

Best Practices

August 2020

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Training Objectives

This presentation contains considerations and advice, based on the experiences of the CPFDD Software engineering services and support groups.

The material in this presentation is intended to serve as a quick reference guide, rather than a complete working tutorial.

Much of the advice would be classified as “recommendations” rather than absolute rules. These recommendations will save you time for many typical problems.

Have a Good Process Description

Before creating a Barracuda model, or even before creating an STL file, it is important to have a good understanding of the process you wish to simulate.

- Goal of the simulation – what problem do you wish to solve?
- Geometry & region of interest (a process diagram is very useful)
- Operating conditions
 - All fluid flow boundary conditions
 - All particle flow boundary conditions (be careful to distinguish between fluid, particle and overall flow rates)
 - Anything else known about the system operation
- Material properties
 - Fluid properties
 - Particle composition, size distribution, behavior
- Thermal behavior of fluids, particles and overall system
- Chemical reactions and rates
- Any data available for comparison including anecdotal information from equipment operators
- A list of plots, images and animations desired
- A list of assumptions
- References for all of the above

CAD Creation

CAD input to Barracuda is via STL format.

- ASCII or binary STL options are both supported; binary is preferred.
- Export STL files with a high resolution so geometry is well-represented.

The STL file must come from a 3D solid model of the internal flow region of interest.

- A thin-walled model of the vessel structure is not useful within Barracuda.

Many geometries are cylindrical in nature. It is typically useful for the model origin to be centered at the bottom of the geometry with one axis up the middle.

- If the z-axis is pointing up (i.e. gravity in the $-z$ direction), mouse rotations will be more natural in Tecplot.

CAD Creation (Continued)

Consider carefully how to handle small geometric features in large vessels.

- Some features can be neglected (e.g. individual sparger shrouds when studying overall entrainment in a large vessel).
- Some features may be made larger in the CAD to facilitate gridding (e.g. a wall separating the vortex tube from a cyclone body).
- Some features must be left as is. This is true if the actual size is relevant to the objectives of a simulation (e.g. individual sparger shroud when studying jet penetration). In such cases, your options include:
 - Run a fine model of the overall vessel. The runtime may be impractical if the characteristic length scale of the feature is orders of magnitude smaller than a characteristic vessel dimension.
 - Run a local model of the region in the immediate vicinity of the small feature. Boundary conditions for this may be extremely challenging to define.

Model Size

Barracuda is used to simulate a wide variety of fluid-particle flow problems for a wide variety of industries. Spatial dimensions, flow rates and the time required to reach a quasi-steady solution can vary by several orders of magnitude. Thus, it is not possible provide rigid guidelines for computational cell and particle counts.

However, it is important to remember that the CPFDF method obtains solution resolution from both the Eulerian (grid) and Lagrangian (discrete) phases – thus the number of cells in a CPFDF grid is typically much lower than that in a CFD grid, where solution resolution is primarily tied to grid resolution alone. Many Barracuda projects can be run with:

- Between 100,000 and 500,000 real computational cells
- Between 1,000,000 and 20,000,000 computational particles

Be aware of the effect of model size on calculation run time

- Doubling the number of computational particles for a given grid, can roughly double the run time
- Doubling the cell count will automatically double the number of computational particles as well. Doubling the number of cells thus results in problem with 3-4 times the original run time.

Grid Definition

Check STL units. Incorrect assumptions here are a common source of error.

Do not put a large cell next to a small cell.

- This is bad practice with any CFD.

Avoid widely varying cell sizes on a global scale.

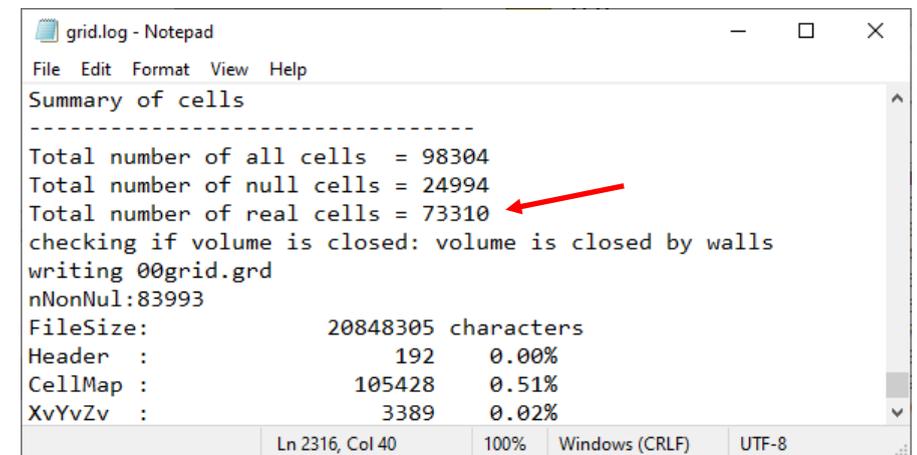
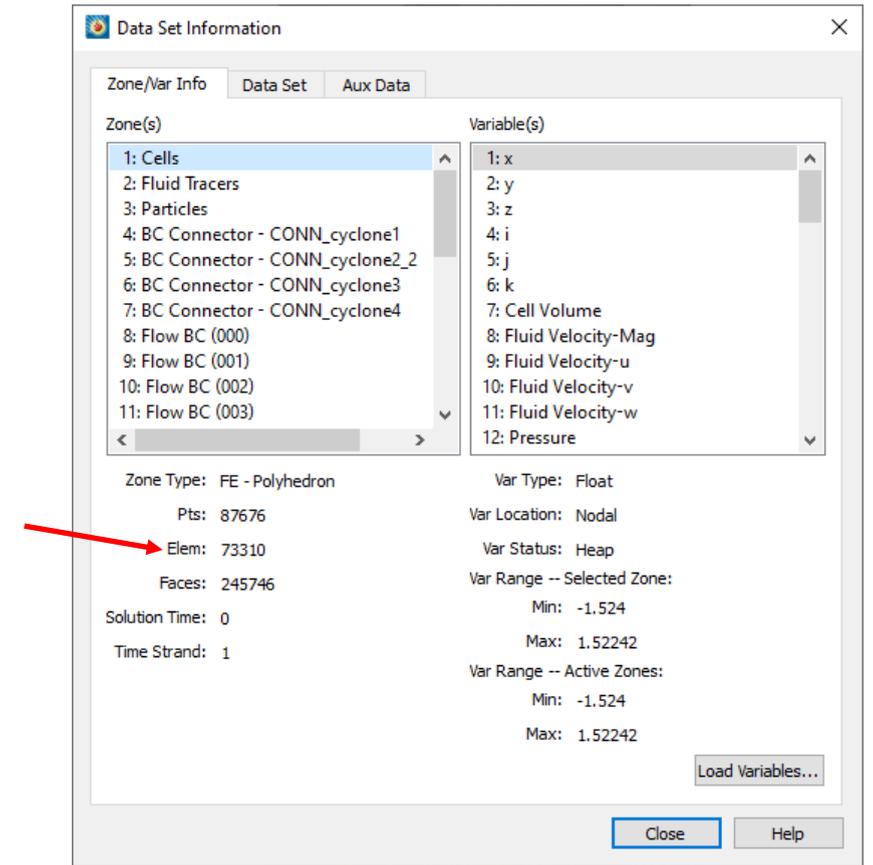
- Try to keep the largest cell size < 3.0 times the smallest cell size in any linear direction.

Use the “Check Grid” button in the Barracuda GUI to see how uniform your grid is.

Check your cell count before running the solver.

- In Tecplot: Data → Data Set Info..., selecting the Cells zone, and reading the term after Elem.
- Also found near the end of the grid.log file. Look for the “Total number of real cells”.

Do not rerun your grid generator in the same directory after starting the solver.



Special Grid and Particle Physics Considerations

If smooth wall surfaces are important, use “Merge and remove small cells”

- Grid Controls → Advanced options → Merge and remove small cells
- Usually not important for primarily axial flow
- Important for modeling flow within cyclones

If modeling very small particles, consider if other physics are important which are not directly computed by Barracuda.

- For example, small particles tend to cluster or agglomerate. It may be important to enable the agglomeration model when modeling small particles.

Initial Conditions (ICs)

Unless you are trying to resolve shocks, ensure your initial pressure and boundary pressures agree.

For Particle ICs, use the “Global Cloud Resolution” slider bar whenever possible.

- A “medium” or “medium-high” value often works best.

Consider initializing particles slightly below close pack, rather than at close pack. This is easier on the solver.

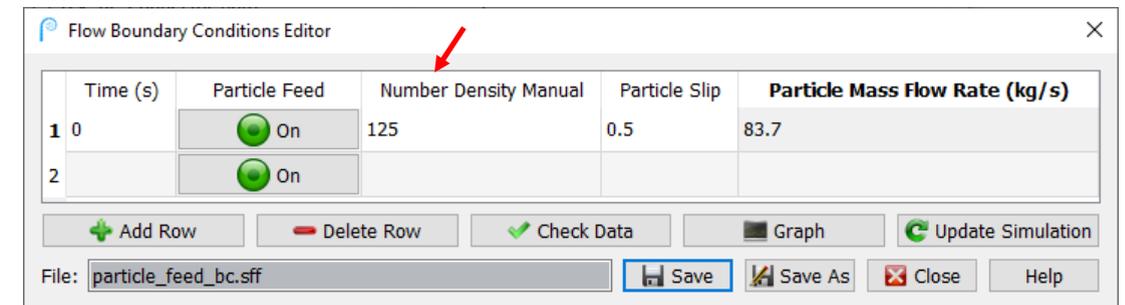
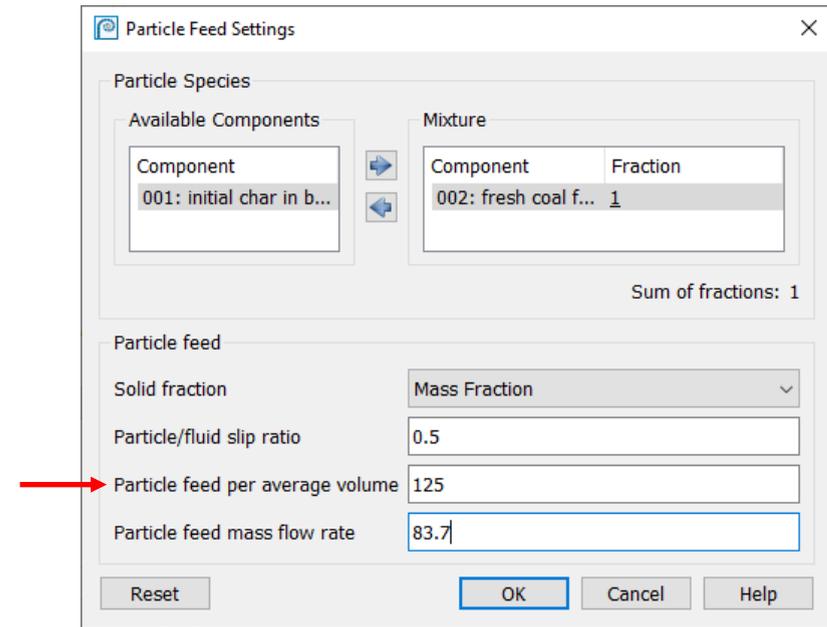
Boundary Conditions (BCs)

Avoid placing a boundary condition in the location of a strong gradient. It is not always possible to avoid this.

Define boundary conditions as transient (.sff files) even if you do not intend for them to change with time. This will allow you to change this interactively, or on restart, if later desired.

When feeding particles at BCs, check your cloud resolution carefully.

- The GUI label for the input parameter controlling cloud resolution at feed BCs is **Number Density Manual** in .sff files, or **Particle feed per average volume** in the Particle Feed Settings dialog.
- Check visually in Tecplot. You want a statistically significant number of clouds in each cell.
- Perform some analysis. A conservative algorithm is to divide 50 by the volume fraction you hope to resolve with the feed particles:
 - Example 1: Particles are flowing in at 50% by volume. $50/0.5 = 100$. Use **100** as the Number Density Manual at the feed BC.
 - Example 2: You have a dilute feed stream coming in at 1% solids by volume. $50/0.01 = 5,000$. Use **5000** as the Number Density Manual at the feed BC.



Calculation Start-Up and Setup Review

Are your BCs specified correctly?

- Especially check particle feed BCs carefully. The local, transient physics of a problem may prevent particles from entering at the specified rate. Always plot particle mass flow rates at inlets to ensure the desired mass flow is achieved. Check this over time as well.

Are your particles initialized in the right location?

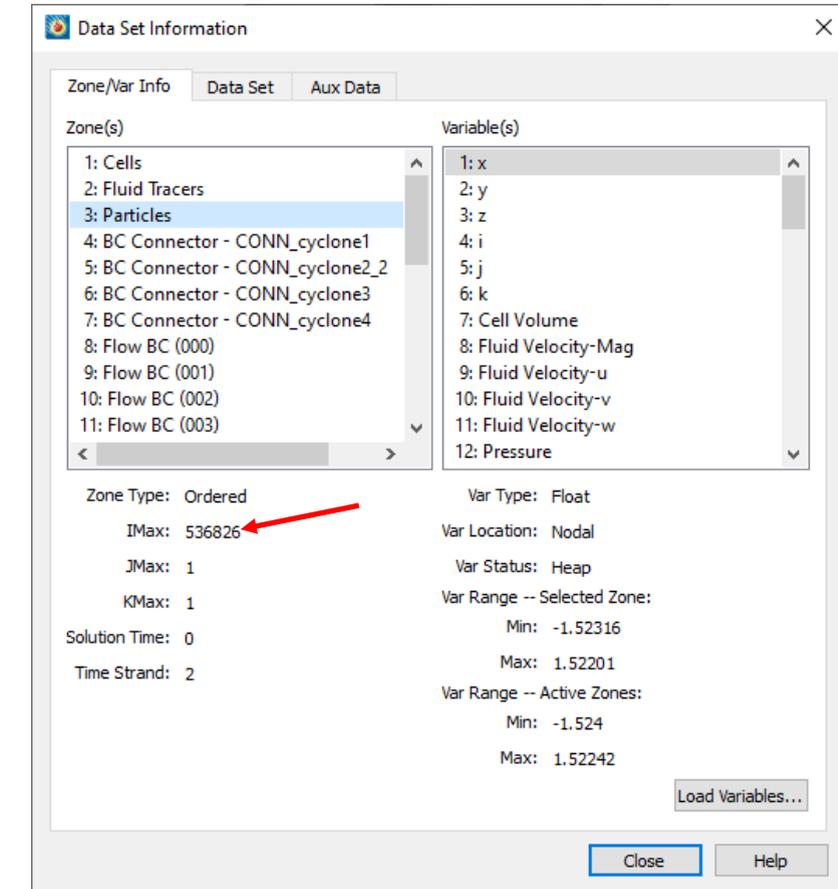
Check the number of clouds in the calculation. This can be found:

- In POPUL* files.
- In the history.log file.
- In Tecplot: the value of Imax found in Data → Data Set Info... in the Particles zone is the number of clouds.

Monitor how the number of clouds changes with time.

Are your flux planes and data points properly defined?

Does the first Tecplot file contain all the information you desire?



Calculation Start-Up and Setup Review (Continued)

Check velocities early on.

- Incorrect boundary conditions will often be apparent when checking velocities.

Check your time step:

- Shortly after startup
- After the calculation has been running for some time

Check the number of Tecplot files produced.

- Too few, and you won't have smooth animations.
- Too many and you'll fill your hard drive!

Do you have enough disk space to run the calculation?

- Check how the directory size grows after a day or so.

Have someone else review your work.

- It's OK if the other person is not a Barracuda user – just explain to them your process sheet and show them your model.

Data Output

It is usually a good idea to use flux planes liberally.

- Use at every boundary.
- Put several across your entire domain.
- If using multiple gaseous species, be sure to activate the gas species output option on flux planes, particularly at the model exits.
- If you want to track PSD crossing a flux plane, be sure to activate the Subdivide by radius option. Alternatively, Raw Particle Data at a flux plane can give you this information.

Begin post-processing as soon as possible after your calculation is running.

- The calculation need not be complete.
- This will ensure everything is set up correctly and all desired data is available.
- If there is a problem requiring a change in setup, it is better to find this out early, rather than after the calculation has completed.

Thermal Calculations

Check temperatures carefully on setup:

- Initial fluid temperatures
- Initial particle temperatures
- Boundary temperatures.

Check material properties over the range of expected temperatures.

Consider wall effects.

- Is the system adiabatic?
- If a wall temperature is known, where is that temperature (inside, outside)? Consider appropriate heat transfer coefficients.
- If a heat flux is known, you can change your wall temperatures interactively while monitoring the heat flux reported.

Consider physical time-scales to equilibrium. For a large fluidized bed of solids, the thermal time-scales may be much longer than the hydrodynamic time-scales.

Calculations with Chemistry

Carefully check material properties:

- Consistent molecular weights are necessary in order to conserve mass.
- Heats of formation are used to calculate heats of reaction.

Check units on reactions very carefully.

If using discrete particle chemistry, ensure the rate you input is based on the solid material (mol/s or kg/s), and not per unit volume (mol/m³/s or kg/m³/s).

Perform a single-cell chemistry project for each reaction to verify reaction kinetics against theoretical calculations.

Calculations with Chemistry (Continued)

You will usually want gas species information through flux planes when modeling chemistry.

- Select an output format that is meaningful to you (mass fraction, mole fraction, mass concentration, or mole concentration).

Time averaged gas species information is often desired when modeling chemistry.

Generally it's best to start with chemistry on from time = 0.

- The calculation can be started with chemistry off, and then chemistry can be toggled on at a later time. However, do not use this feature if reactants for fast reactions are building up in the system (unless you are trying to model an explosion!).

Project Directory and File Management

Barracuda creates many output files as it runs. Be sure to run each calculation in a different directory.

When running multiple simulations for the same project, be sure to uniquely name each directory

- If the names are not fully descriptive of the contents (run1, run2, etc.), then be sure to keep a text file containing notes and explanations.

Be mindful of disk space as you run.

- Check the amount of space remaining before starting a new calculation. Look at other directory sizes to estimate roughly how much space is needed.
- For very long running calculations, check space periodically.
- Archive files as needed.

Follow file naming conventions to make your life easier.

- Use recommended file extensions (i.e. “.sff” for input files). This will facilitate support and archiving
- Start flux plane names with either “Flux” or “FLUX”. This will facilitate support and archiving. Also, the file viewing defaults in Barracuda look for flux plane files following these naming conventions.

Starting New Simulations Based On Old Simulations

When starting additional calculations based on an existing calculation, certain files must be copied to the new directory. Use the Save Case As... tool.

A minimum set of files includes the following. In this case, the grid will need to be regenerated in the new directory:

- Project file (*.prj)
- Transient input files (*.sff)
- Particle size distribution files (*.sff)
- CAD (*.stl, *.STL)

If you do not need to change your grid, copy the grid files as well.

In general, it is a good idea to also copy the following:

- Tecplot layout files (*.lay)
- Analysis scripts you have written (*.ipynb, *.py, *.sh)

Restarting a Barracuda Virtual Reactor Simulation

It is possible to restart a Barracuda calculation from a restart (IC) file

Click “Restart Solver” on the Run page

An IC file name must be specified

Other information should only be entered if you want that information to change from the current run

The screenshot shows the 'Restart Calculation' dialog box with the following fields and options:

- IC:** A text input field with a 'Browse' button next to it, circled in red.
- Time step:** A text input field.
- End time:** A text input field.
- Iterations/Residual:** A table with two columns: 'Iterations' and 'Residual'.

	Iterations	Residual
Volume	<input type="text"/>	<input type="text"/>
Pressure	<input type="text"/>	<input type="text"/>
Velocity	<input type="text"/>	<input type="text"/>
- Output intervals:** A section with four text input fields: 'Terminal and log files', 'Visualization files', 'Restart files (IC_###)', and 'Backtrack files (IC_)'.

Field	Value
Terminal and log files	<input type="text"/>
Visualization files	<input type="text"/>
Restart files (IC_###)	<input type="text"/>
Backtrack files (IC_)	<input type="text"/>
- Min CFL:** A text input field.
- Max CFL:** A text input field.
- Options:**
 - Reread BC input files
 - Reread BC particle size distribution tables
 - Reset attrition
 - Reset wear
 - Reset average data variables
 - Turn thermal calculations ON if they are not
 - Change chemistry state
 - Turn on chemistry
 - Ramp on from s to s
 - Turn off chemistry
 - Change wear state
 - Turn on wear
 - Turn off wear

Buttons: OK, Cancel, Help

Archiving Project Results

After completing a project, you may need to archive results in order to free disk space on the computer.

When archiving, it is recommended to save the following as a minimum set:

- Files needed to rerun (Project file (*.prj), Transient input files (*.sff), Particle size distribution files (*.sff), CAD (*.stl, *.STL))
- Grid (grid.grd, viewgrid.plt, 00*.gmv, 00grid.grd, grid.log, VIEWGRID.gmv)
- Some Tecplot files (maybe every 2nd, 10th, 50th or 100th)
- Restart file (at least the final IC file)
- Other output files (history.log, flux planes (FLUX*, Flux*), data points (trans.data*), data planes (*.dat))
- Post-processing files (any scripts created and files referenced (*.ipynb, *.py, *.sh), Tecplot views (*.lay))
- Images, animations and plots (*.png, *.eps, *.mpg, *.avi, *.mp4)

Use the Create Support Package utility (discussed in the next slide) as a way to quickly collect and compress the most relevant project setup files.

See this support site post: [Archiving Barracuda VR Simulation Results](#) (includes the script swee.py)

Contacting Support

If you have questions about this material, or a specific question about a Barracuda simulation project you are working on, contact the CPF D Software support team at: support@cpfd-software.com

If your question relates to a specific project, please include a “support file” if possible

To create a support file, click on the “Create support file” button on the Post-run dialogue. Be sure to include the CAD.

