Advanced Best Practices: Effective Modeling with Barracuda VR

Barracuda Virtual Reactor Users' Conference

September 30 – October 2, 2015

Santa Ana Pueblo, New Mexico

Purpose of Training Course

Provide techniques to:

- Improve the value of Barracuda VR simulations
- Avoid setup mistakes

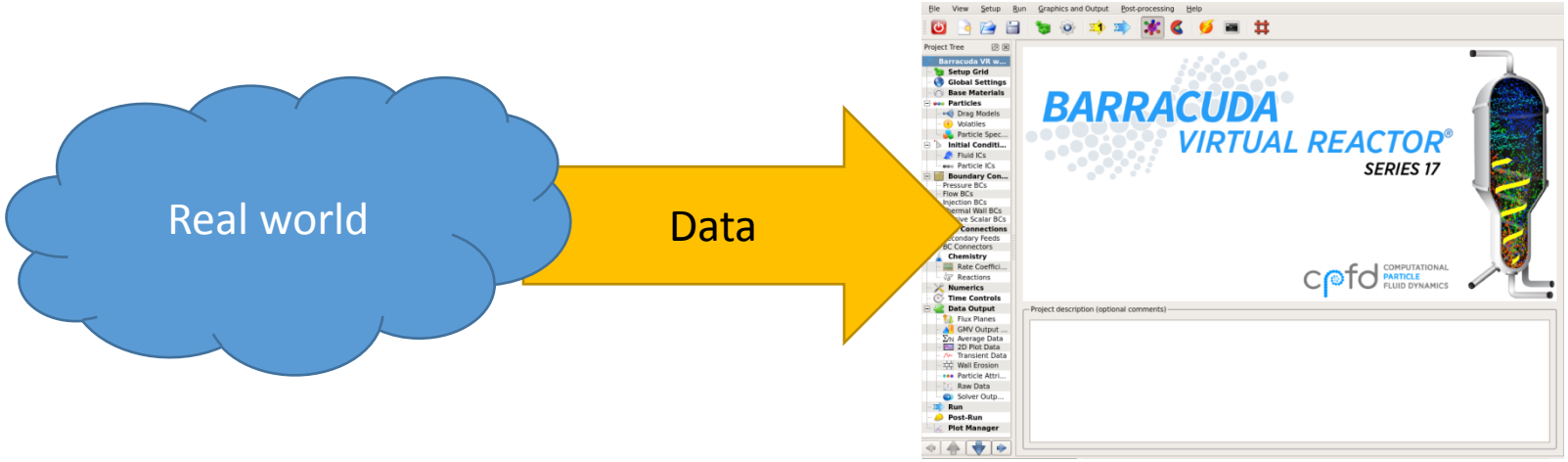
Training Course Outline

Topics:

- Validating model inputs 4
- Using better boundaries 15
- Implementing complex chemistry in Barracuda VR 33
- Selecting key data outputs 45
- Monitoring Barracuda VR simulations 48
- Getting help from CPFD support 50

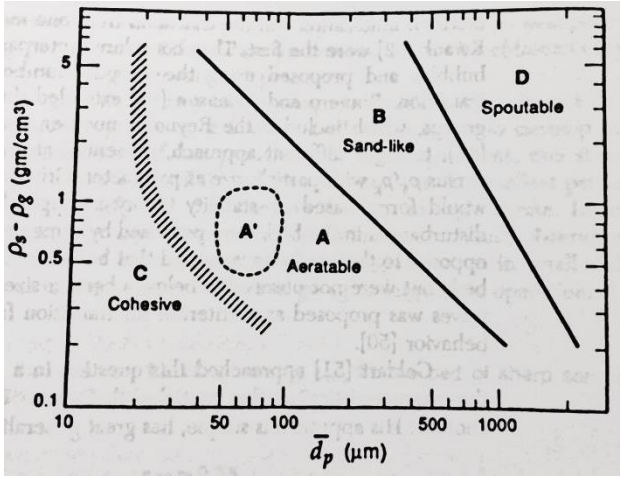
Validating Model Inputs

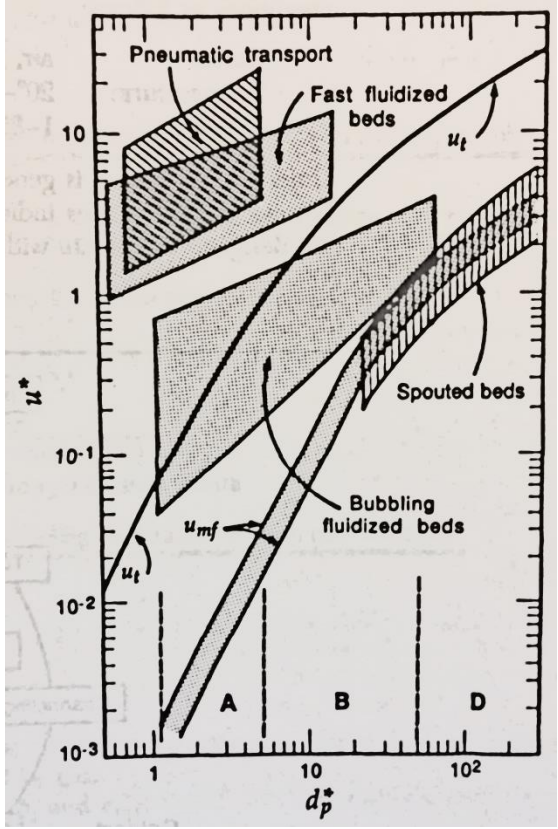
Save time and energy by ensuring input data is **accurate** and **self-consistent**



Tip #1: Know expected fluidization

- Geldart particle classification
- Flow regime





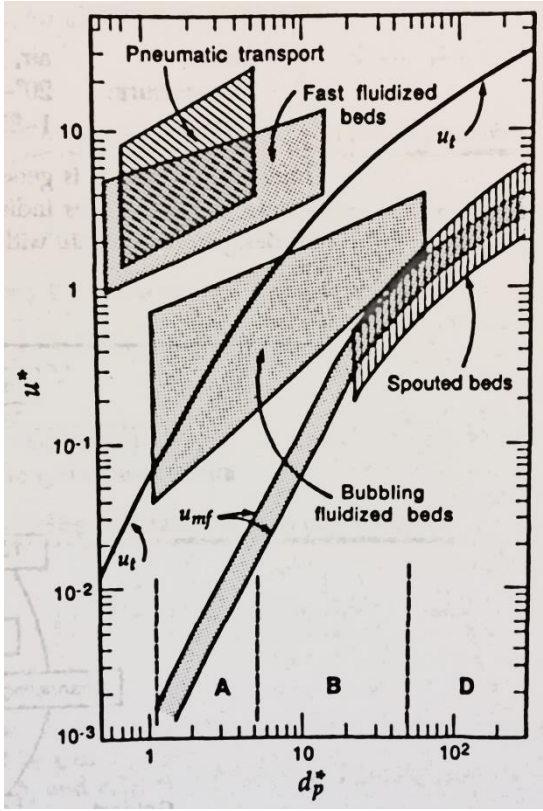
Kunii, D. and Levenspiel, O. (1991) *Fluidization Engineering.* Butterworth-Heinemann, Boston.

Calculation of flow regime

- Calculation is quick with basic material and superficial velocity

$$d_p^* = d_p \left[\frac{\rho_g \left(\rho_s - \rho_g \right) g}{\mu^2} \right]^{1/3} \qquad u^* = u \left[\frac{\rho_g^{\,2}}{\mu \left(\rho_s - \rho_g \right) g} \right]^{1/3}$$

- PSRI tools make this easy too



Kunii, D. and Levenspiel, O. (1991) *Fluidization Engineering.* Butterworth-Heinemann, Boston.

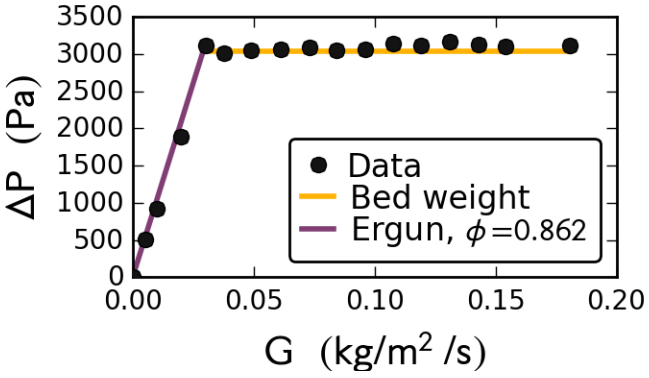
Tip #2: Use available data to improve particle characterization

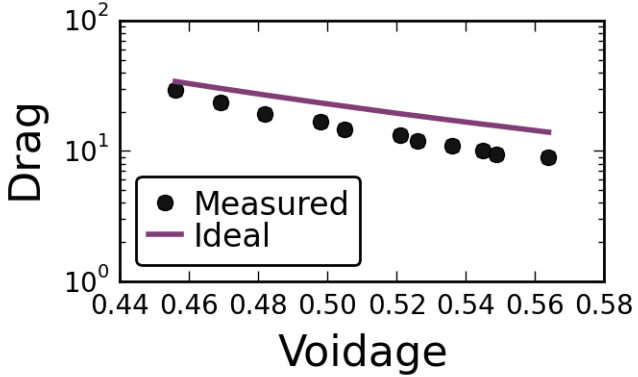
Verify that the particle specifications are consistent with experimental data

- PSD and d_{32}
- Sphericity, ϕ
- Close-pack particle volume fraction, ε_{mf}

Packed bed: $$\frac{\Delta P}{L} = \frac{18(1-\varepsilon_{mf})\mu U_0}{d_{32}^{\,3}\varepsilon_{mf}}\left(\frac{a}{18}\frac{(1-\varepsilon_{mf})}{\phi^2\varepsilon_{mf}^{\,2}} + \frac{b}{18}\frac{\mathrm{Re}}{\phi\varepsilon_{mf}^{\,2}}\right)$$

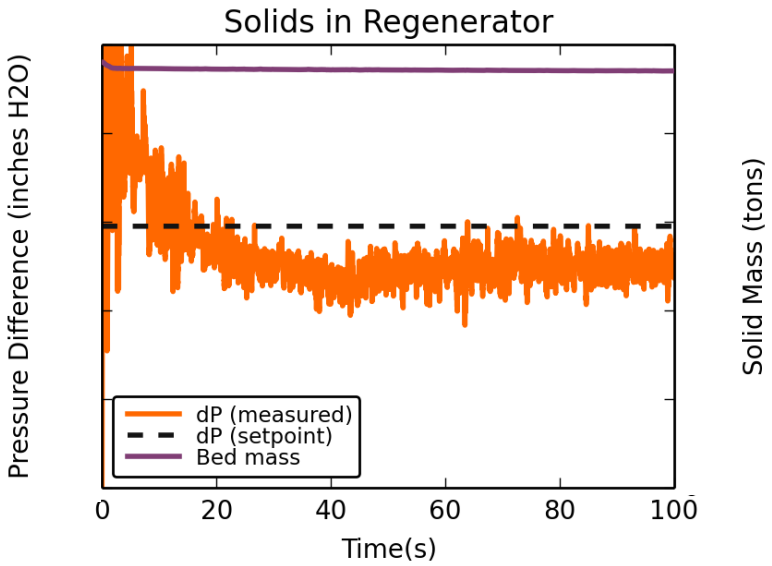
Fluidized: $$F_{meas}(\varepsilon,\mathrm{Re}) = \frac{d_p^{\,3}\rho_f(\rho_s-\rho_f)g}{\mu_f^{\,2}}\frac{\varepsilon}{18\,\mathrm{Re}}$$





Tip #3: Verify the bed mass

- **history.log** contains a more complete inventory of solids than the estimate from pressure drop
- Understand the bed mass estimate
- Place transient data points for pressure in the model to compare simulated pressure drop with operation



Tip #4: Use a Mass and Energy balance

Mass and energy balances are important when system contains any of the following:

- Complex reaction scheme
- Inexact components (ie biomass, coal, etc)
- Strongly exothermic / endothermic reactions

Tip #4: Use a Mass and Energy balance

- Verify that reactant feeds and reaction scheme can produce expected gas composition under any conditions
- Inform assumptions about material thermal properties such as heat of formation and heat capacity
- Determine whether any significant reactions, heat losses, inputs are missing

Sample M&E Balance From FCC Regenerator

System Inflows			Total	Solids			Gases					Notes
				Cat base	C	H	N2	O2	H2O	CO	CO2	
INPUTS												
Spent Catalyst	Flow rate	kg/s	###	###	###	###						
	Composition	wt%	###	###	###	###						
	Temperature	K	###	###	###	###						
	Enthalpy	MJ/s	###	###	-###	-###						
AIR #1	Flow rate	kg/s	###				###	###	###			
	Composition	wt%	###				###	###	###			
	Temperature	K	###				###	###	###			
	Enthalpy	MJ/s	-###				###	###	-###			
AIR #2	Flow rate	kg/s	###				###	###	###			
	Composition	wt%	###				###	###	###			
	Temperature	K	###				###	###	###			
	Enthalpy	MJ/s	-###				###	###	-###			
Torch Oil	Flow rate	kg/s	###						###			
	Composition	wt%	###						###			
	Temperature	K	###						###			
	Enthalpy	MJ/s	-###						-###			
Total Feeds	Flow rate	kg/s	###	###	###	###	###	###	###			
	Enthalpy	MJ/s	###	###	-###	-###	###	###	-###			

	Combined Enthalpy		###		Diff*1000	###					
Combined Inflows	Flow rate	kg/s	###	###	###	###	###	###	###		To calculate equivelent inlet temperature (combined)
	Composition	wt%	###	###	###	###	###	###	###		
	Temperature	K	###	###	###	###	###	###	###		
	Enthalpy	MJ/s	###	###	-###	-###	###	###	-###		

Air Compositon Calculation

		N2	O2	H2O	MW
Dry	mol%	###	###	###	###
	wt%	###	###	###	
Wet	mol%	###	###	###	###
	wt%	###	###	###	

Flow rate of Wet Air

	#1	#2
mscfh	###	###
kg/s	###	###

Sample M&E Balance From FCC Regenerator

Overall Reactions			Total	Solids			Gases					Notes
				Cat base	C	H	N2	O2	H2O	CO	CO2	
Params	Feed	kg/s	###	###	###	###	###	###	###	###	###	
	O2 Reaction	%	###									
	CO/CO2 molar	-	###									
	C/H in Coke	wt/wt	###									
Reaction: Coke + O2 --> alpha*CO + beta*CO2 + gamma*H2O												
Extents	alpha	-	###									
	beta	-	###									
	gamma	-	###									
	Delta	mol/s	-###	###	-###	-###	###	-###	###	###	###	
	Delta	kg/s	###	###	-###	-###	###	-###	###	###	###	

System Outflows			Total	Solids			Gases					Notes
				Cat base	C	H	N2	O2	H2O	CO	CO2	
Regen. Catalyst	Flow rate	kg/s	###	###	###	###						
	Composition	wt%	###	###	###	###						
	Temperature	K	###	###	###	###						
	Enthalpy	MJ/s	###	###	-###	-###						
Flue Gas	Flow rate	kg/s	###				###	###	###	###	###	
	Composition	wt%	###				###	###	###	###	###	
	Temperature	K	###				###	###	###	###	###	
	Enthalpy	MJ/s	-###				###	###	-###	-###	-###	
Total Outflow	Flow rate	kg/s	###	###	###	###	###	###	###	###	###	
	Enthalpy	MJ/s	###	###	-###	-###	###	###	-###	-###	-###	

Flue Gas Calcs	Flow rate	kg/s	###				###	###	###	###	###	
	Composition	wt%	###				###	###	###	###	###	
	Flow rate	kmol/s	###				###	###	###	###	###	
	Composition	mol%	###				###	###	###	###	###	
	Dry mol%	mol%	###				###	###		###	###	

Coke properties		Mass Balance			Enthalpy			Temperatures			Delta Coke		
Heat Desorp (MJ/kg)	###	In	kg/s	###	In	MJ/s	###	RCSP	K	###	Coke in	wt%	###
Heat capacity J/kg/K	###	Out	kg/s	###	Out	MJ/s	###	DT	K	###	Coke Out	wt%	###
		Bal.	kg/s	###	Bal.	kg/s	-###	Flue	K	###	Delta	wt%	###

Tip #4: Use a Mass and Energy balance

Guidelines for successful material and energy balance:

- Use material properties *as defined* in Barracuda VR.
- Define reactions with adjustable extents
- Sanity-check any conclusion drawn from an M&E balance

Q & A: Validating Model Inputs

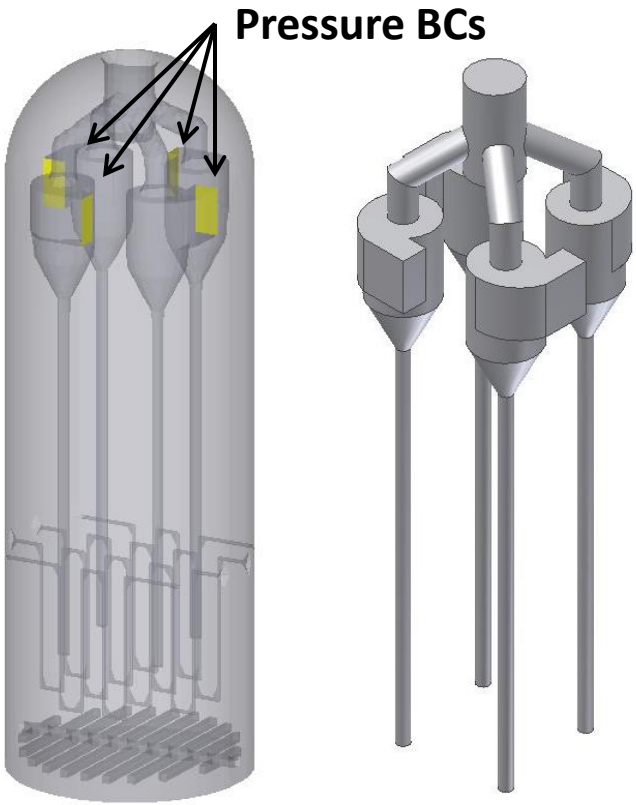
- Are you already doing this type of input validation in your own modeling? If so, have you found it to be valuable?
- Is there other input validation that I haven't considered here?
- Any questions about doing this for your own system?

Using Better Boundary Conditions

- Pressure at an internal cyclone
- Particle withdrawal
- Non-uniform distributor

Internal Cyclones

- Outside walls of internal cyclones act as blockages
- Particles and gas leave the computational domain at inlets to cyclone
- Location of pressure BC at cyclone inlet is not ideal but unavoidable



Reactor model

Internal cyclones structure

Internal cyclones

- Pressure at inlet to cyclone is not equal to the vessel pressure
- Acceleration of particles toward cyclone inlets creates a pressure drop

$$\Delta P_{gas} \approx 0.5 \rho_g (v_{inlet}^2 - v_{vessel}^2)$$

$$\Delta P_{particles} = L \cdot v_{inlet} (v_{p,inlet} - v_{p,vessel})$$

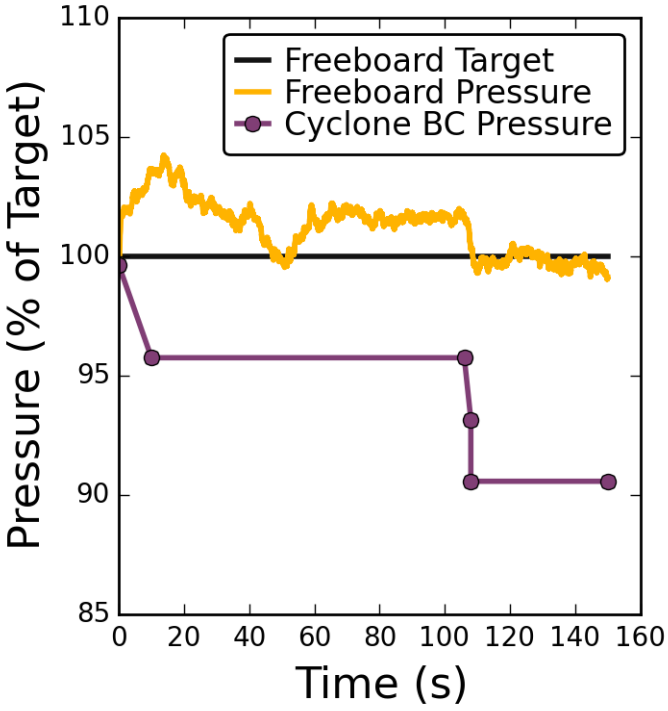
L = particle mass loading
v_{inlet} = inlet velocity
v_{vessel} = vessel velocity

Tip #5: Use cyclone inlet pressure to control vessel pressure

- Place a transient data point for pressure at the location where vessel pressure is measured.
- Use SFF file for pressure BC. Initially set BC pressure to vessel pressure.
- Periodically update SFF file to minimize difference between simulated vessel pressure and target vessel pressure
- Reread BC's through **Interact**

Implementation of control scheme

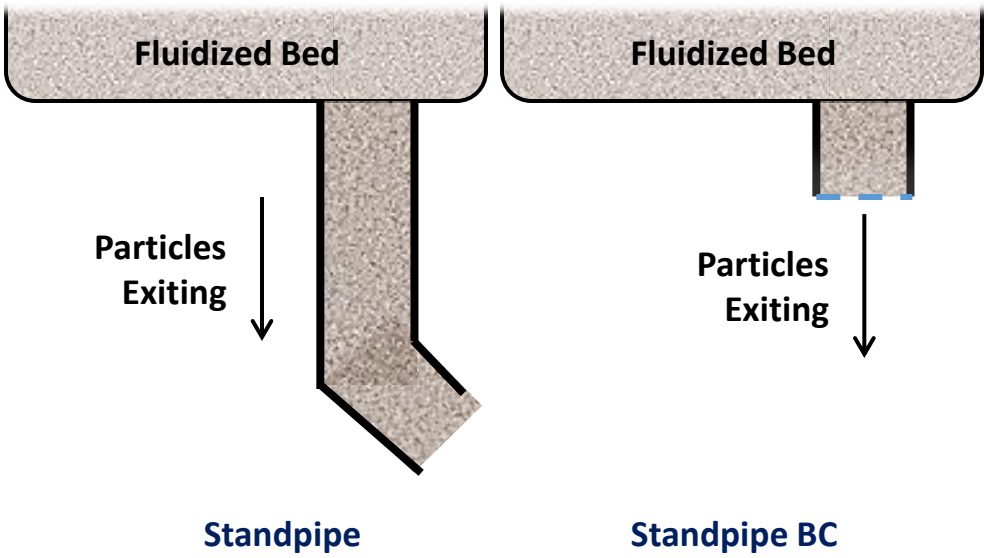
- Manual control
  - Easy implementation
  - Requires frequent user intervention
- Automated control script
  - Can be done in various scripting languages
  - Adjusts for changes in particle loading, particle velocity, etc.
  - See "How to use Interact features from a script or the command line" on support site



Manual pressure control in FCC regenerator

Particle withdrawals at Standpipes

- A boundary condition a short way into a standpipe eliminates the balancing force from particles below it



Particle Withdrawals at Standpipes

- A few possibilities:
  - Negative flow BC
  - Negative flow BC with control
  - Pressure BC
  - **Pressure BC with control**

Tip #6: Control particle flow rate out of standpipe using a pressure BC

- Use SFF file for pressure BC. Initially set BC pressure to neighboring fluid IC pressure.
- Periodically update SFF file to minimize difference between average solids flow rate leaving standpipe and target
- Reread BC's through interact
- Can be done manually or automatically with a script

Standpipe controller warnings and recommendations

- This requires solids to be present near the standpipe. If for some reason solids cannot reach the standpipe, an automatic controller can run away.
- Use gentle PID settings for automatic controller, because of time delays, there is a high risk of overshoot
- If pressure is too high, gas can start flowing back into the system. Solids flow rate will be zero and controller will get no response to adjustments
- Include a small amount of aeration – real or numerical

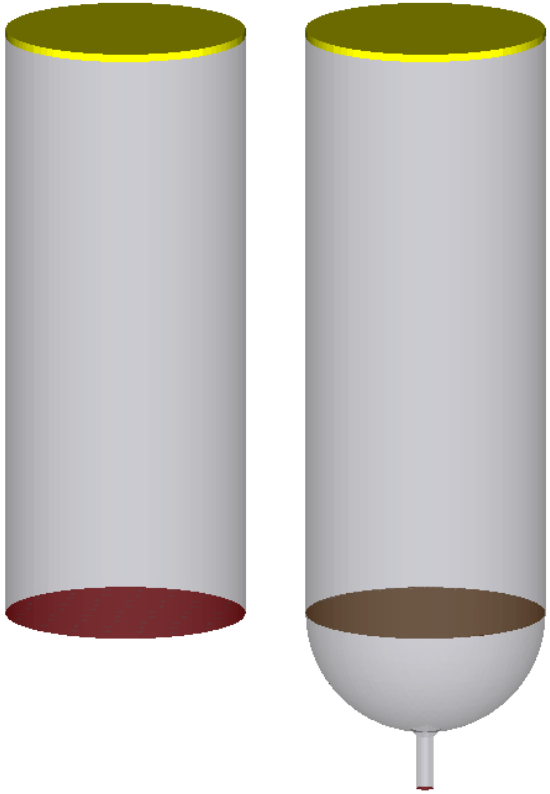
Distributors

- A uniform flow BC is commonly used but users often have questions
- Is the gas really distributed uniformly across the plate?
- Is there interaction between the bed and the plenum space below?

Reactor model with uniform flow BC

Barracuda VR Baffles

- Use a baffle as a distributor
- Not the intended purpose for this feature
- Baffles block all particle flow
- Baffles create a pressure drop across when fluid flows through



Reactor model with uniform flow BC

Reactor model with baffle distributor

Orifice pressure drop

Pressure drop of gas flowing through orifice

$$\Delta P = \frac{0.5\rho_g u_{or}^{\ 2}}{C_{d,or}} \qquad u_{or} = u_0 / A_r \qquad \mathrm{Re}_t = \frac{d_t u_0 \rho_g}{\mu}$$

Re_t	100	300	500	1000	2000	>3000
$C_{d,or}$	0.68	0.7	0.68	0.64	0.61	0.6

where A_r = open area, u_0 is superficial velocity, u_{or} is orifice velocity, d_t = vessel diameter

Baffle K-factor

- K-factor of baffles relates pressure drop across baffle to gas velocity

$$\Delta P = 0.5 K \rho_g u_0^{\ 2}$$

- For perforated plate,

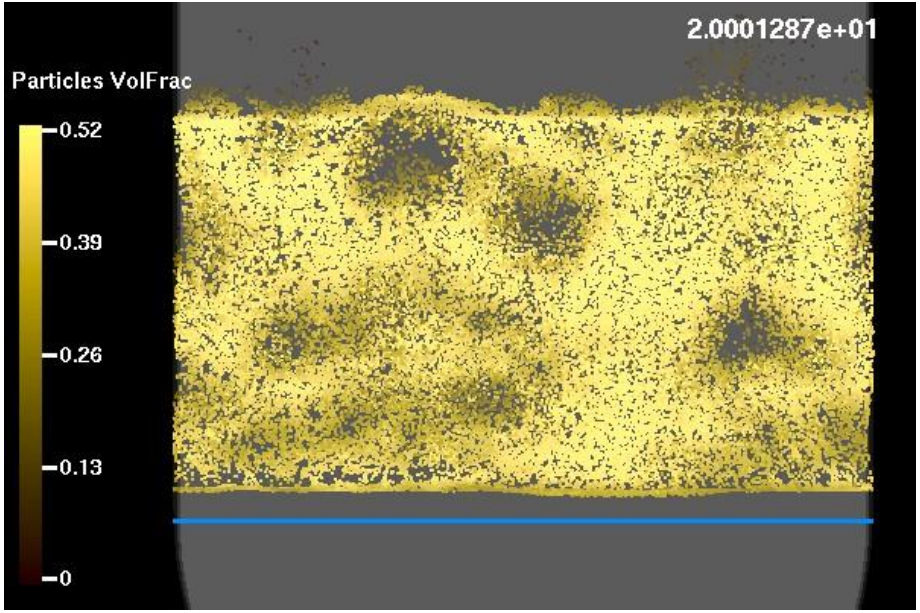
$$K = \frac{1}{\left(C_{d,or} A_r\right)^2}$$

Demonstration using textbook example (Kunii-Levenspiel 2nd ed., Chapter 4:)

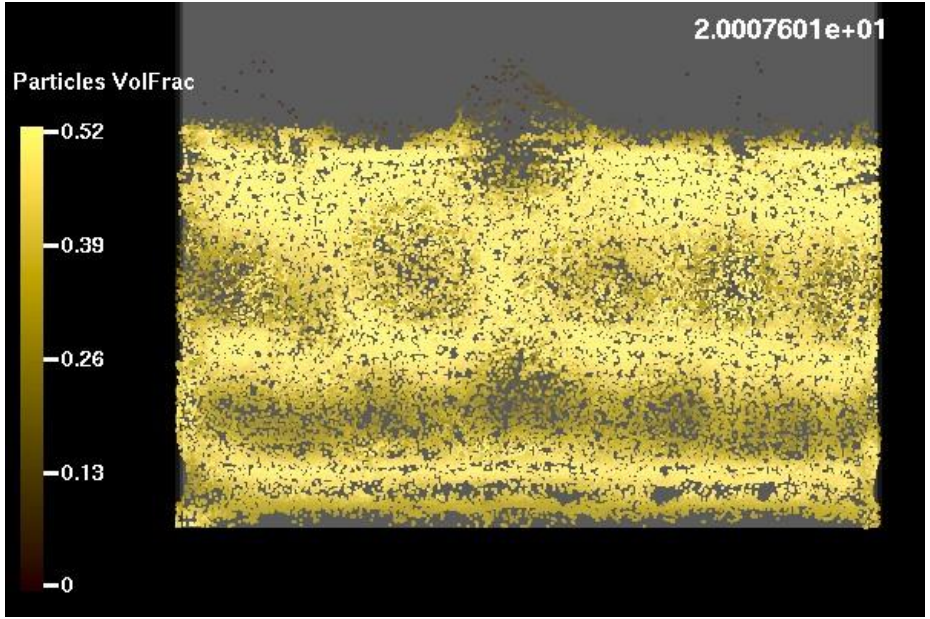
- 4 m diameter reactor
- 2 m of solids at close pack
- Close pack vol frac = 0.52
- Solids density = 1500 kg/m3
- Gas density = 3.6 kg/m3
- Viscosity = 2E-5 kg/m/s
- Pressure = 3 bar
- Superficial velocity = 0.4 m/s

- Particle size not provided, assume 400 microns
- Open area should be 1.3% to give pressure drop that is 30% of bed weight (*20 to 40% of bed weight is recommended*).
- $C_{d,or}$ = 0.6
- K-baffle = 15885

Designed Perforated plate vs Uniform flow

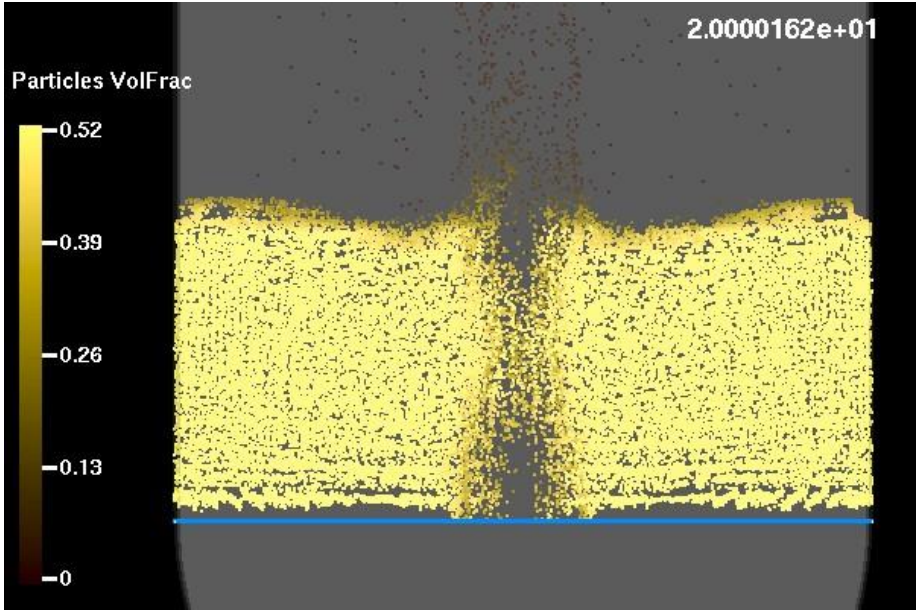


Baffle distributor,
ΔP = 30% of bed weight

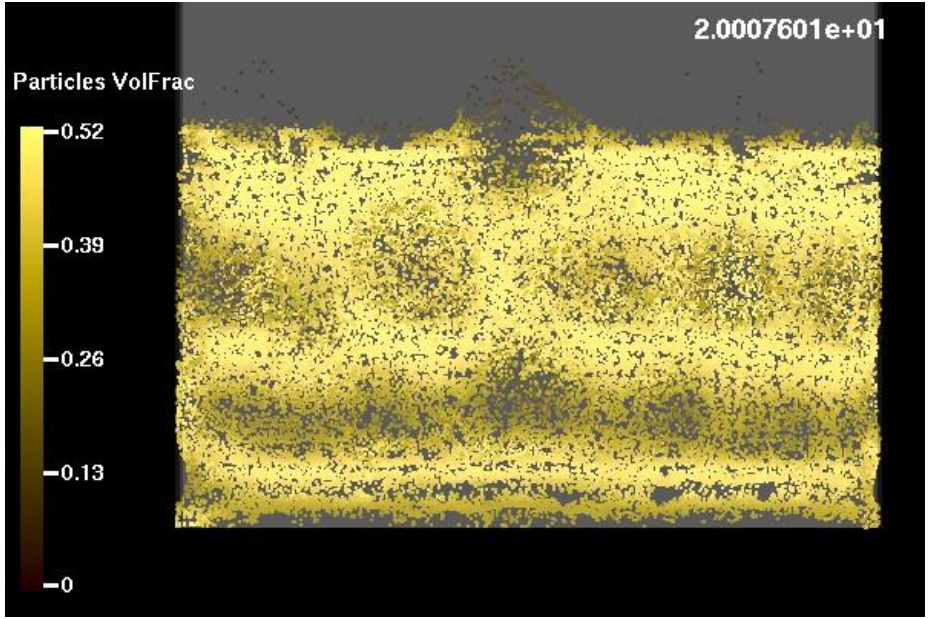


Uniform flow BC

Poor perforated plate vs Uniform flow



Baffle distributor,
ΔP = 0% of bed weight



Uniform flow BC

Tip #7: Use a uniform flow BC… unless you have reason not to

- Flow BCs work well for a distributor… unless the flow isn't uniform!
- They are easy to implement whereas other options take more work
- Consider more complicated distributor BCs only if needed

Q & A: Better Boundary Conditions

- Do you have internal cyclones or standpipes in your own modeling? If so, have these been a struggle in the past?
- Any questions about scripting or applying these tips to your own system?
- Any other questions about Boundary Conditions – even those not discussed here?

Implementing Chemical Reactions in Barracuda VR

- Chemistry is the main mechanism in Barracuda VR for converting mass from one material to another material

- As Barracuda VR users, it is necessary to understand how chemistry is being solved numerically to ensure that reactions are being solved in a way that is both accurate and stable.

Volume average chemistry

- Volume average chemistry uses “volume averaged” particle properties to calculate rate coefficients at the cell level.
- Calculation approach in each cell for each time step
  1. **Calculate rate coefficients** at start of t
  2. Use **ode solver** to calculate change in gas composition over the following time step based on rate coefficients and reaction rate expressions.
  3. Update gas compositions with the values calculated at t+Δt
  4. Add or subtract solid mass from particles based on reaction calculation

Volume average chemistry

Pros

- Uses sub-timesteps to calculate gas reactions. This can be stable and accurate, regardless of speed of reaction

Cons

- Does not conserve mass on each particle for solid → solid reactions
- Calculates rate coefficients only at start of hydrodynamic time step

Discrete particle chemistry

- Calculates reactions on each particle using individual particle properties and surrounding gas.
- Calculation approach at each particle for each time step
  1. Randomly select a reaction and calculate reaction rate.
  2. Update gas and particle compositions based on hydrodynamic time step

     $$\Delta[A] = d[A]/dt * \Delta t$$

  3. Repeat for remaining reactions

Discrete particle chemistry

Pros

- Reaction rates are calculated using individual particle properties
- Conserves particle mass for solid→solid reactions

Cons

- Does not use sub-timesteps to increase stability and accuracy for faster reactions
- Does not consider simultaneous gas reactions
- Cannot handle solid catalyzed gas reactions (input issue)

Types of chemistry where calculation form should be considered

1. **Solid catalyzed gas chemistry:** Gas phase chemistry is catalyzed by solid product.
2. **Solid transformation reactions** : Solid material is transformed into another solid material. Some part of original solid doesn't ever leave the particle
3. **Fast equilibrium chemistry:** Forward and reverse reactions which produce gas equilibrium
4. **Fast competing reactions:** Multiple reactions have the same reactants but produce different products
5. **Fast solid chemistry:** Particle properties are changing quickly

Tip #8: Use volume average chemistry for solid catalyzed gas chemistry

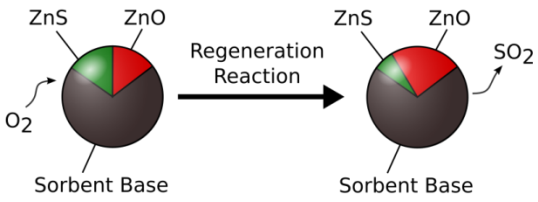
- Gas phase reaction is dependent on presence of solid mass. Does not consume or produce a solid product

- Cannot be implemented in discrete chemistry. Must use **volume average chemistry.**

- Example: Heterogeneous CO combustion used in FCC regenerators and other applications

Tip #9: Use discrete chemistry for solid transformation reactions

- Solid material is transformed into another solid material. Some part of original solid doesn't ever leave the particle.



- If particle composition is going to be analyzed, must use **discrete particle chemistry**
- Examples: desulfurization chemistry, chemical looping combustion, CO_2 adsorption

Tip #10: Use volume-average chemistry for fast competing or fast equilibrium reactions

- Multiple fast reactions that share reactants and/or products
- Must use **volume average** chemistry to ensure accurate gas compositions
- Examples: FCC regen chemistry, FCC cracking chemistry

Tip #11: Minimize the numerical damage when there are no good options

Difficult scenario:

$$A(s) + 3B \leftrightarrow C(s) + D$$

where rates are fast and balanced to give about 50-50 mix of gas

$$A(s) + 3B \rightarrow C(s) + D \quad \text{(endothermic)}$$

$$C(s) + D \rightarrow A(s) + 3\,B \quad \text{(exothermic)}$$

- Volume average chemistry will not preserve composition of particles
- Discrete chemistry will likely cause instability
- Use discrete chemistry with small time step for stability
- Use volume average if particle composition isn't important

Q & A: Implementing Chemistry in Barracuda VR

- Questions about your specific reaction scheme in your models?

Miscellaneous Tips for Setting up and Running Models

- Selecting key data outputs
  - Transient data points
  - Raw data
  - GMV
- Monitoring Barracuda VR simulations
  - Number of computational particles
  - Overpacking
- Getting help

Tip #12: Place transient data points at all real pressure and temperature measurement locations

- Validation of model is important
- Compare same values to the extent possible
- Define point locations using xyz locations

Transient Data Output

Settings

Write frequency: 1 | Flush frequency: 0 | Clear All

Output file name: trans.data | Browse

Type		x (m) / i	y (m) / j	z (m) / k	Comment
Fluid temp	xyz	-0.235	0.235	0.2	K1
Fluid temp	xyz	-0.235	0.235	0.9366	K2
Fluid temp	xyz	-0.235	0.235	1.851	K3
Fluid temp	xyz	-0.235	0.235	3.071	K4
Fluid temp	xyz	-0.235	0.235	4.291	K5
Fluid temp	xyz	-0.235	0.235	6.57	K6
Fluid temp	xyz	0.235	-0.235	0.2	K7
Pressure	xyz	-0.235	-0.235	3.6	P1
Pressure	xyz	-0.235	0.235	3.6	P2
Pressure	xyz	0.235	-0.235	3.6	P3
Pressure	xyz	0.235	0.235	3.6	P4
Pressure	xyz	-0.235	-0.235	3.8	P5
Pressure	xyz	-0.235	0.235	3.8	P6
Pressure	xyz	0.235	-0.235	3.8	P7
Pressure	xyz	0.235	0.235	3.8	P8
Pressure	xyz	-0.235	-0.235	4	P9
Pressure	xyz	-0.235	0.235	4	P10
Pressure	xyz	0.235	-0.235	4	P11

Tip #13: Raw Data output

Raw Data

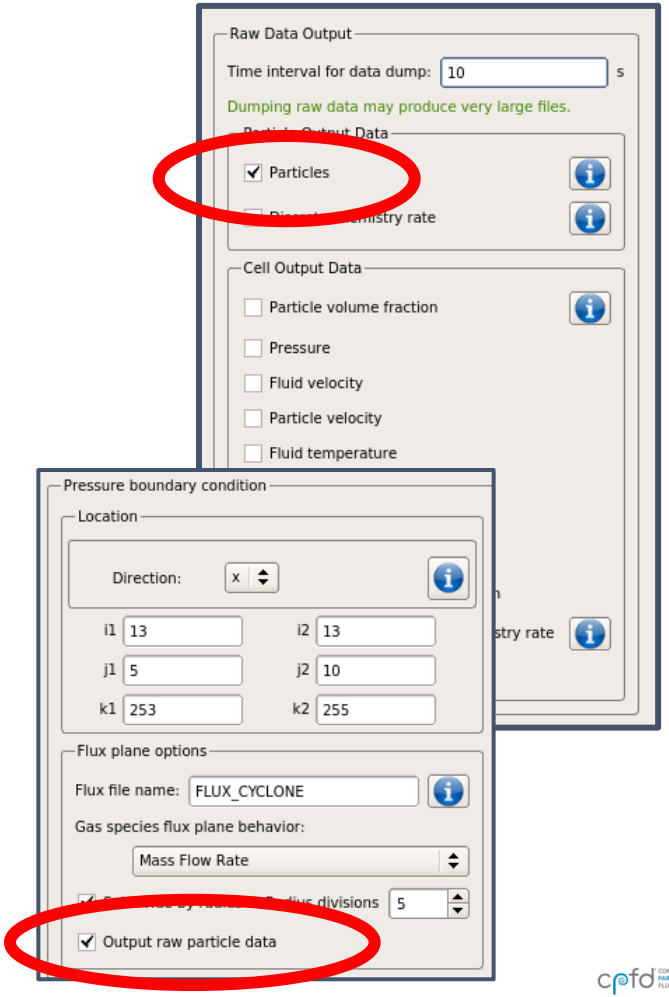
- Output all raw particle data every 10 seconds or so
- Can be used for quantifying segregation, bypassing, …

Flux planes

- Select raw particle data output at boundary flux planes
- Can be used for PSDs and particle composition

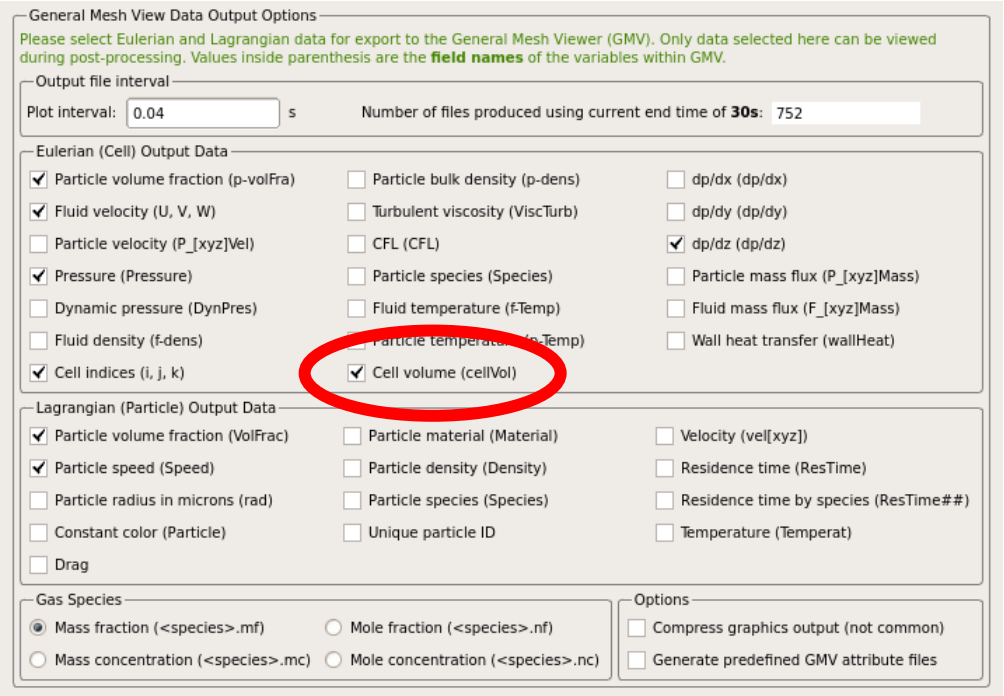
Support site help:

- "Analyzing data with Python and NumPy"
- "Using Python to Calculate PSDs from Raw Particle Data Files"



Tip #14: Don't forget to output cell volume as GMV output

- Scripts are available for creating raw text data from Gmv files
- See "Data-mining GMV files using gmv2txt.py" on support site
- Cell volume is critical for calculating weighted averages



Tip #15: Maintain size of computational particles

- Systems with particle inlets and outlets
- Check that number of computational particles per mass at inlets is comparable to particles initialized in bed
- **POPUL*** files have information for each species
- **history.log** has total number of computational particles
- Adjust number of computational particles in SFF files as necessary ("Number density manual")

Tip #16: Watch for Overpacking

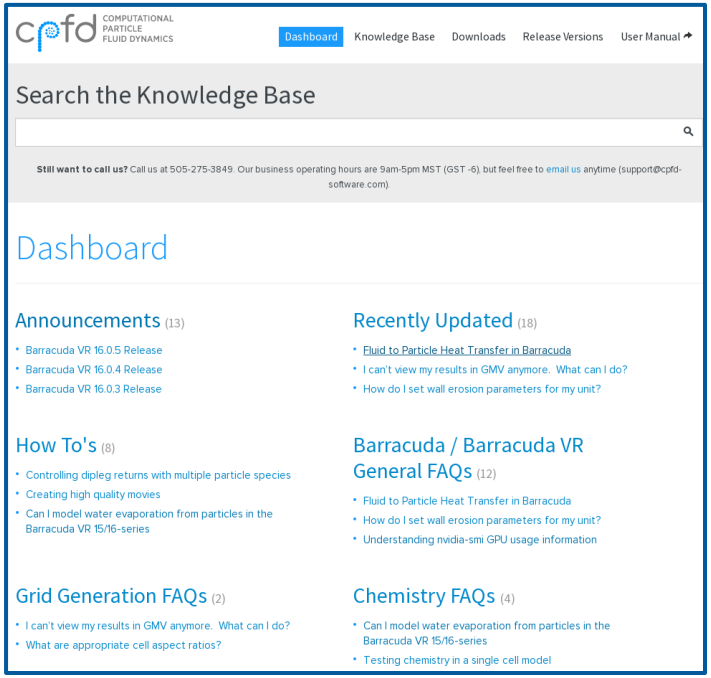
- Persistent overpacking of cells (“Low”, “Med”, “Hi” columns) should be avoided.
- Reducing time step will often fix serious overpacking problems
- Increasing computational particles

Low	Med	Hi	R
32	0	0	2
28	0	0	2
30	0	0	2
30	0	0	2
[illegible]	6	0	1
116	12	0	0
262	17	[illegible]	0
415	25	[illegible]	0
152	0	0	2
[illegible]	[illegible]	0	2
57	0	0	2

Tip #17: Get help when you need it

The Barracuda VR support website at www.cpfd-software.com contains:

- Access to knowledge base posts
- Tips for successful modeling
- Barracuda VR user manual



General Q & A

- Anything!