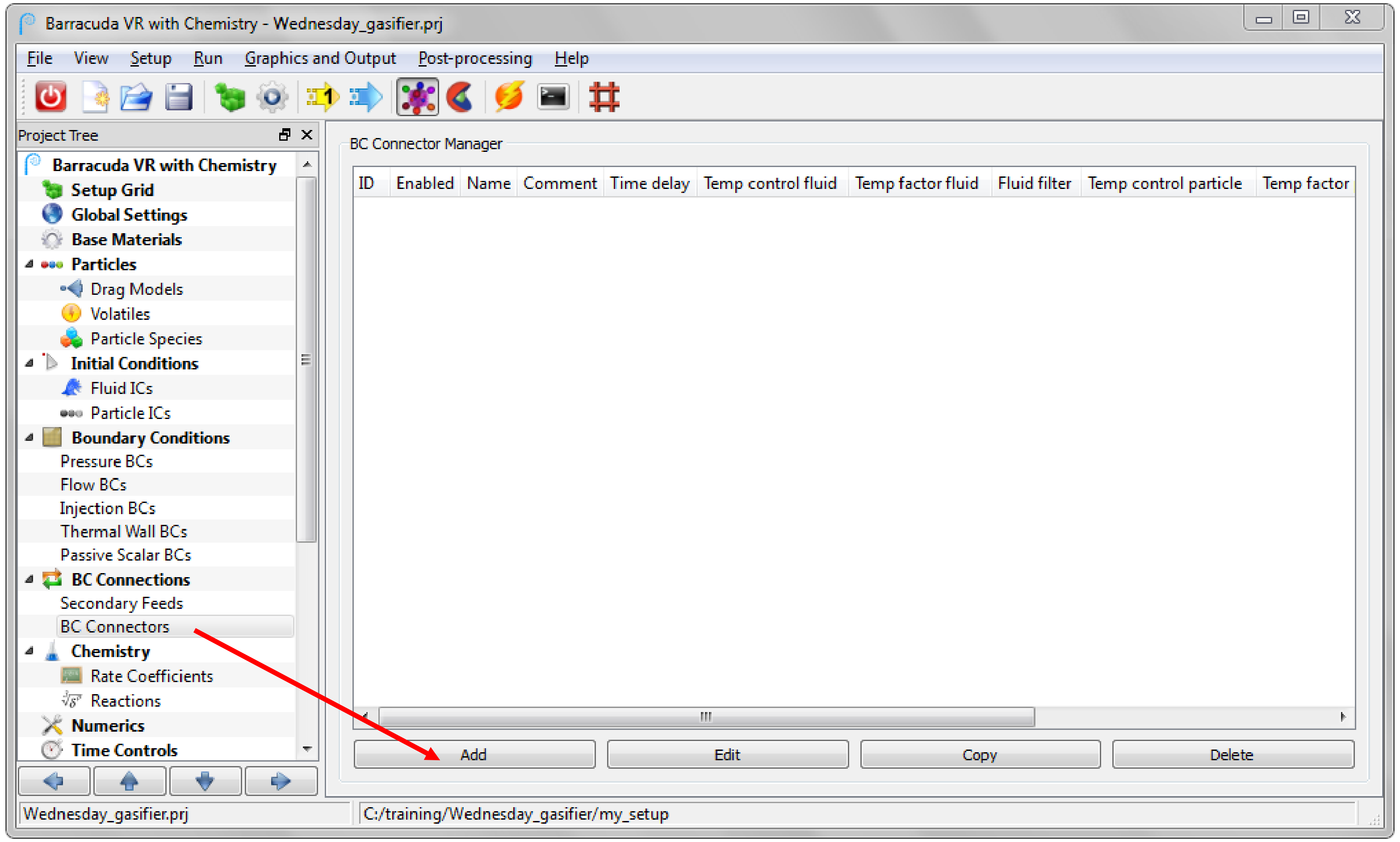
- Wednesday gasifier from Barracuda training (coal gasification unit with internal cyclone/diplegs)
- Previously, entrained coal and char particles were returned to the unit through overall mass control or simple control loop. Particle and gas properties were estimated.
- BC connectors allow recycle of exact particles and gas – improved simplicity, accuracy, and control.

BC Connections – Example Setup (continued)



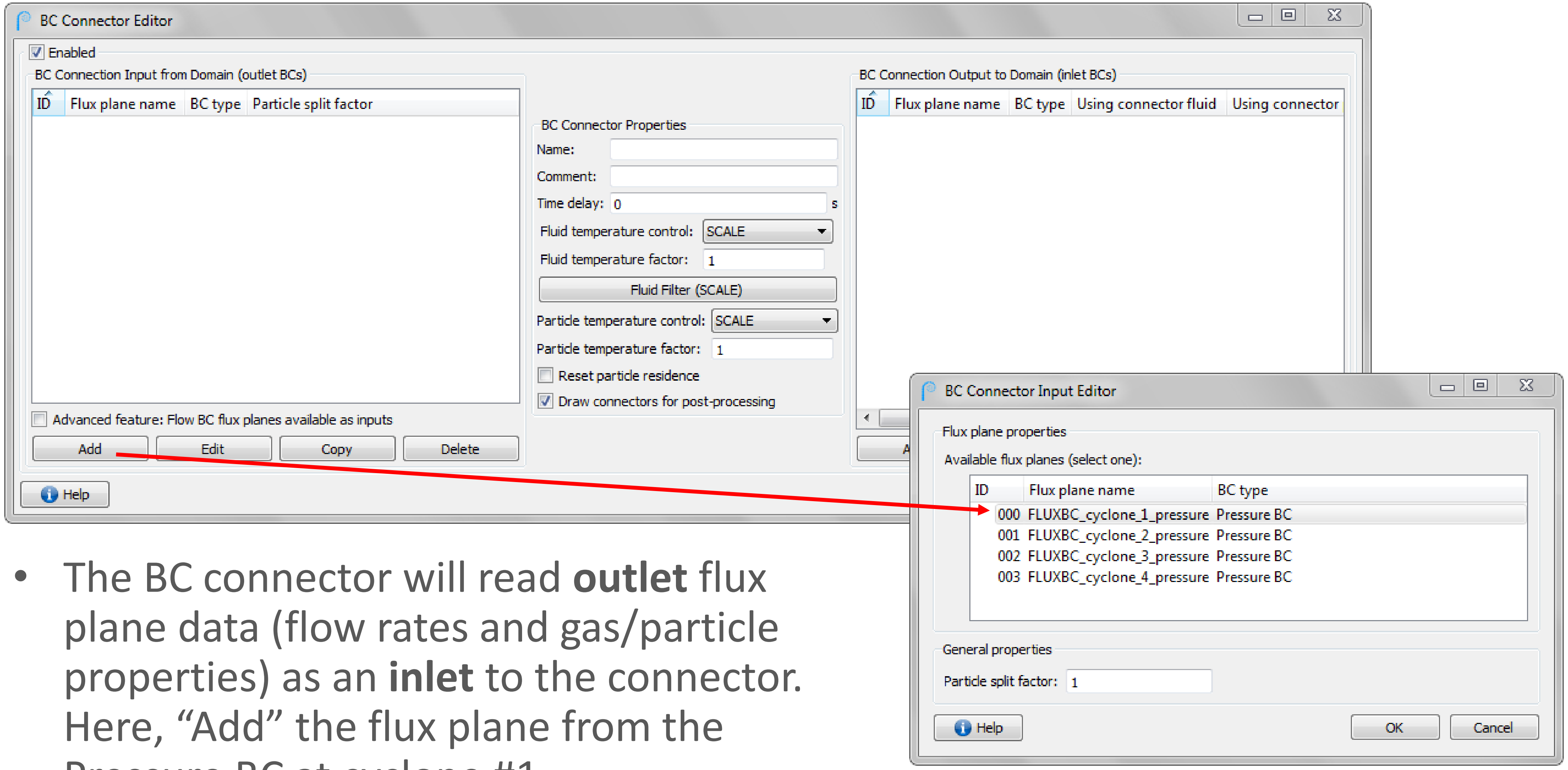
- Flow BC for dipleg – set up the geometry as normal. For fluid and particle behavior at boundary, select new option “Use BC Connector data”.

BC Connections – Example Setup (continued)



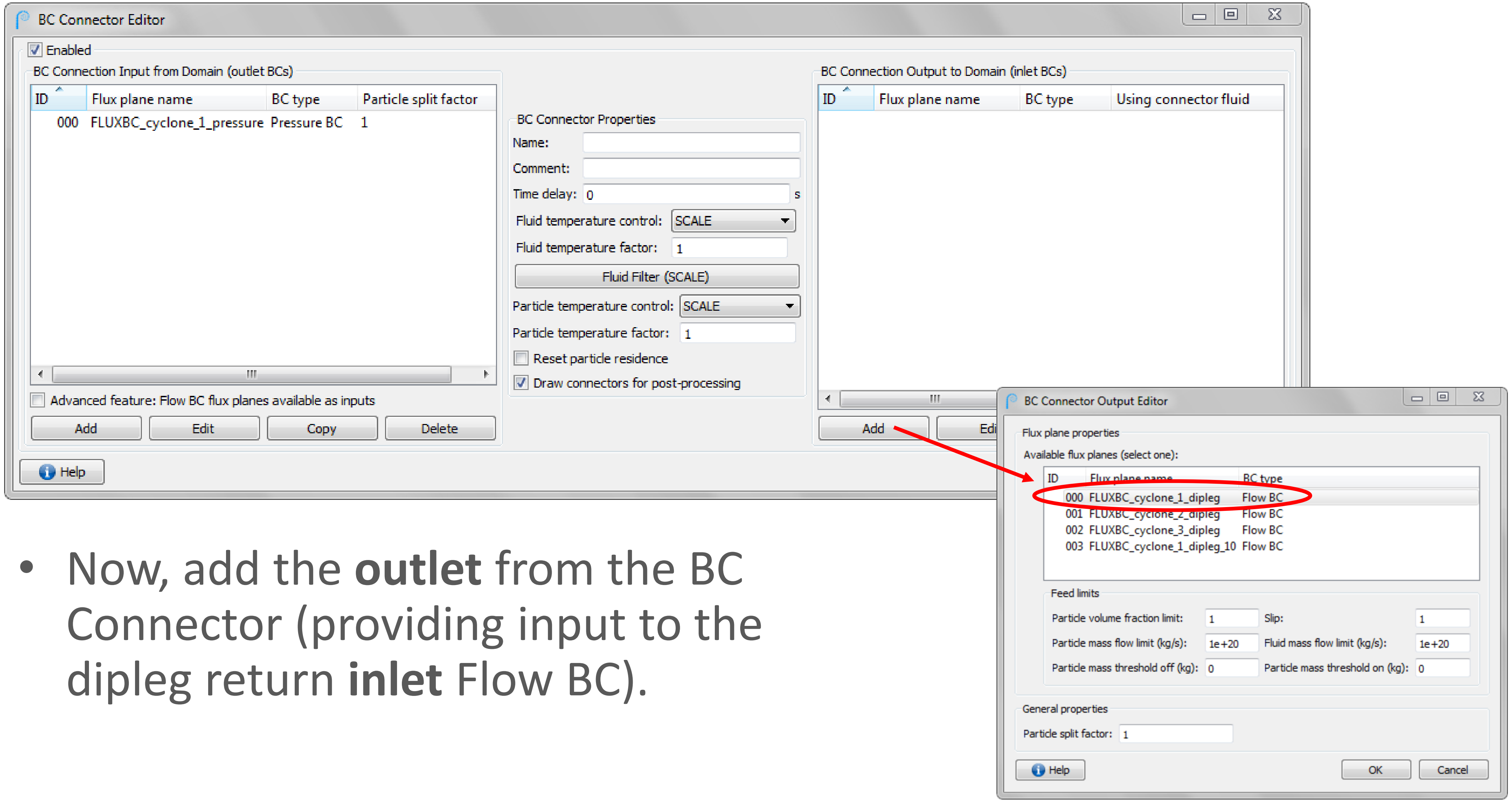
- Add a new BC Connector to simulate the dipleg return.

BC Connections – Example Setup (continued)



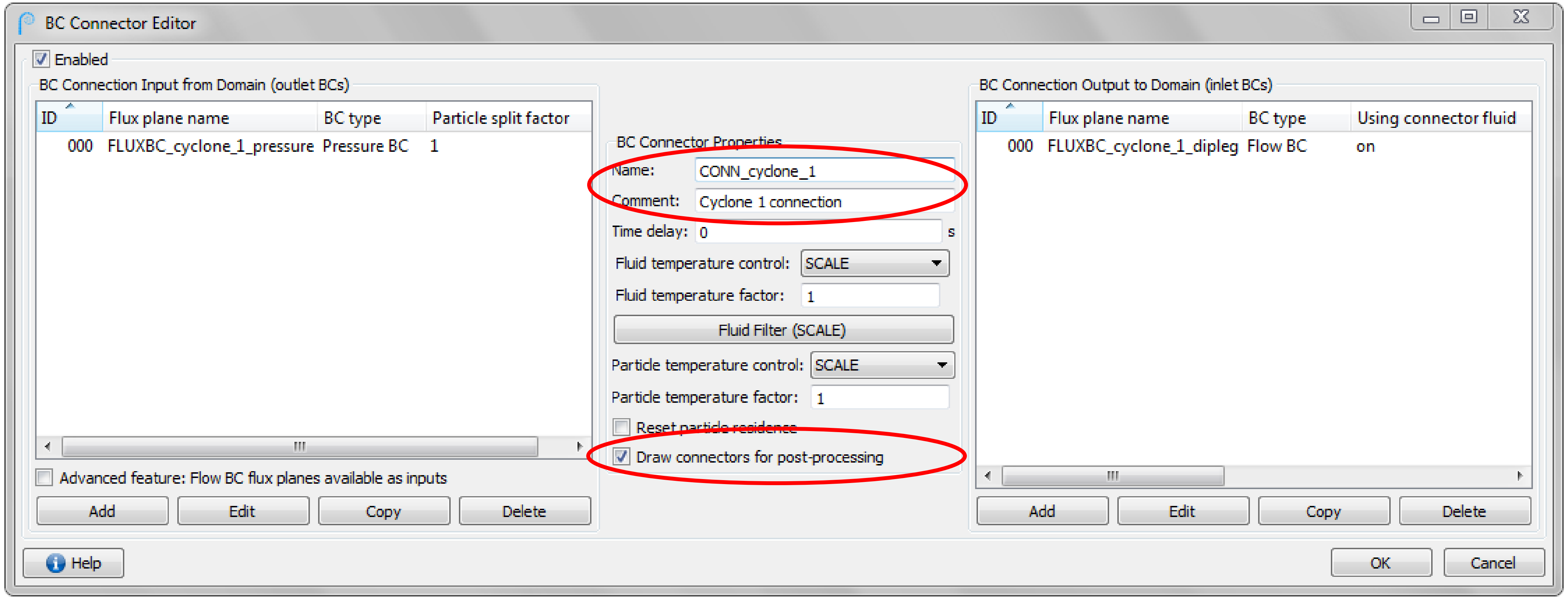
- The BC connector will read **outlet** flux plane data (flow rates and gas/particle properties) as an **inlet** to the connector. Here, “Add” the flux plane from the Pressure BC at cyclone #1.

BC Connections – Example Setup (continued)



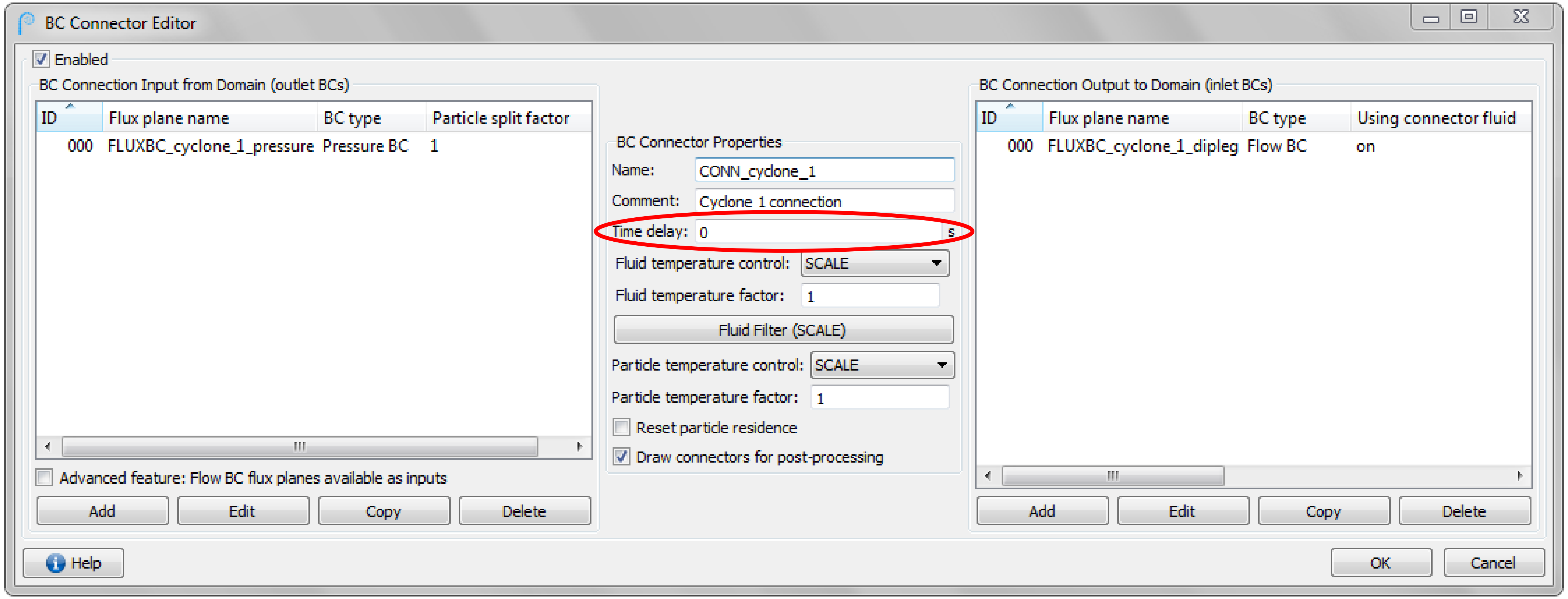
- Now, add the **outlet** from the BC Connector (providing input to the dipleg return **inlet** Flow BC).

BC Connections – Example Setup (continued)



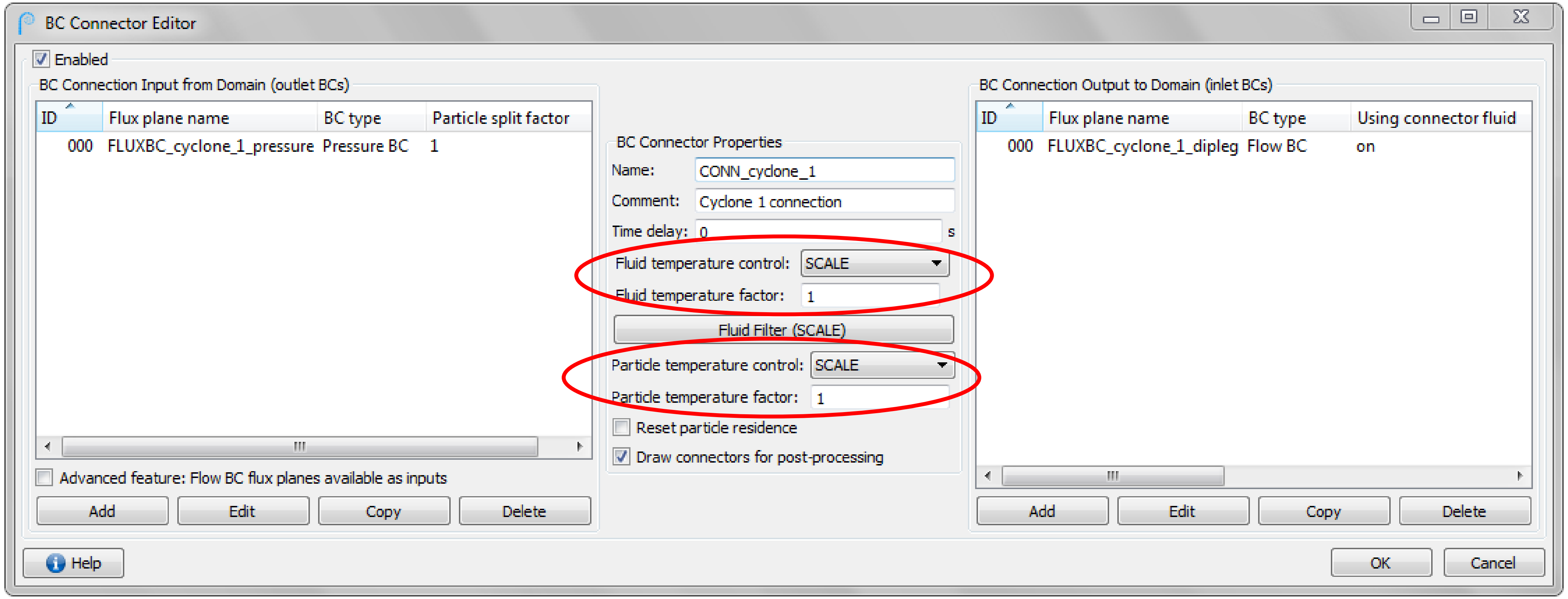
- In the center of the dialog, define a **Name** (which will be the name of the flux plane file for the BC Connection) and an optional **Comment.**
- "Draw connector for post-processing" allows the connections to be seen in Run => View Boundary Conditions.

BC Connections – Other Options



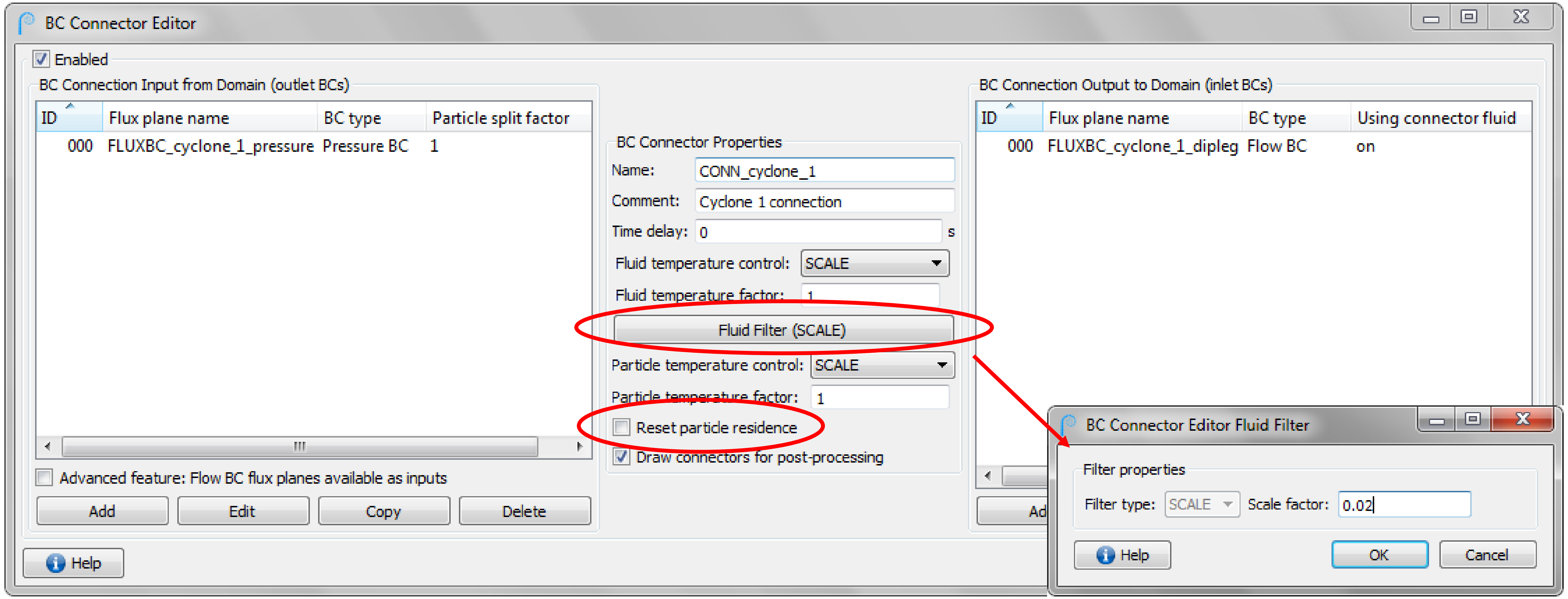
- **Time delay** specifies an interval before materials are returned to the system through the BC Connector outlet.

BC Connections – Other Options (continued)



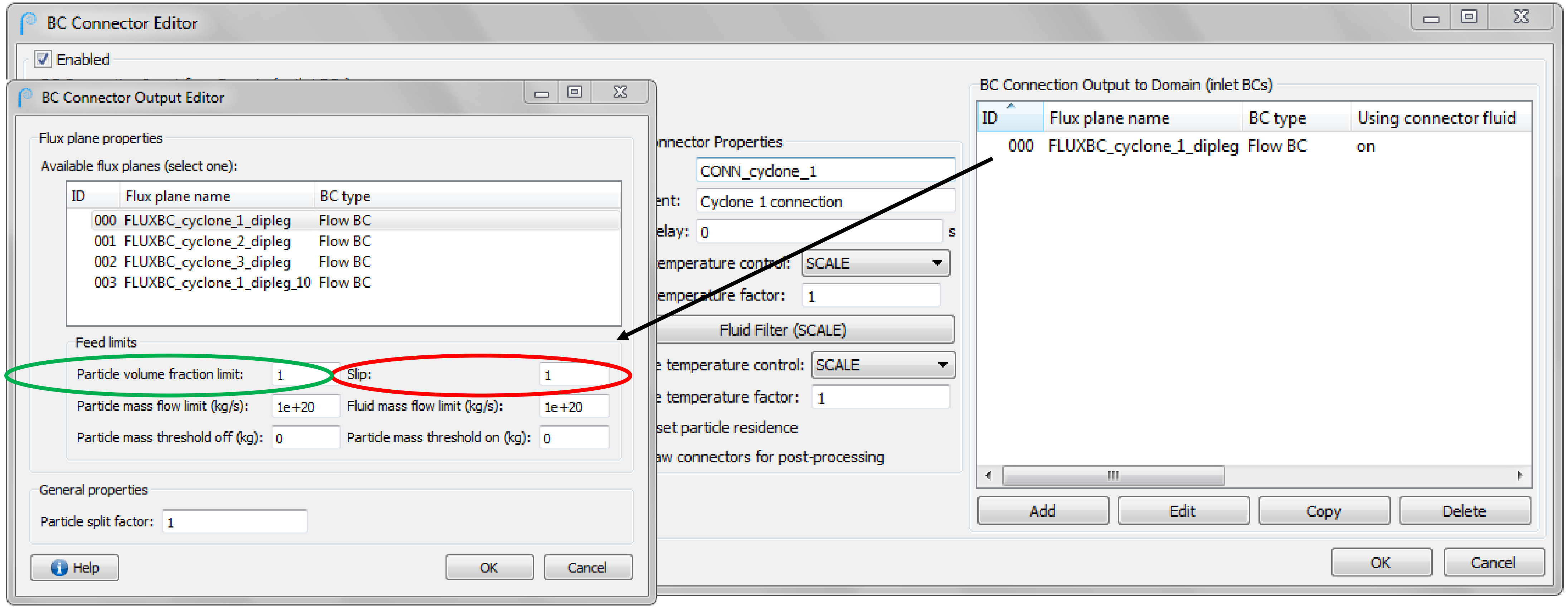
- **Fluid temperature control** allows the user to **scale** (multiply) the incoming fluid temperature by the temperature factor, **set** the outgoing fluid temperature to the temperature factor, or **offset** (add or subtract) the incoming fluid temperature by the temperature factor.
- Can perform similar operations independently for temperature of particles.

BC Connections – Other Options (continued)



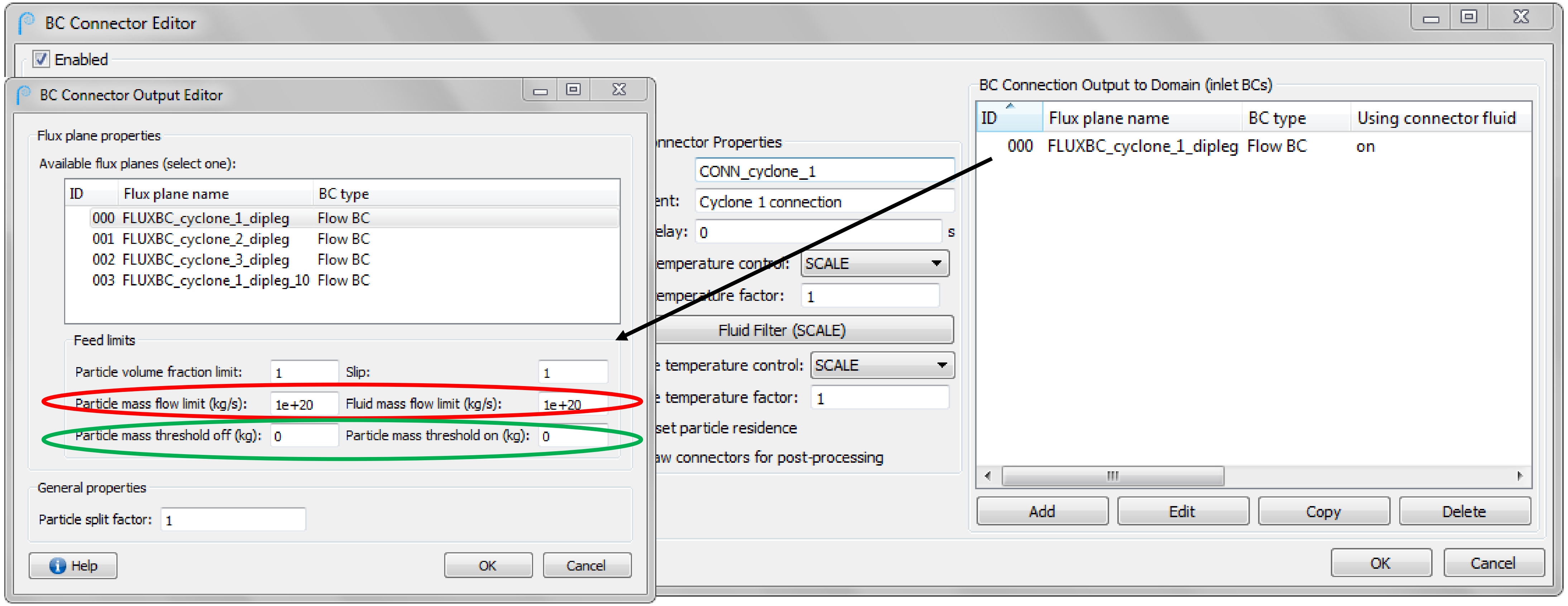
- The **Fluid Filter** allows the user to return only a portion of the outgoing gas (a very common application). Here, the fluid filter is set to return 2% of the exiting gas through the dipleg.
- **Reset particle residence** can be selected to track freshly recycled particles. Otherwise, particles "remember" their residence time from being previously in the domain.

BC Connections – Other Options (continued)



- In the Output Editor, the user can set **Slip** to increase (>1) or decrease (<1) particle speed relative to fluid speed.
- The user can decrease the **Particle volume fraction limit** to limit particle feed to packed cells. For example, if the volume fraction limit is set to 0.4, particles will not be fed to a cell beyond 40% of the total cell volume. This limit can promote smoother overall particle feed.

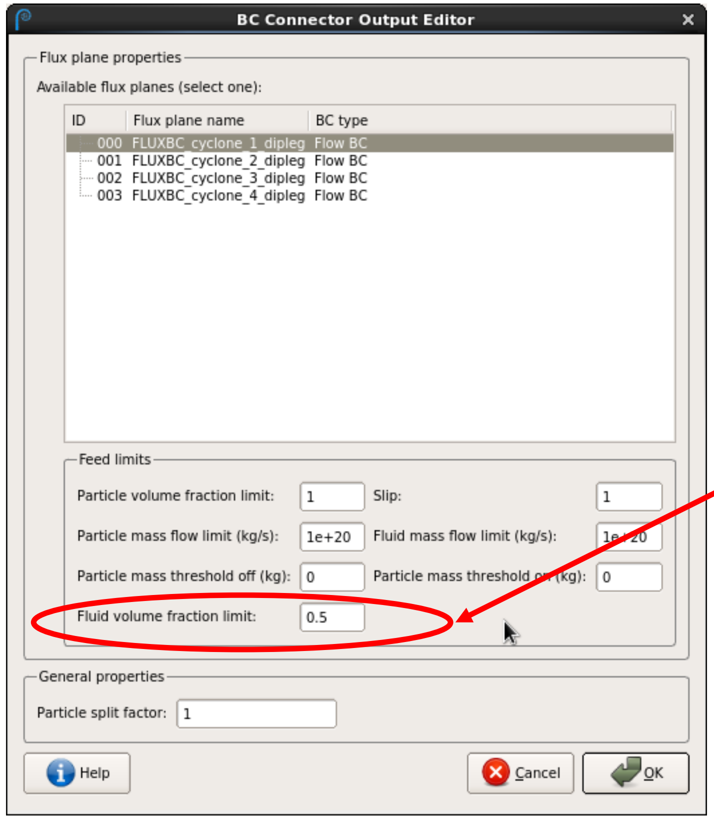
BC Connections – Other Options (continued)

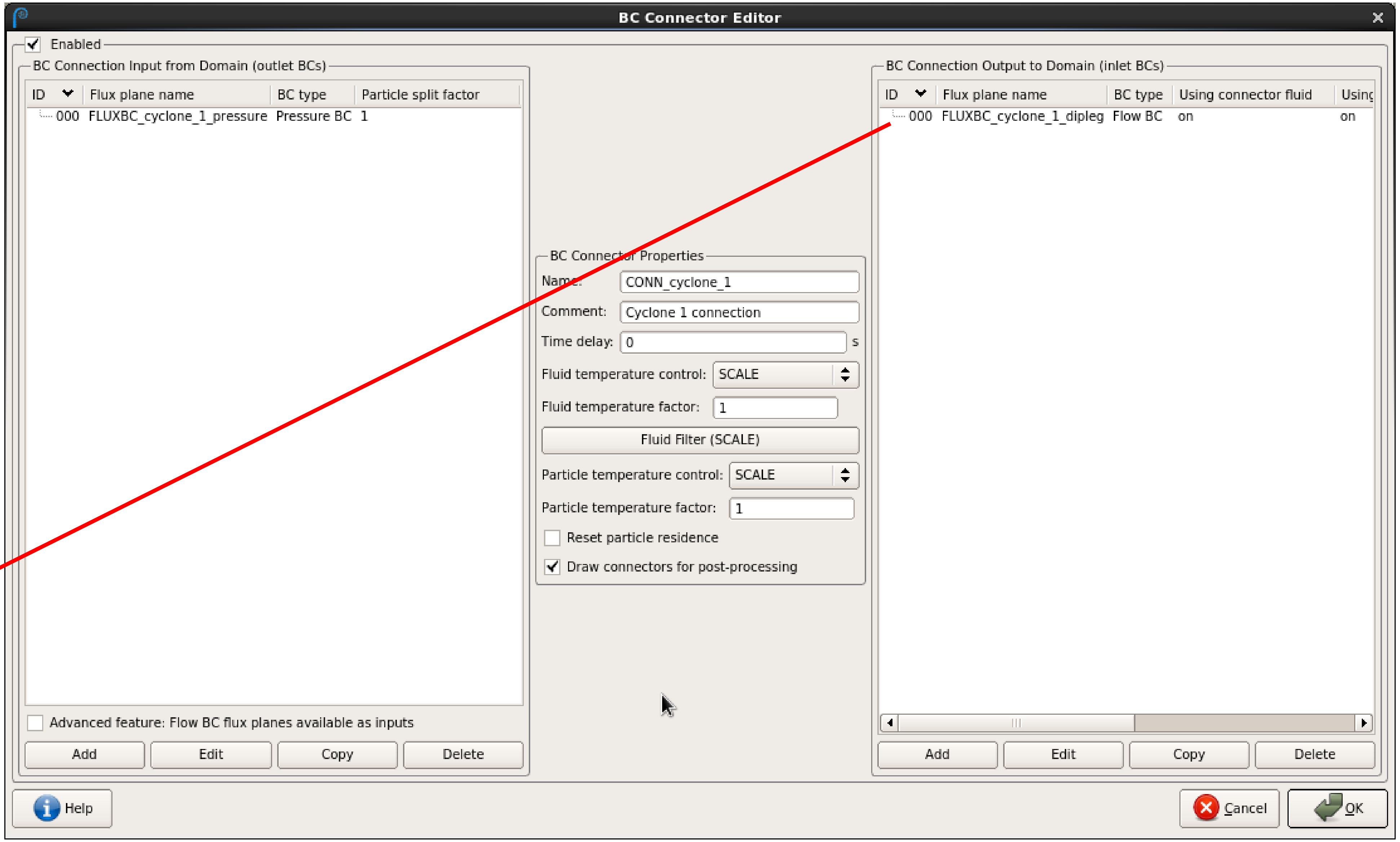


- In the Output Editor, the user can limit total flow of fluid and/or particles (red). Default limits are very high, allowing unlimited flow.
- User can also set on/off mass thresholds (green). Typical example: flapper valve on secondary dipleg for intermittent release – flow commences when a certain mass accumulates in the dipleg.

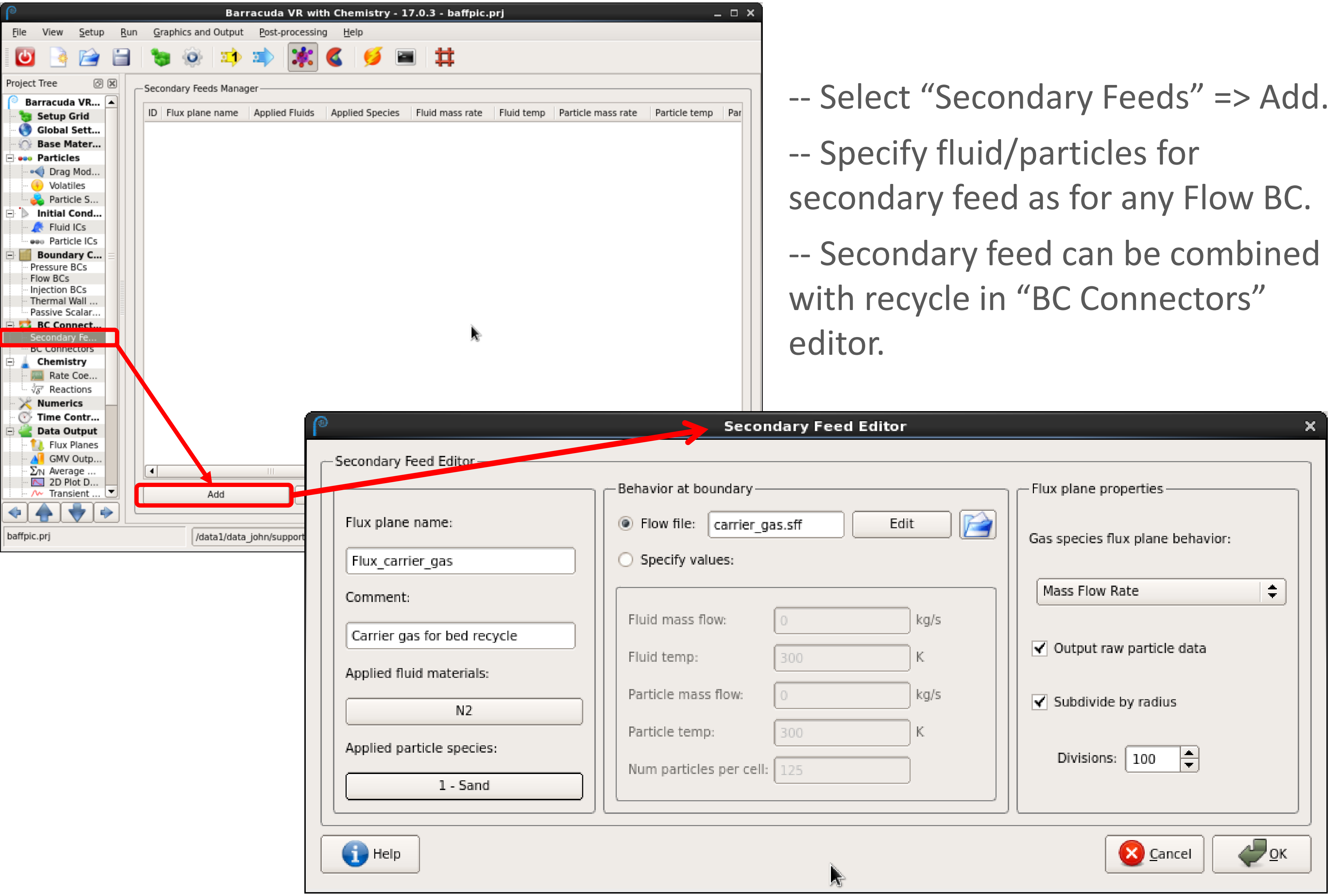
BC Connections – Other Options (continued)

- The **Fluid volume fraction limit** allows the fluid return to be scaled to the rate of particle return. In this example, fluid will be returned at a maximum volume fraction of 0.5; this might be a realistic representation of dense dipleg particle return.





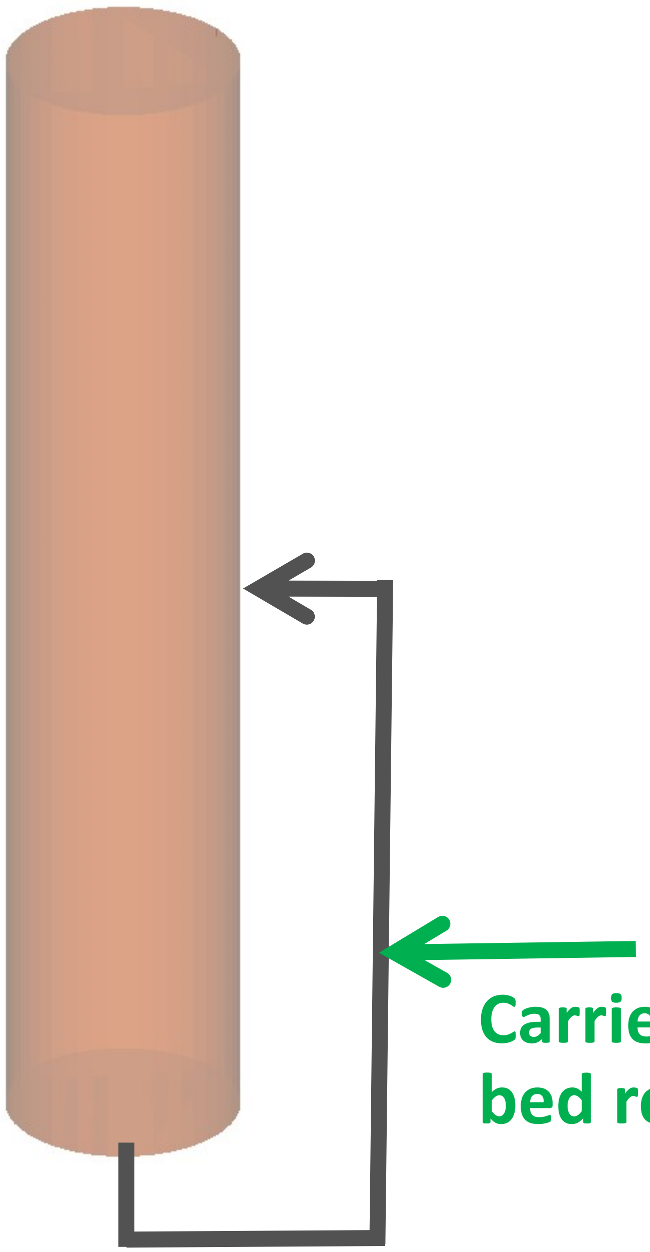
BC Connections – Secondary Feeds



-- Select “Secondary Feeds” => Add.

-- Specify fluid/particles for secondary feed as for any Flow BC.

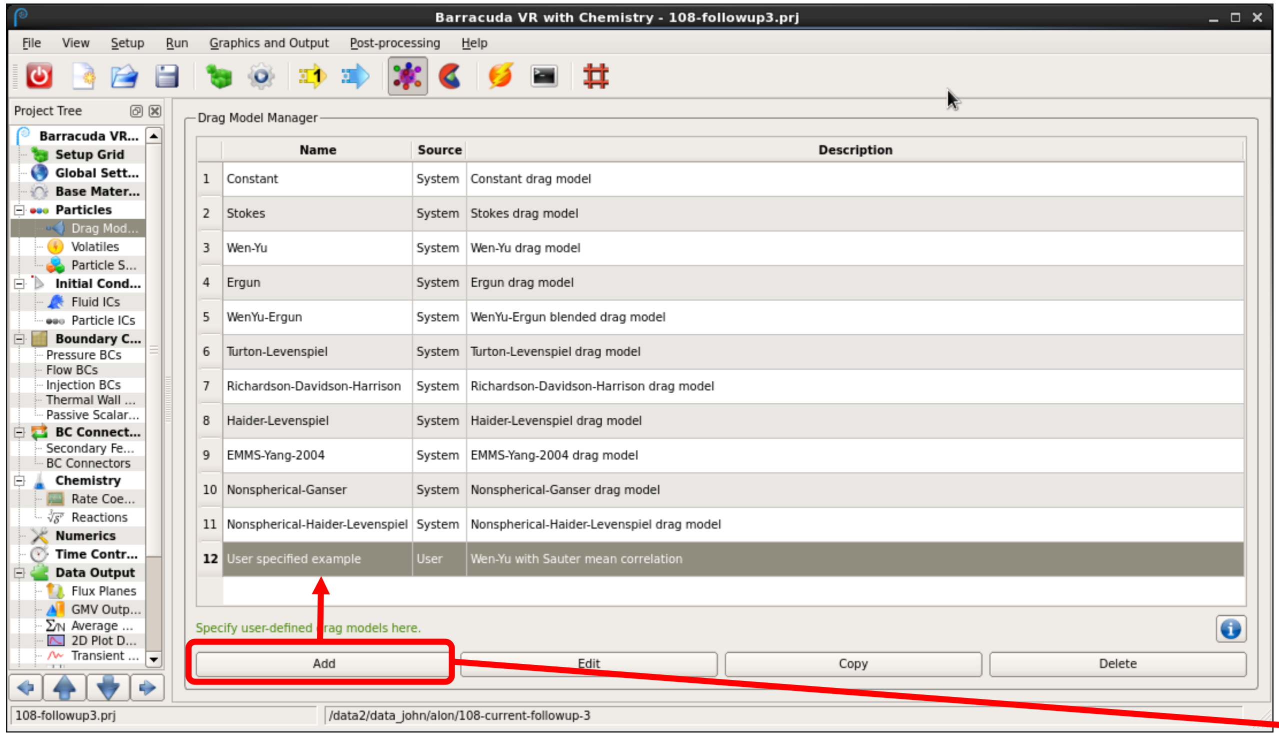
-- Secondary feed can be combined with recycle in “BC Connectors” editor.

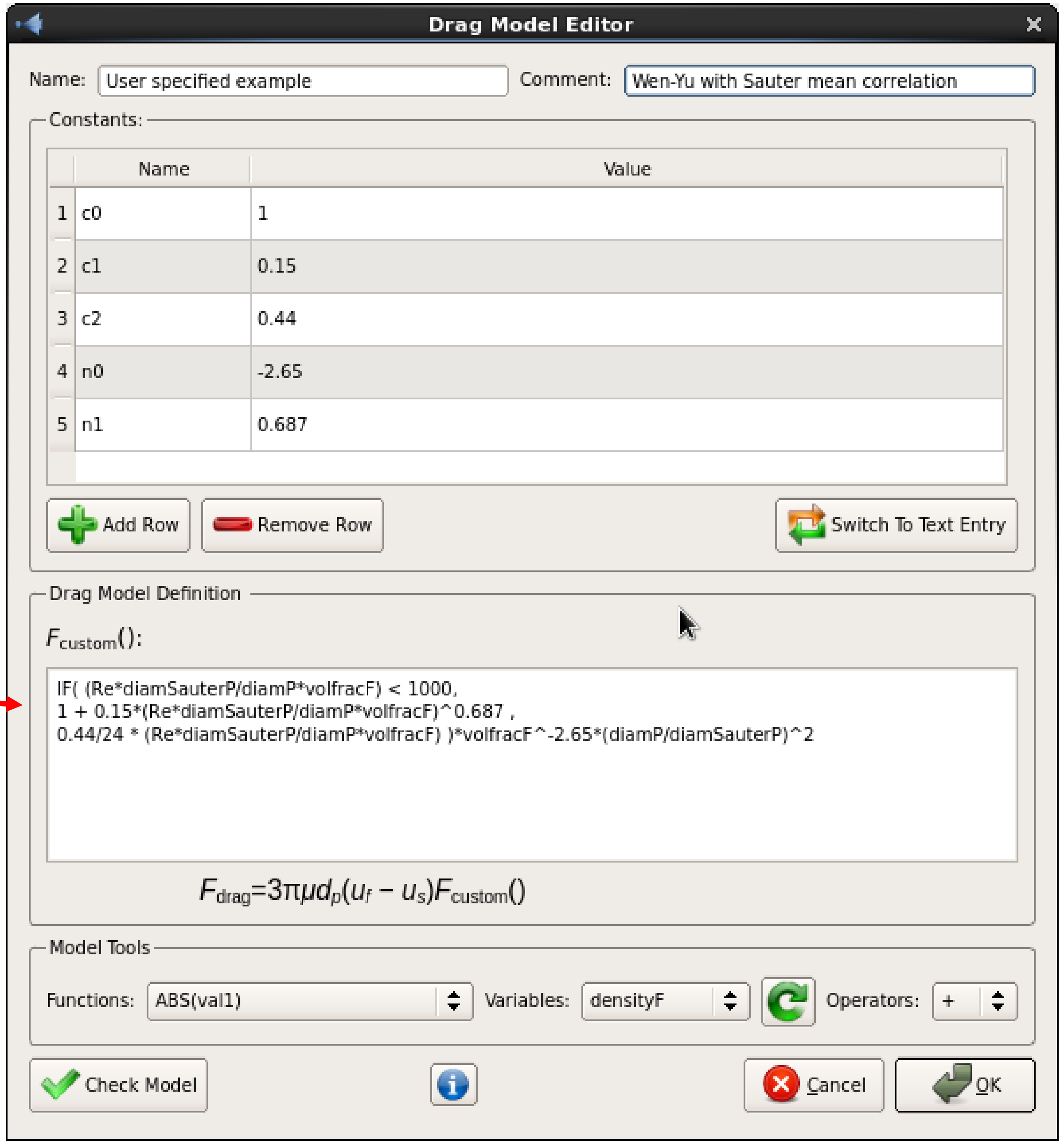


Carrier gas for bed recycle

Enhancements to Drag Models

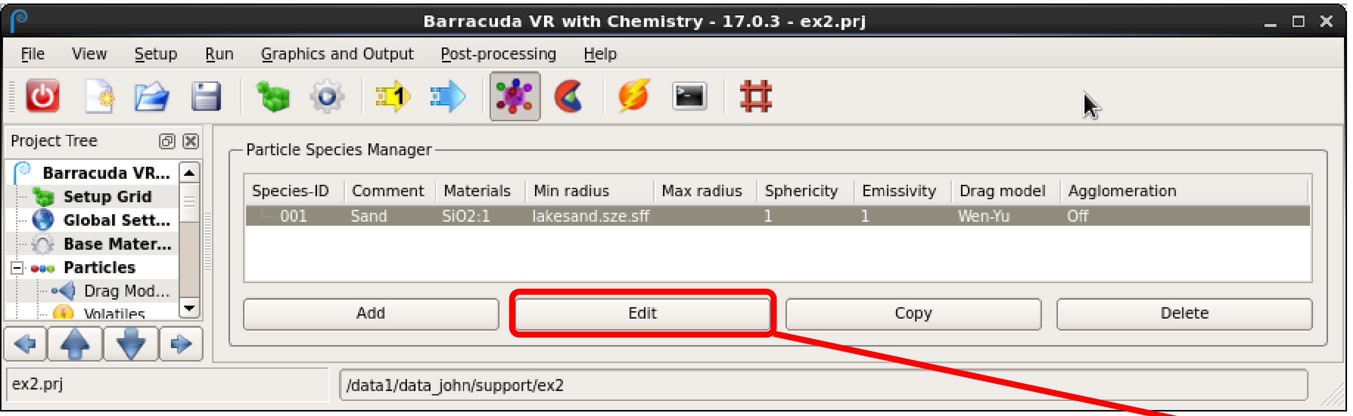
User-Defined Drag Models

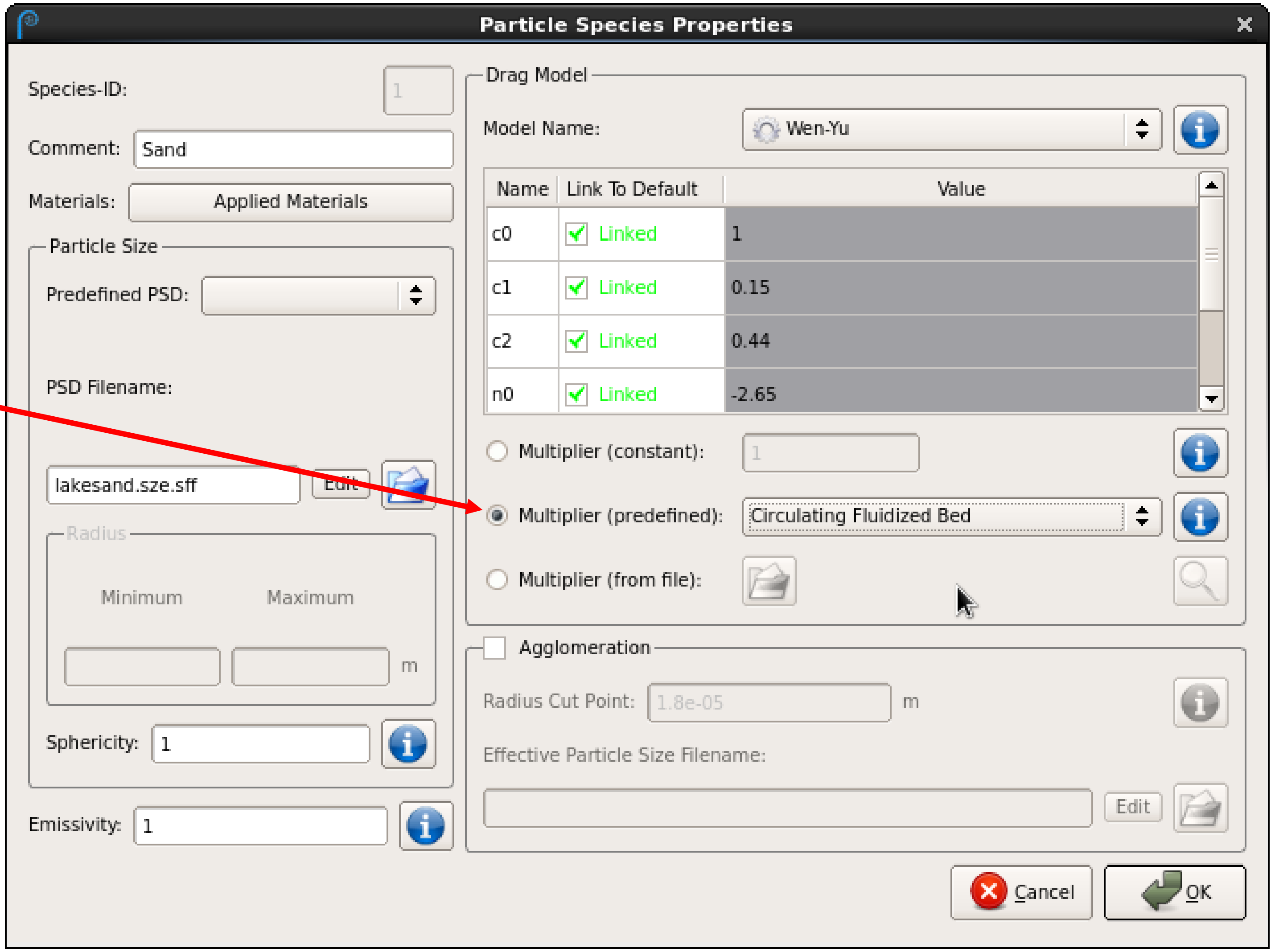




Drag model editor includes parsing of user-defined expressions. Functions, variables, and operators can be selected from "Model Tools" section at bottom.

Predefined Drag Multipliers



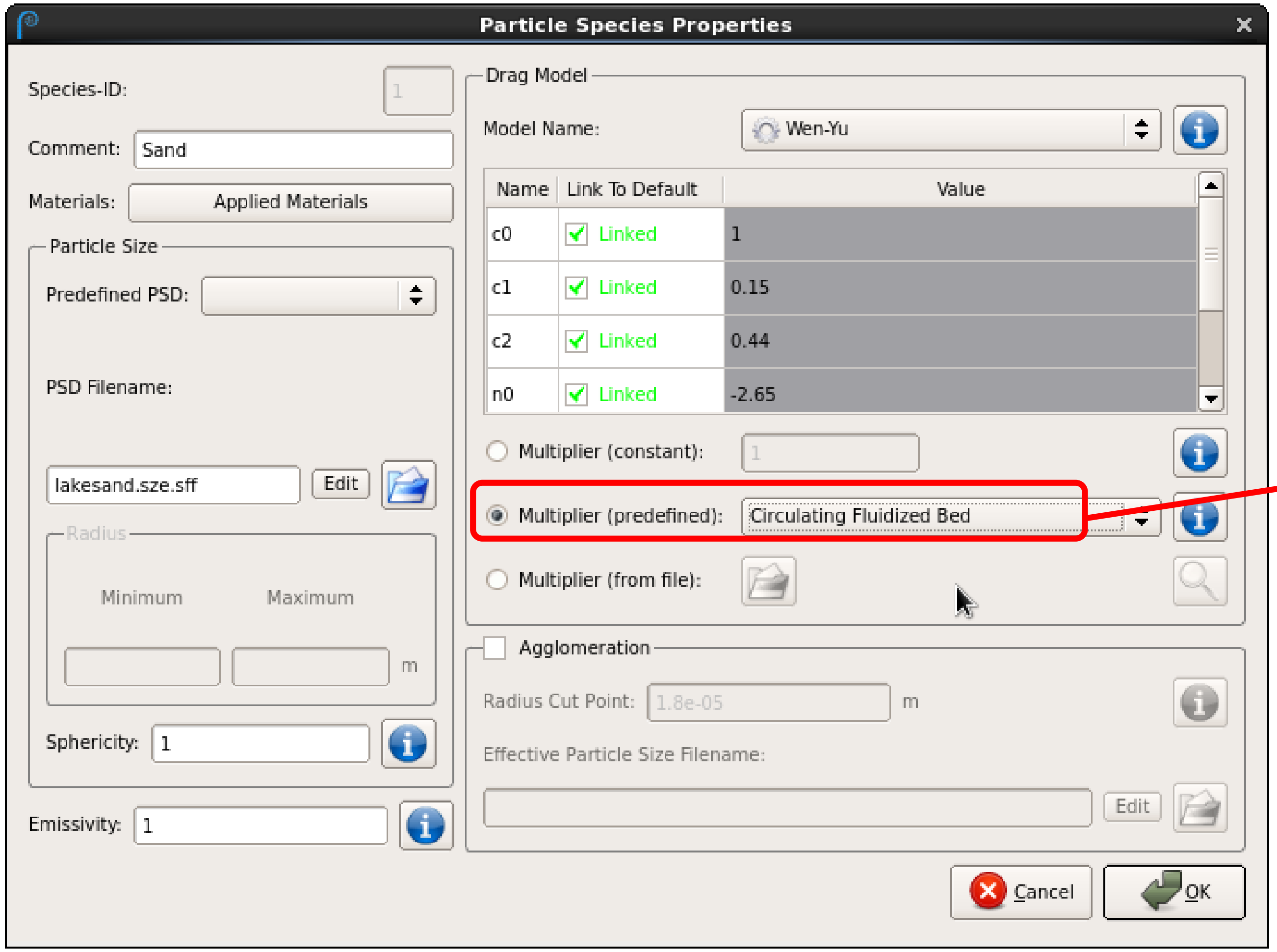


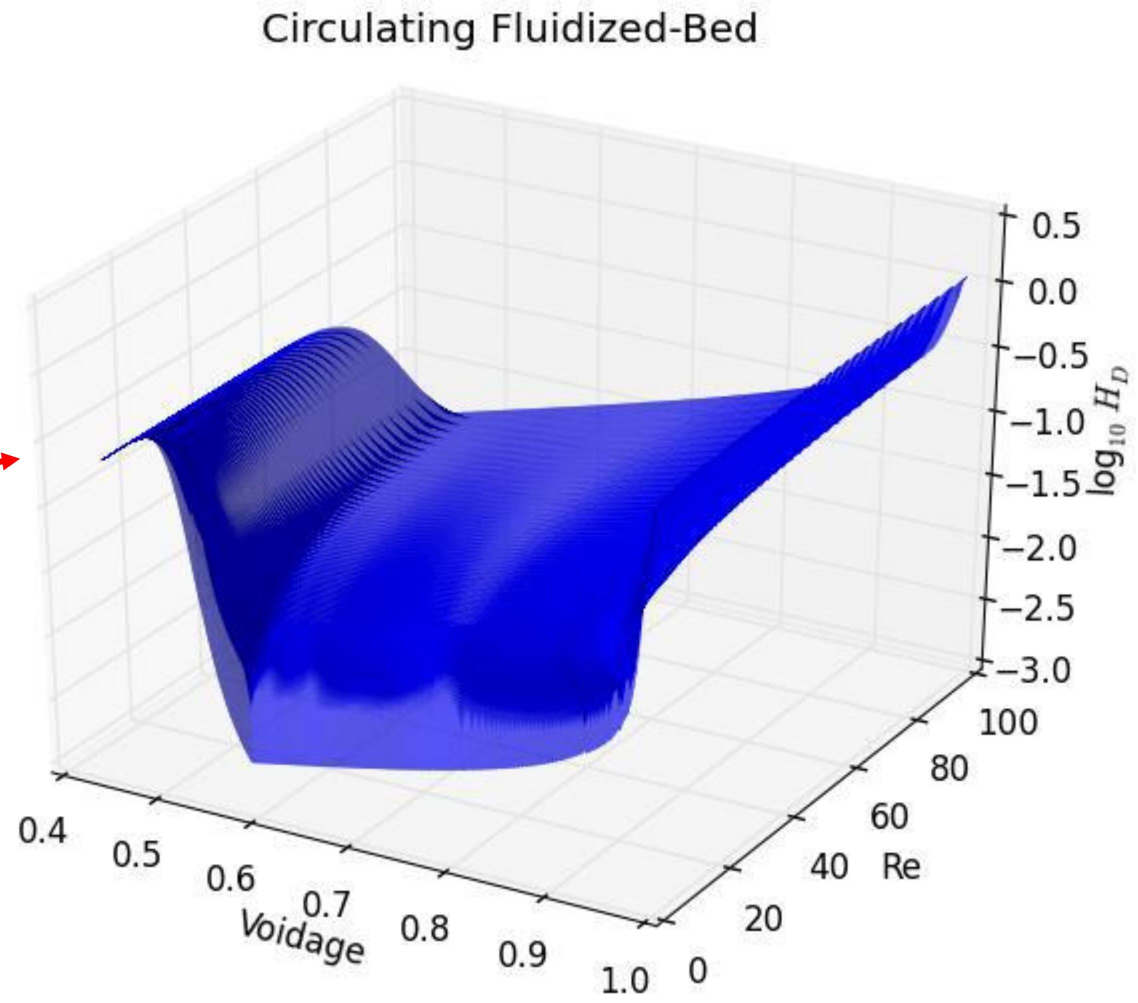
-- Predefined drag multipliers are available for a set of typical fluidized bed hydrodynamic regimes.

-- Selection of the predefined multiplier generates a text table of drag ratios based on the energy minimization multi-scale (EMMS) method.

-- The multiplying factors are applied to the base **Wen-Yu** drag model.

Predefined Drag Multipliers (continued)





-- Drag multiplier values have been generated as a function of voidage and Reynolds number (particle slip velocity).

-- Stored as a .txt table for use as the simulation runs.

-- CPFD also has the capacity to generate custom drag coefficient tables for user-defined conditions, using the EMMS software.

Baffles

Baffles (continued)

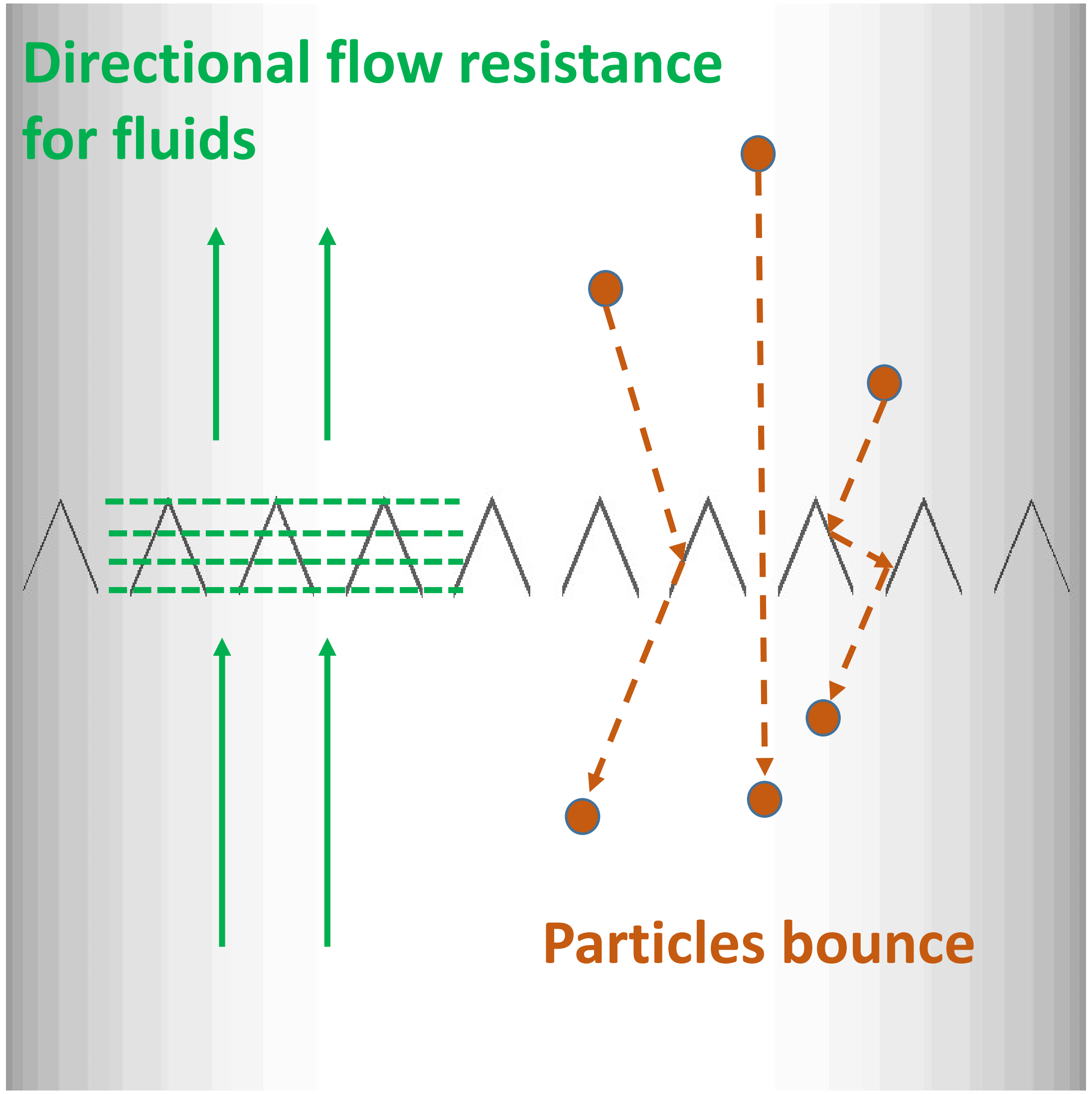
-- Baffles are zero-thickness ***subgrid*** structures that can affect fluid and particle flow. They do not need to be resolved by the grid as regular geometry.

-- ***Fluids*** can experience flow resistance (pressure drop) through application of a k-factor. The k-factor can be specified independently in the x-, y-, and z-directions. *Note: if no k-factor is specified, the fluid is not affected by the baffle.*

-- Pressure drop is a function of k-factor:

$$\Delta P = \frac{1}{2} k \rho v^2$$

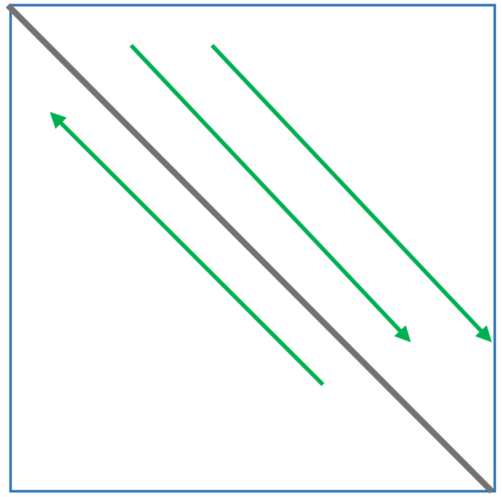
-- ***Particles*** interact with baffles as if they are solid walls.



Baffles (continued)

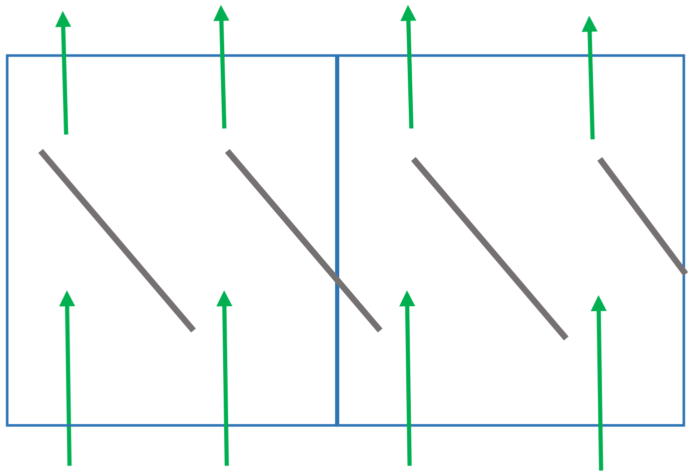
What baffles do not do

-- Baffles do not fully split cells (as thin walls); all the fluid within the cell experiences the same forces and thermal/chemical effects.

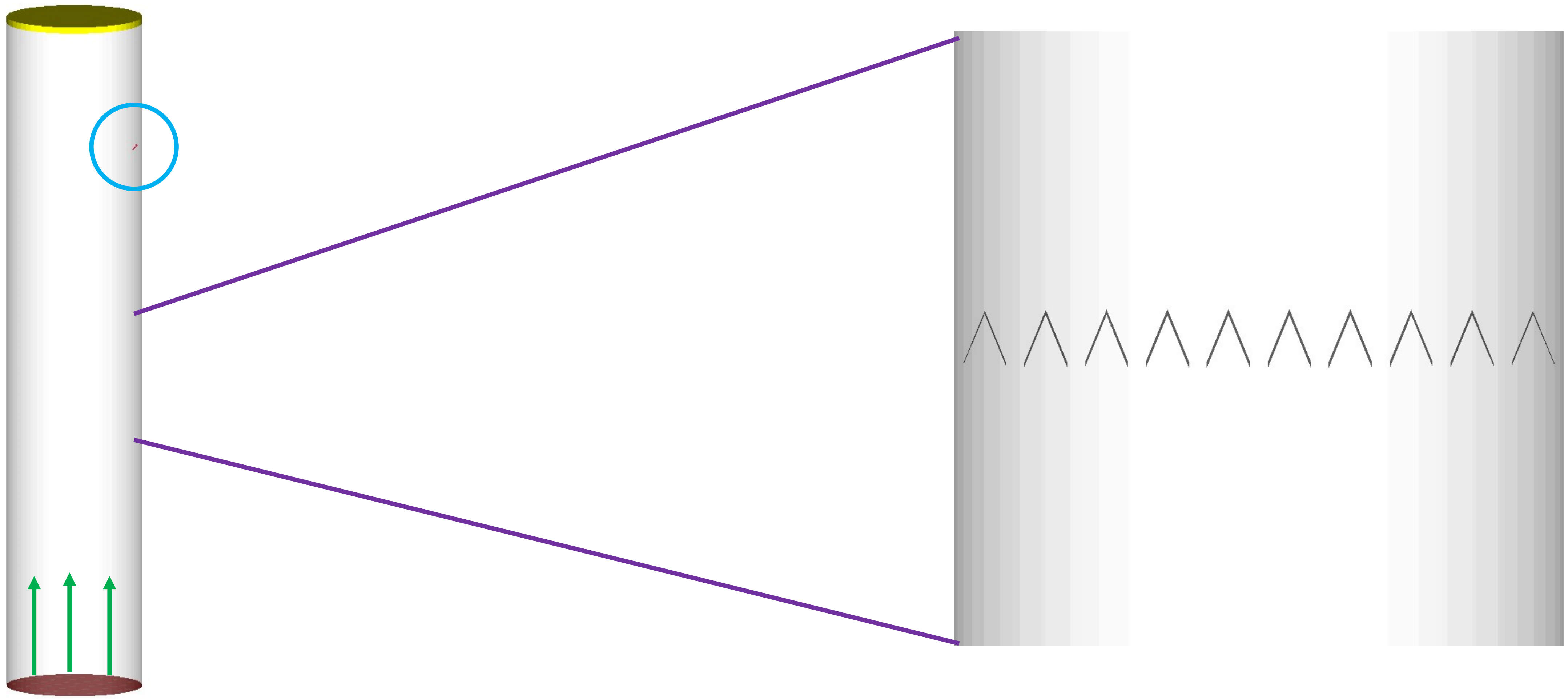


Fluid flow in opposite directions on either side of baffle – not possible

-- The direction of flow is not directly altered by the baffle surface; however, directional flow resistance and particle-fluid drag can act ***indirectly*** to change flow.



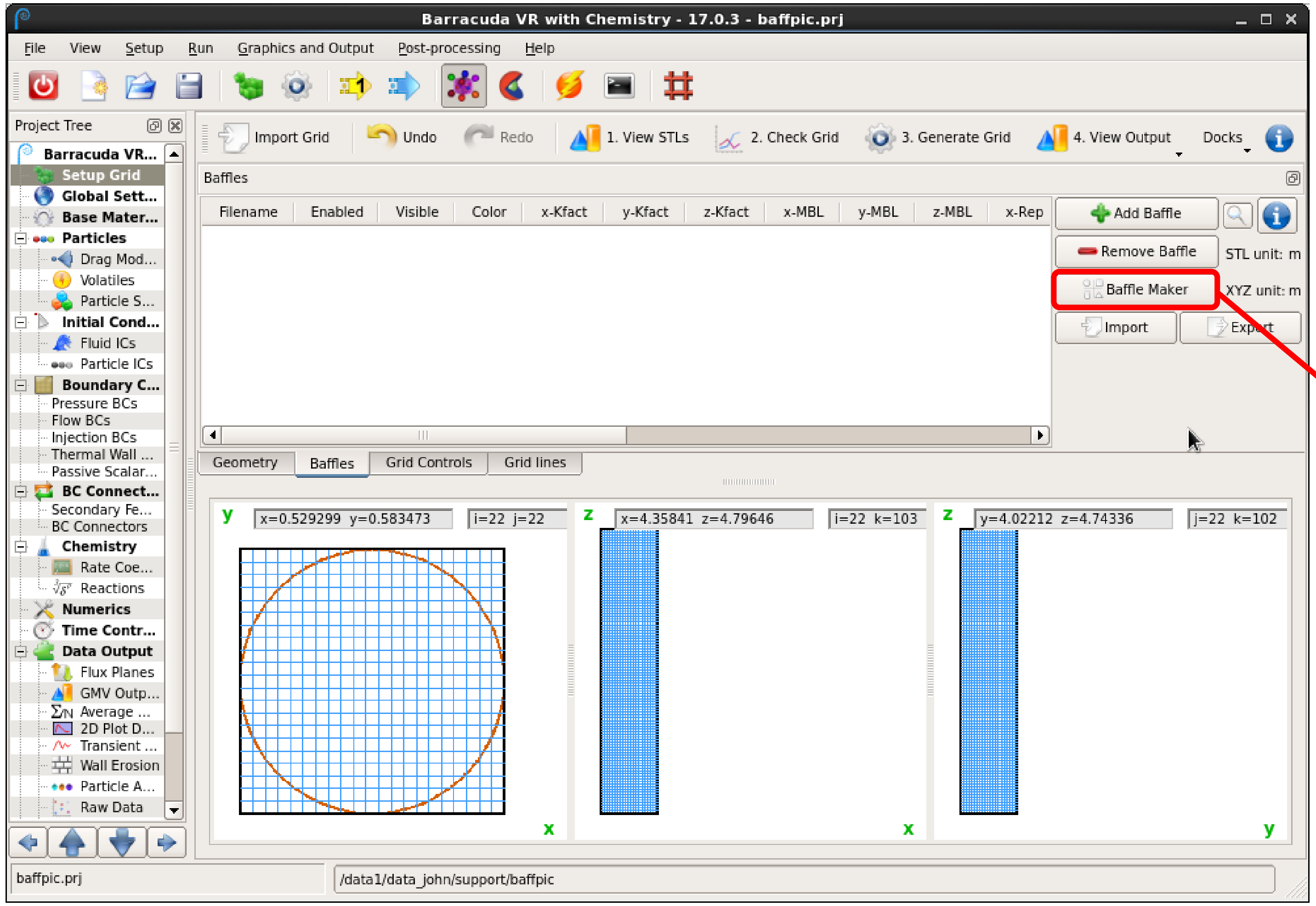
Baffles – Example Setup



Cylinder with upwards fluid flow and downward particle injection (circled)

Desire to add layers of chevron flow internals

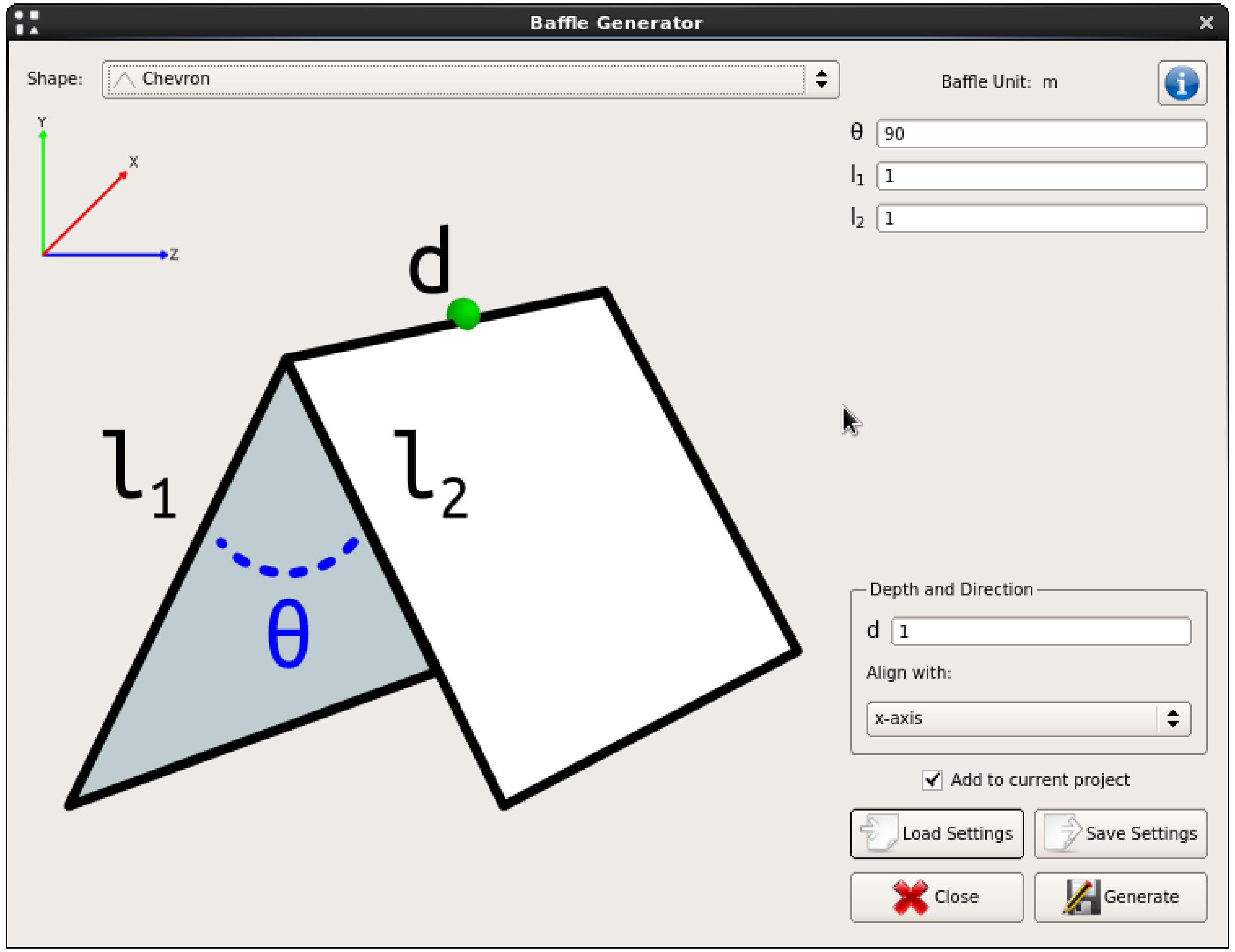
Baffles – Example Setup (continued)



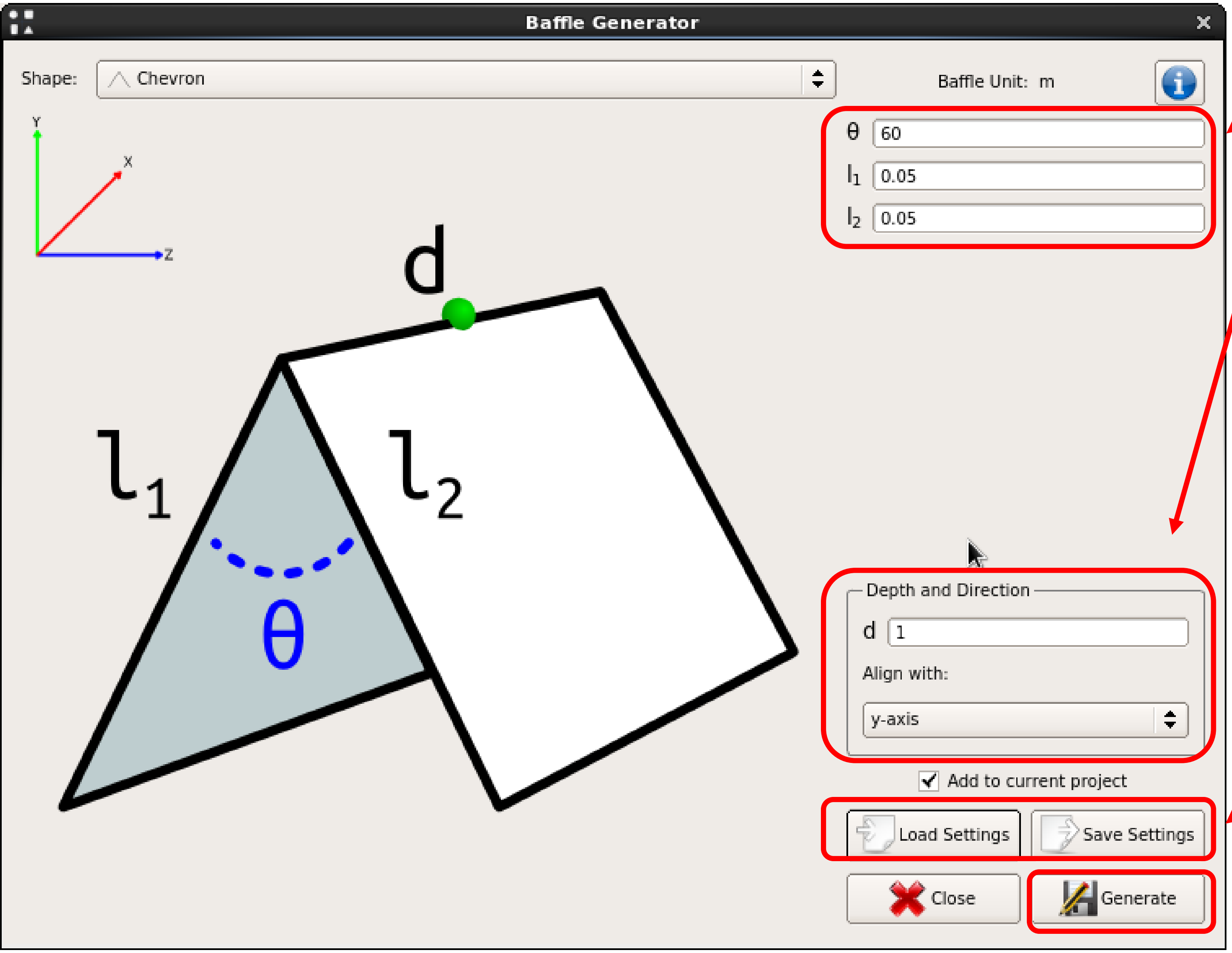
Baffles window under "Setup Grid"

-- Baffle Maker has predefined shapes (arc, chevron, I-Beam, U-Beam, plate

-- Dimension specifications differ for each baffle geometry



Baffles – Example Setup (continued)

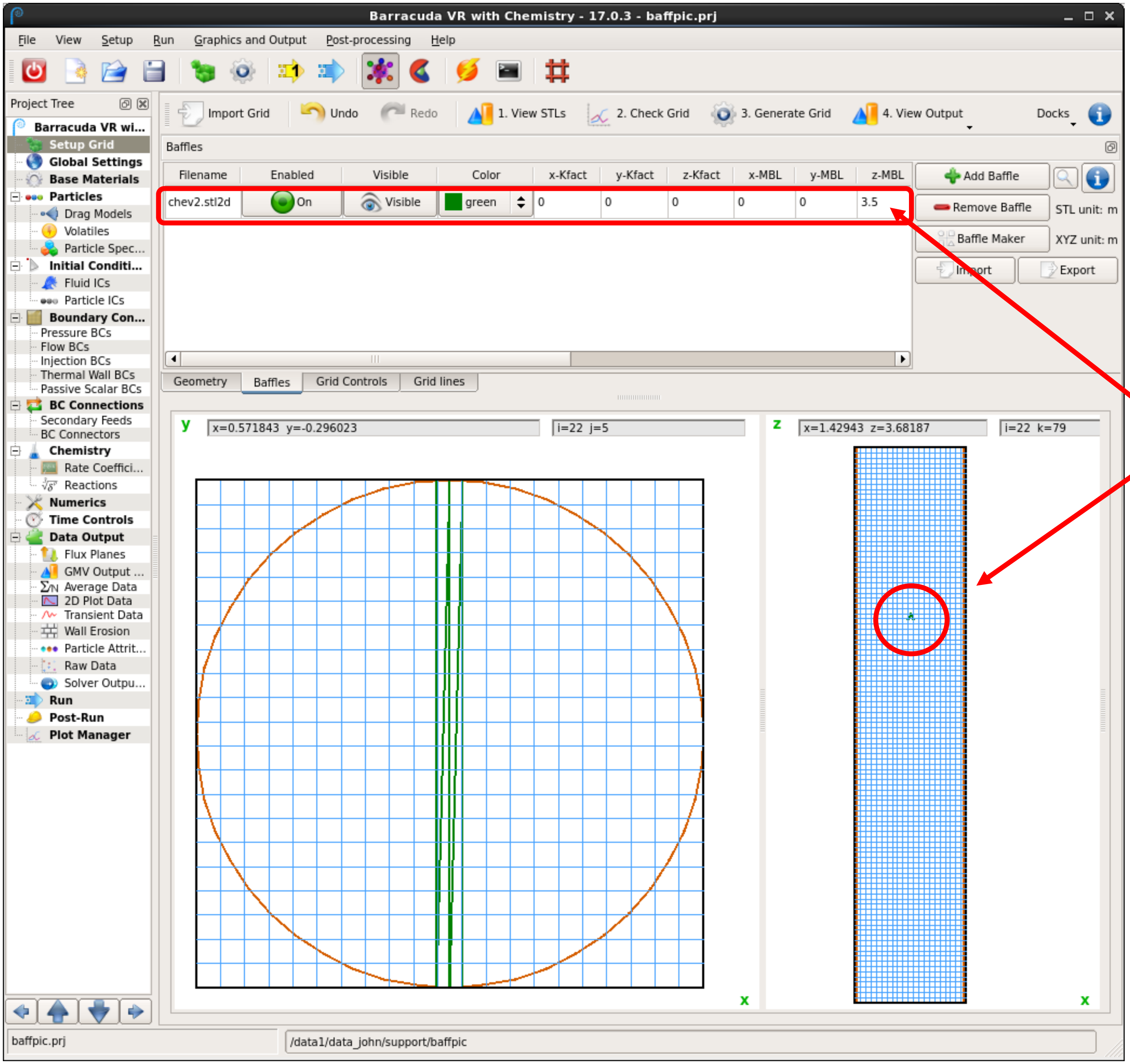


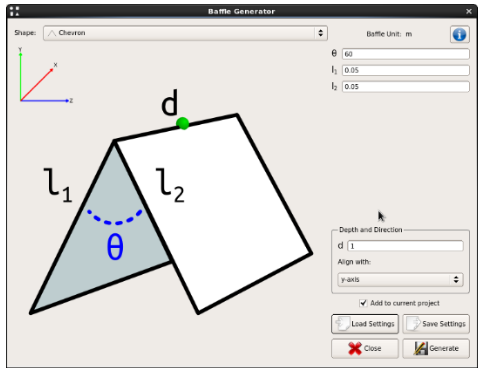
-- Set geometry: d = 1m; $l_1 = l_2$ = 0.05m; angle = 60^o; aligned with y-axis.

-- Save settings to use the same geometry on future setups; load settings to retrieve them.

-- Generate to create a baffle stl file for use in main baffles window.

Baffles – Example Setup (continued)





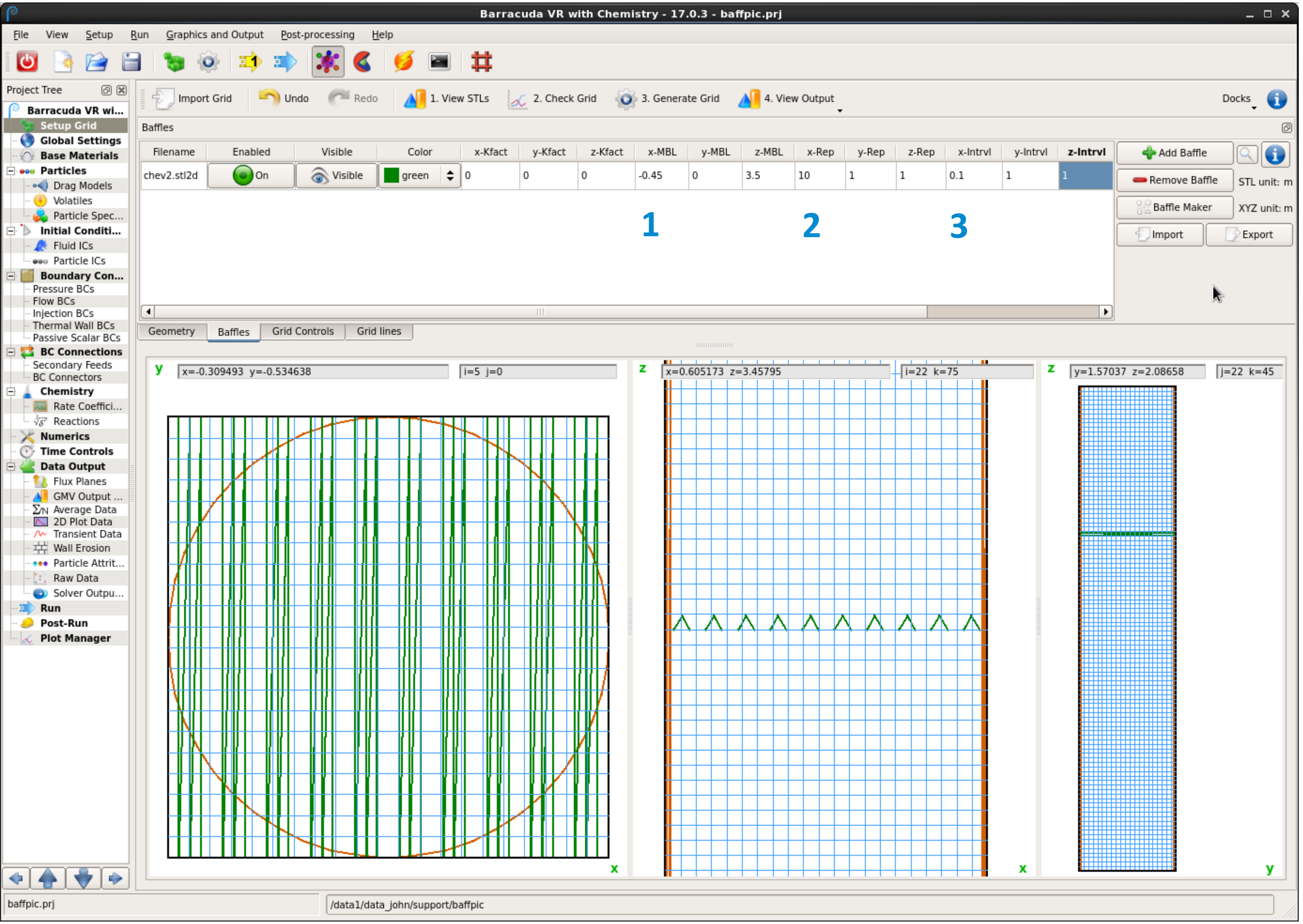
-- Baffle has been generated from sub-window.

-- Elevation has been set to 3.5 meters.

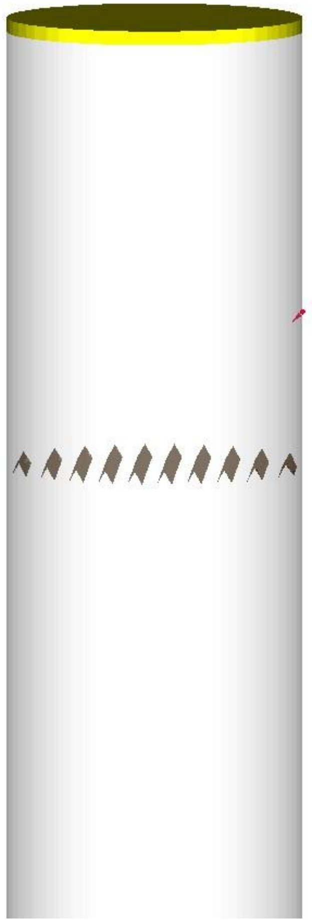
-- Single baffle can be seen in x-y and x-z views

-- Next step is to replicate the baffles across the unit.

Baffles – Example Setup (continued)

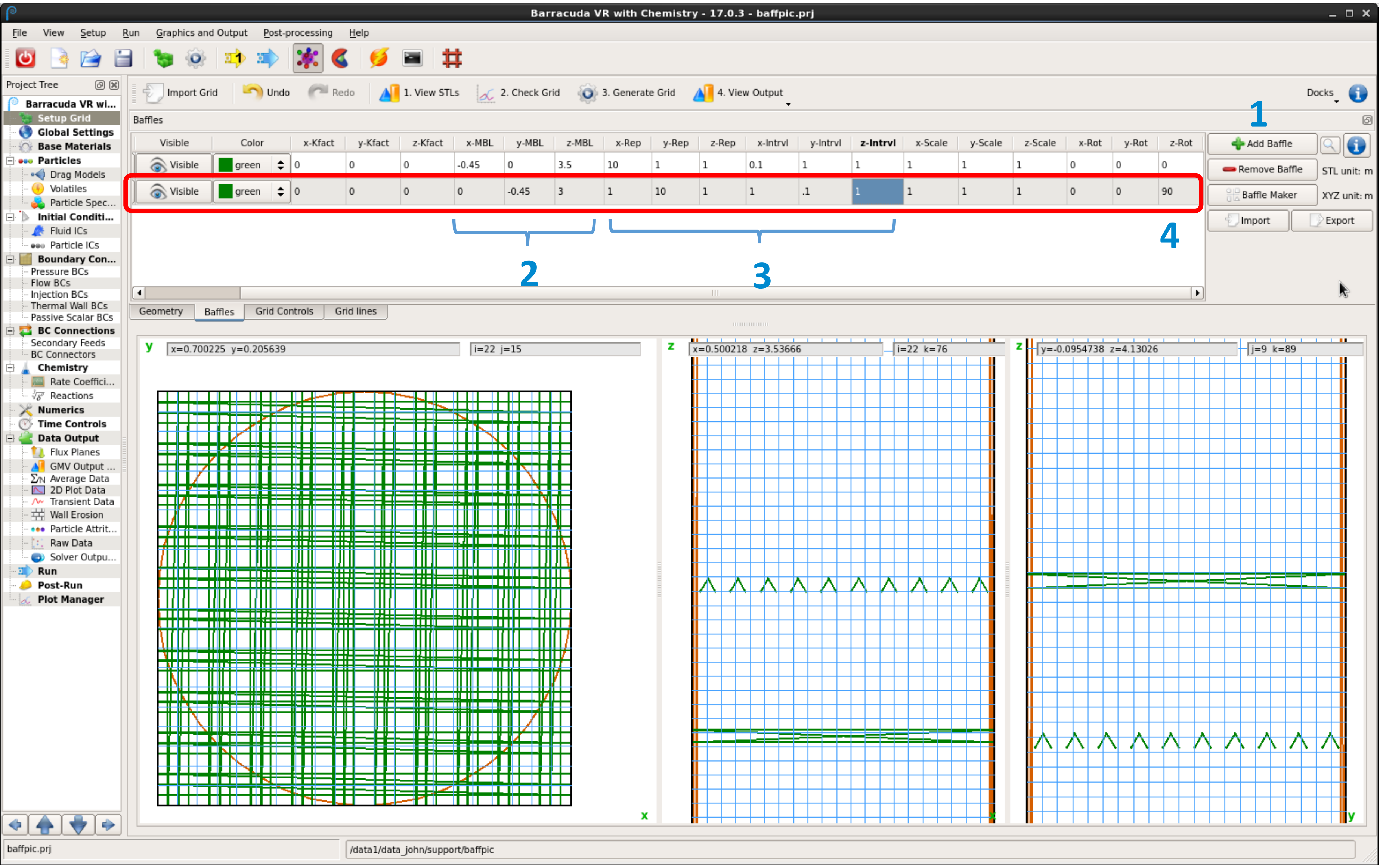


1. Master baffle location (MBL) is set to -0.45 in x-direction.
2. Set to 10 repetitions in x-direction.
3. Interval of 0.1 m between centers of repeating units in x-direction.



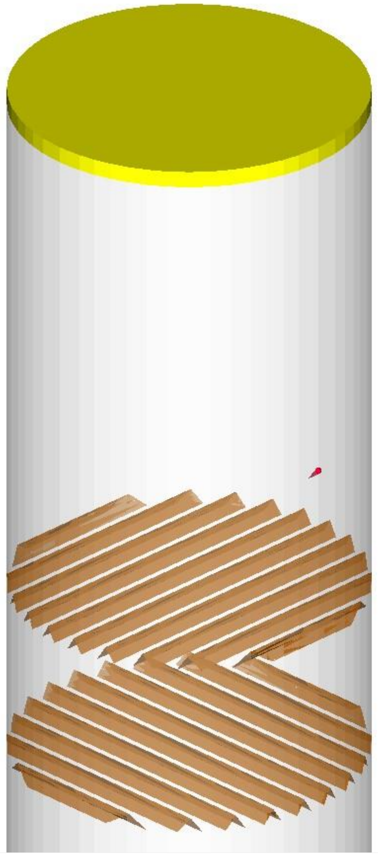
Baffles as generated by Run => Solver Setup

Baffles – Example Setup (continued)



Goal: create a second layer of baffles, rotated 90°, at z = 3.0 m.

1. Use “Add Baffle” and select previously generated stl2d file.
2. Set new master baffle locations, starting at minimum y-value.
3. Set repetitions and spacing in y-direction.
4. Rotate about the z-axis.



Chemistry

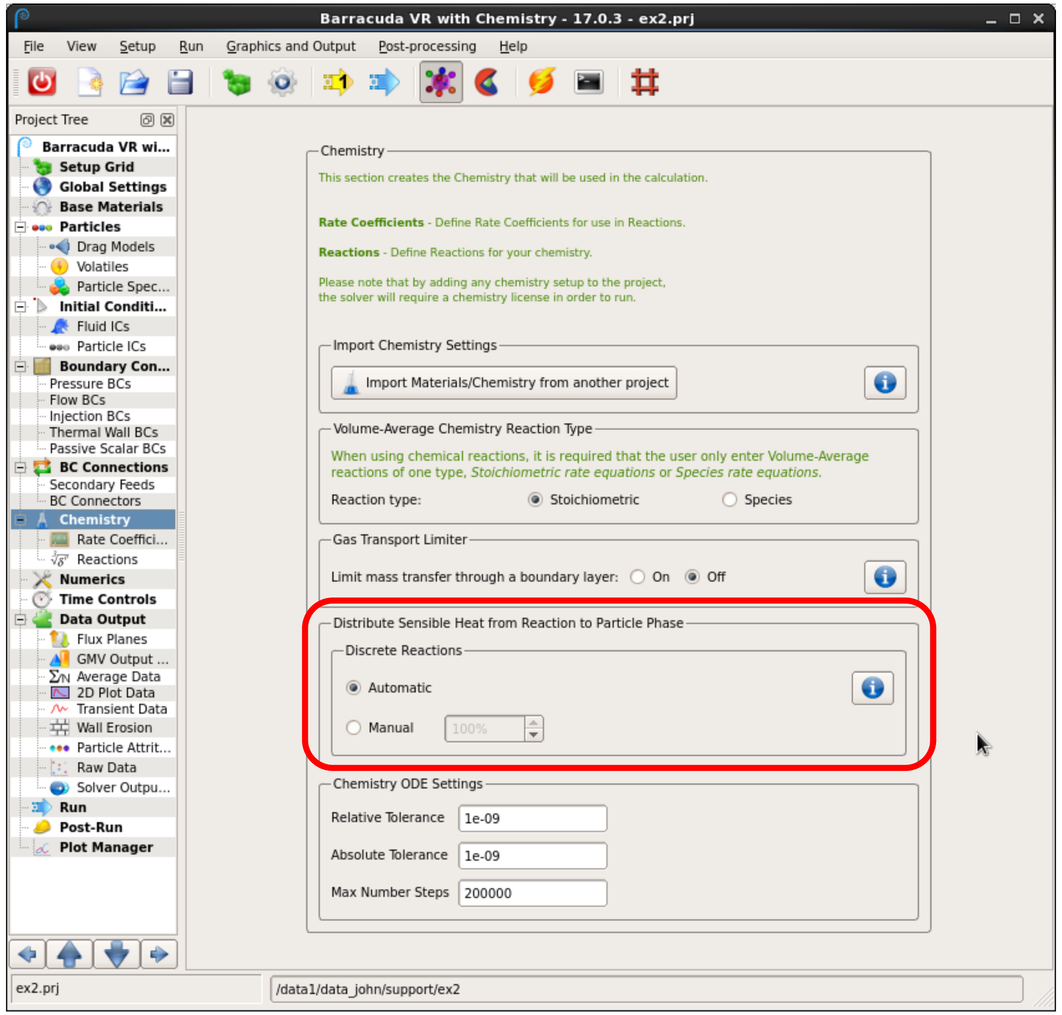
Chemistry – Distribution of Heat of Reaction

-- Applies to discrete particle reactions (volume-average chemistry heat of reaction goes to gas phase).

-- New default (automatic) method of heat Distribution is based on Musser *et al*, Constitutive equation for heat transfer caused by mass transfer, *Chemical Engineering Science*, 123: 436-443.

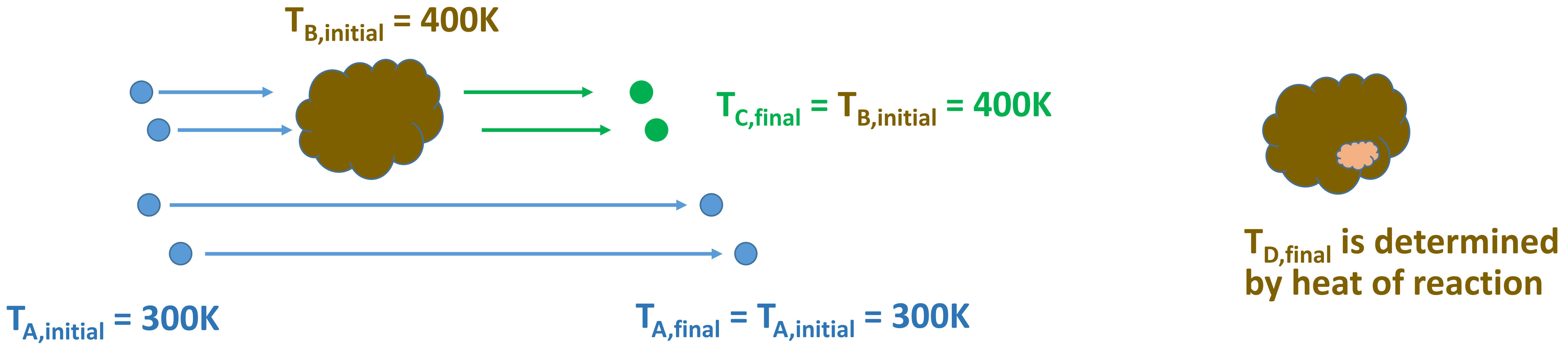
-- New method is physically more accurate and numerically more stable.

-- Legacy method may still be used by selecting "Manual" and specifying heat distribution.



Chemistry – Distribution of Heat of Reaction

Example discrete reaction: $A(g) + B(s) \rightarrow C(g) + D(s)$



- Unreacted gases retain their original temperature (subject to other energy calculations in the cell, including particle-fluid heat transfer).
- Reaction product gases have the ***original*** temperature of the solid reactant.
- Reacting particle has final temperature as calculated from net heat of reaction.

Chemistry – Age Factor

-- Applies to discrete particle reactions with solid **original mass** terms (m_0, m/m_0, $1-m/m_0$) for particle materials.

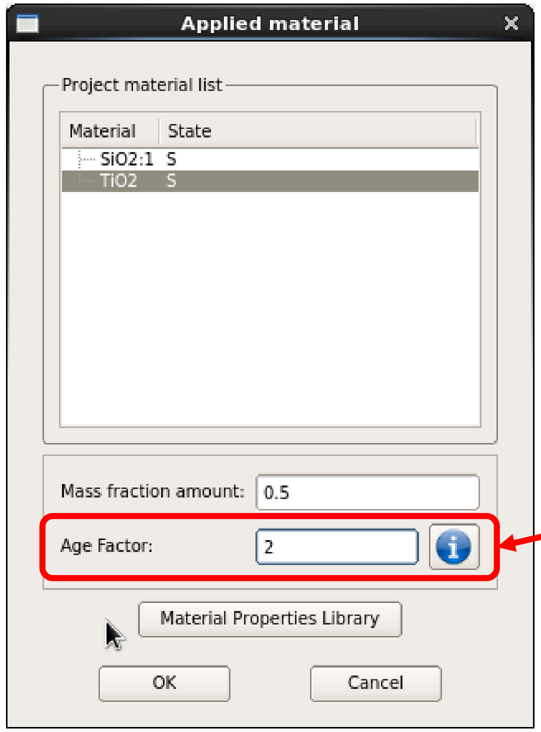
-- Allows the user to specify particles (initial or feed) that have already partially reacted.

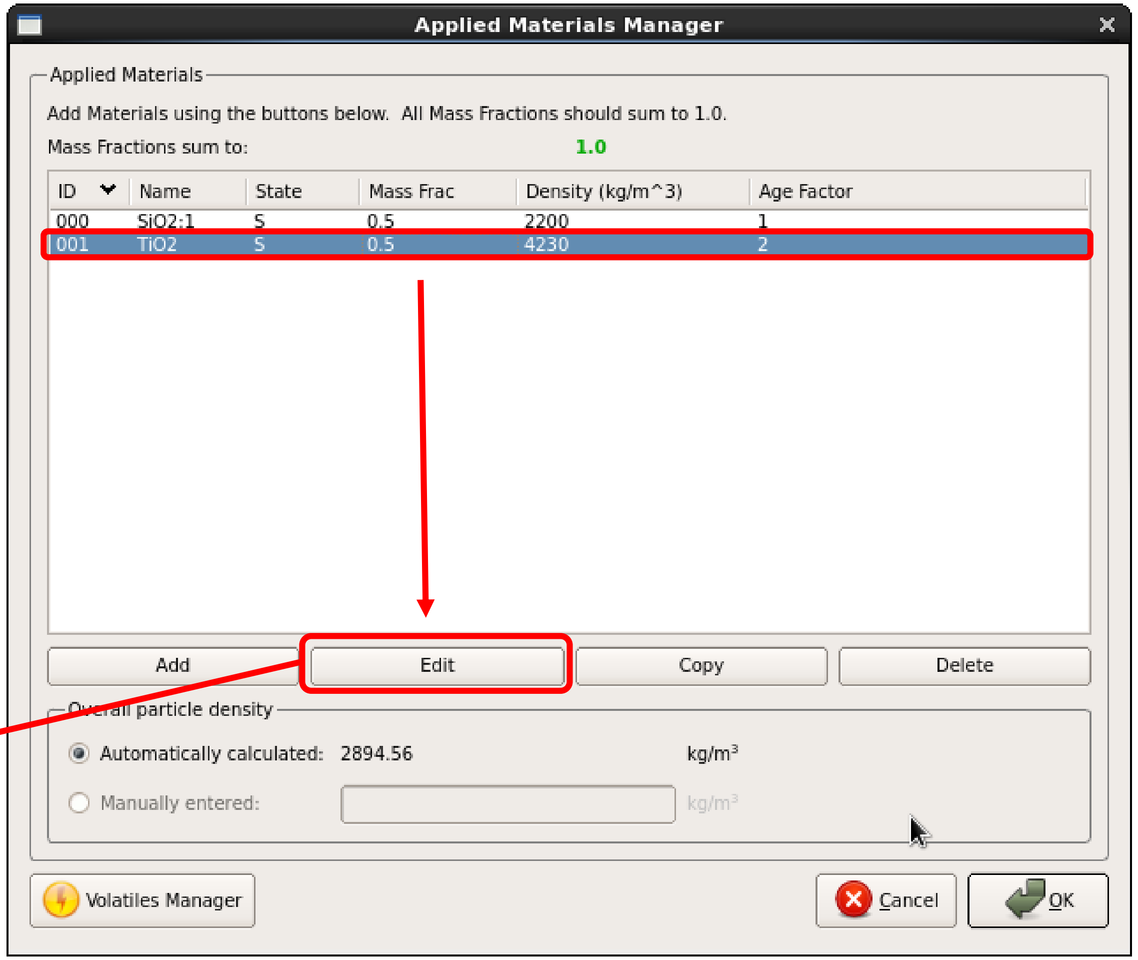
-- The **original mass** is equal to the **current mass** multiplied by the age factor:

$$m_0 = m * (\text{Age Factor})$$

Age Factor > 1 for partially reacted material

-- Specified under Applied Materials Manager for particle composition.

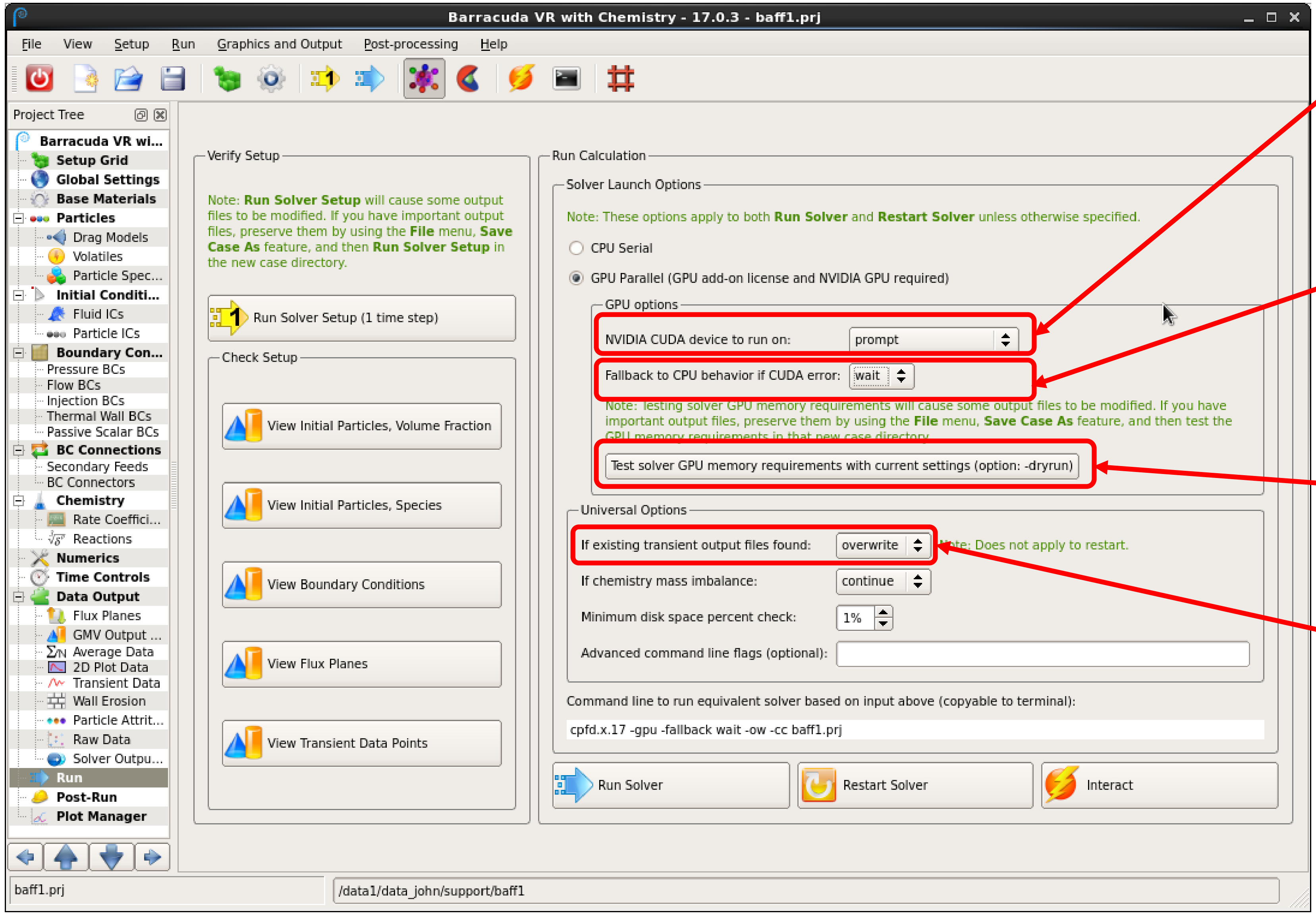




Run Window Options and File Systems

Run Window Options

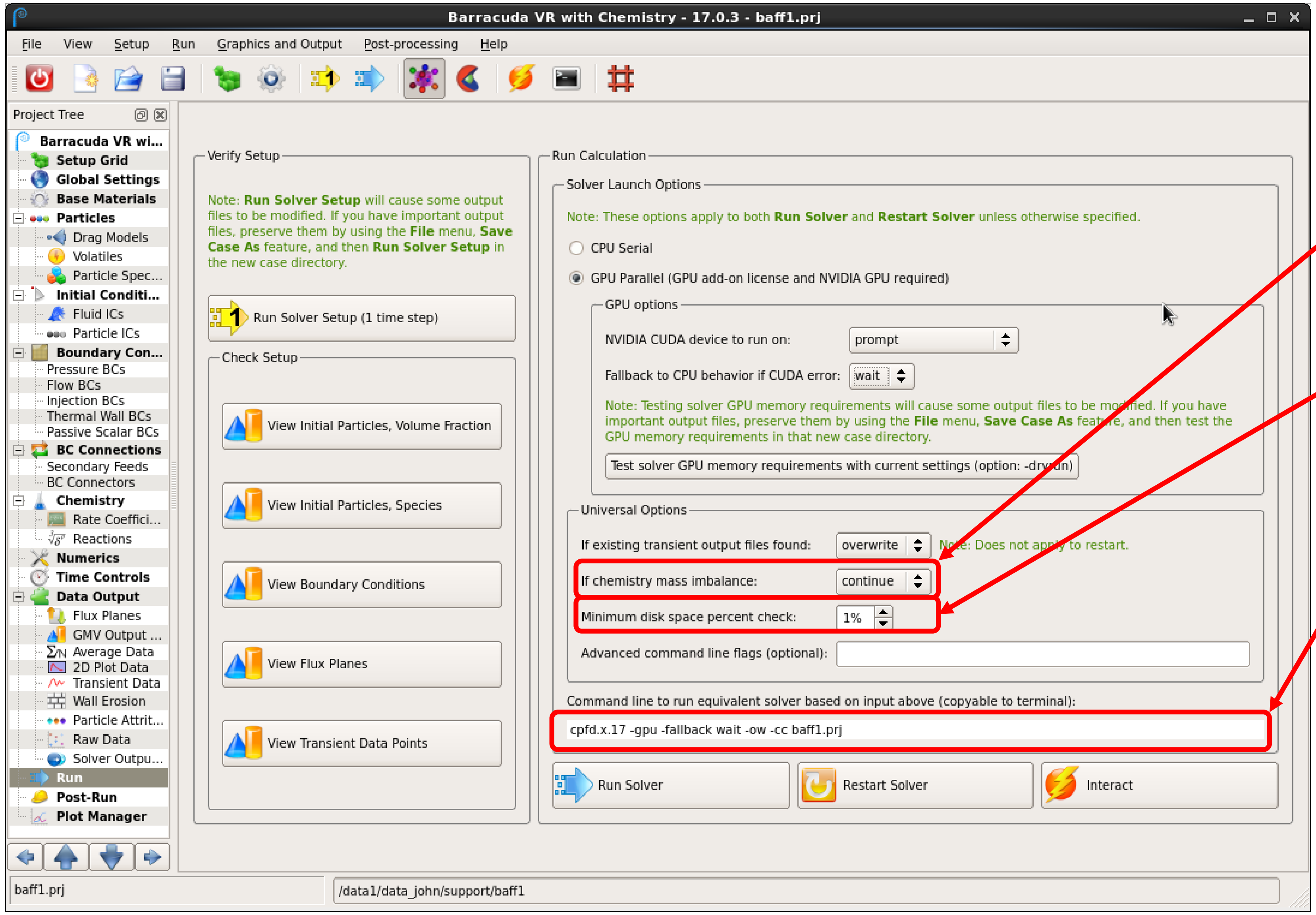
A number of options have been added to the run window:



- Which GPU card to run on – screen prompt, automatic, or preselected
- If there is an error with the GPU run, fall back to CPU automatically or prompt
- Check GPU memory requirements for proposed run
- Automatically overwrite or append to transient data files

Run Window Options (continued)

A number of options have been added to the run window:



- Continue run with chemistry mass imbalance
- Set minimum disk space to prompt for continued simulation
- The selections above are used to automatically generate a command line, which can be used to start runs from the terminal.

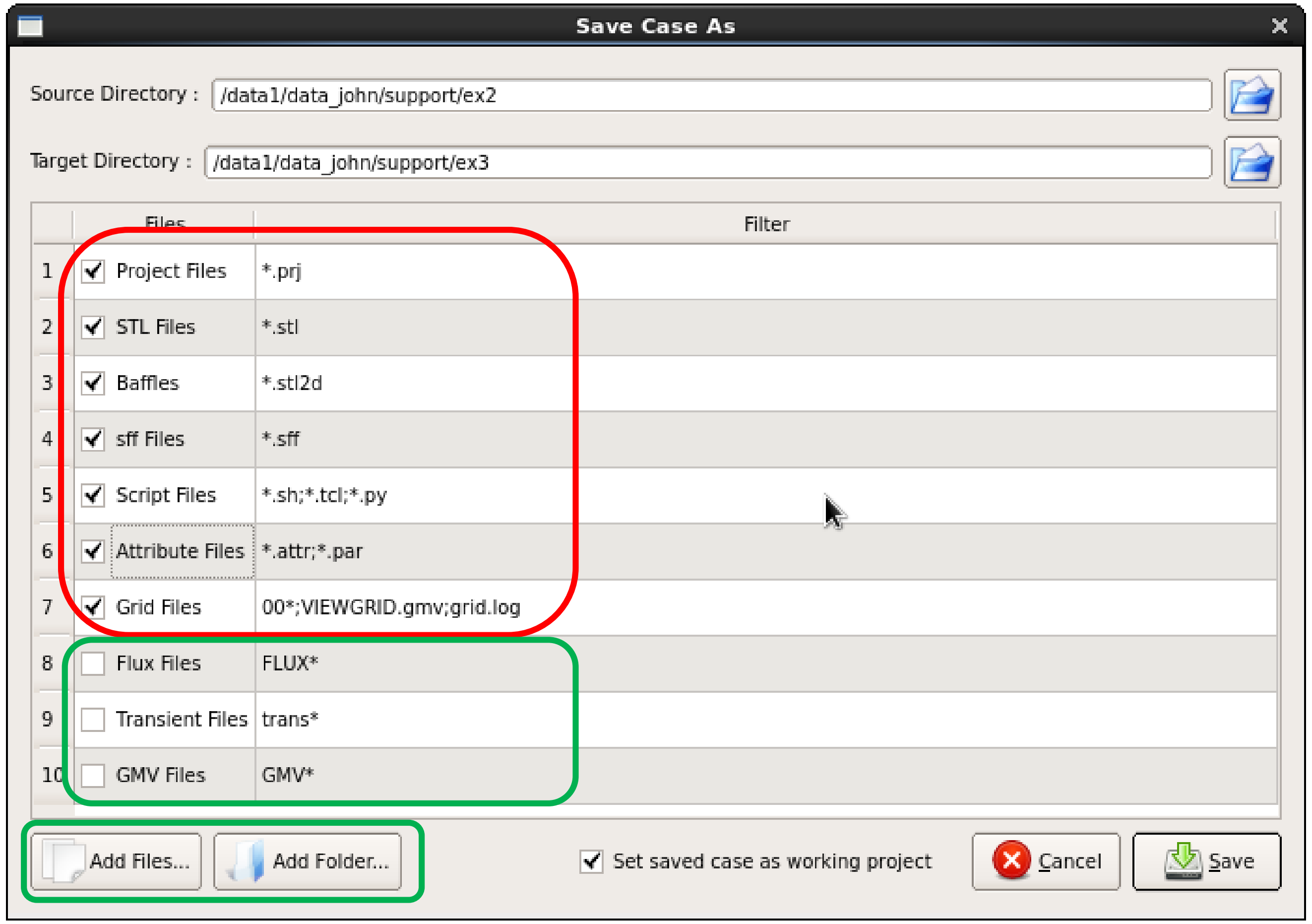
Save Case As

-- Makes it easier to run variations of a simulation.

-- The project (prj) file, along with other user-selected file types, are copied to a new directory.

-- These selections (including the generated grid) have been made to start a new parametric run.

-- Can also copy results, and other selected files or subdirectories.



Conclusion

-- Thank you!

-- All CPFD staff are available to answer questions, discuss features in more depth, or address specific applications.