CPFD Software Updates: Product, R&D, and Q&A

Sam Clark, Andrew Larson, and James Parker

CPFD Software

June 20, 2024

Outline

The Barracuda Virtual Reactor Development Team

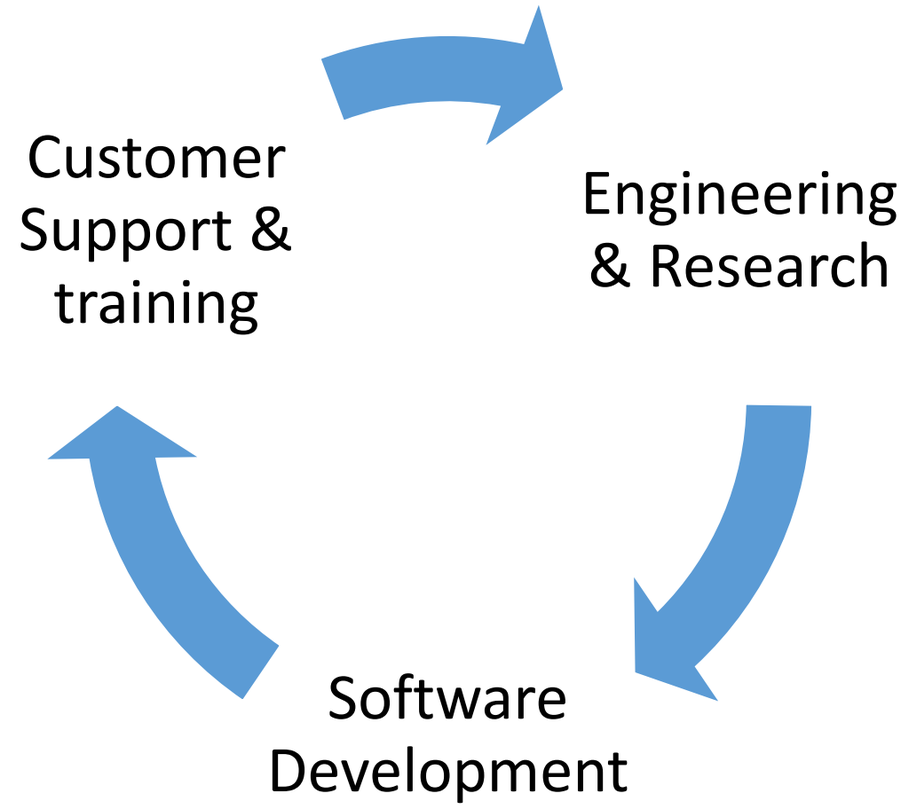
R&D Updates – Dr. James Parker

Product Updates – Andrew Larson

Support and Training Updates – Sam Clark

Q&A

The Barracuda Virtual Reactor Development Team




Paul Zhao


Sam Clark


James Parker


Andrew Larson


Rosemary Clark


Paul Earhart


Hoan Larson


Shashank Karra


Pramod Bangalore


Tanner Stelmach

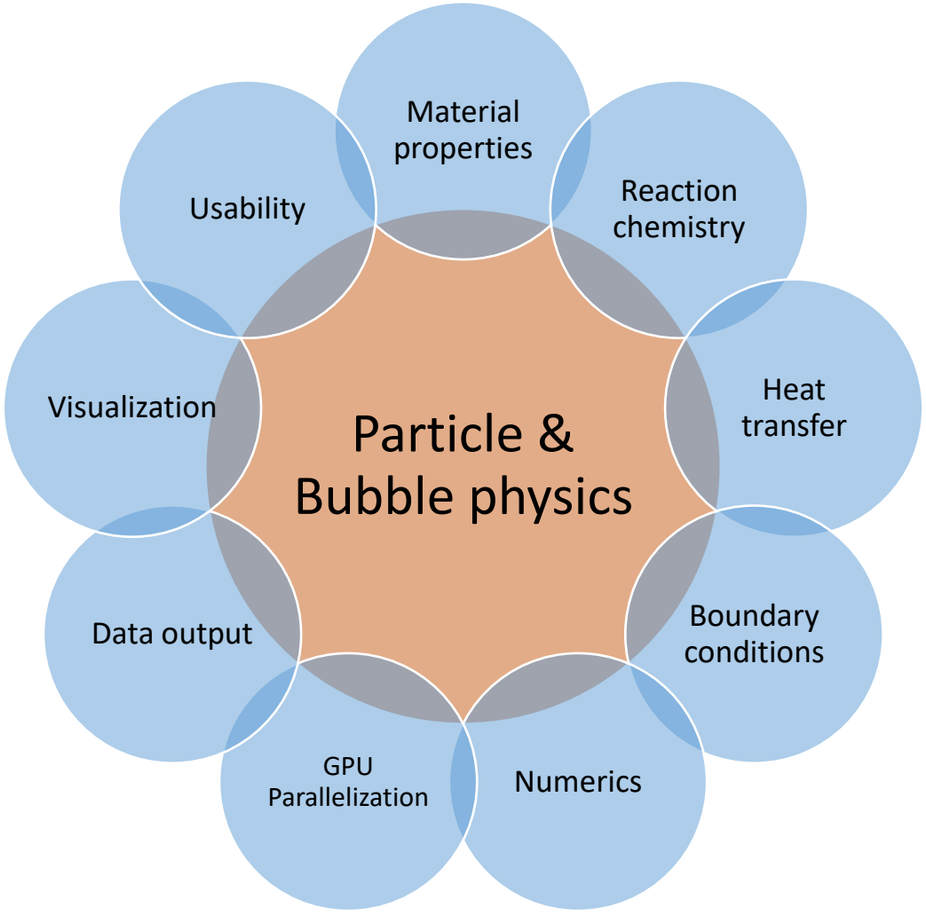
Engineering and Research

R&D areas:

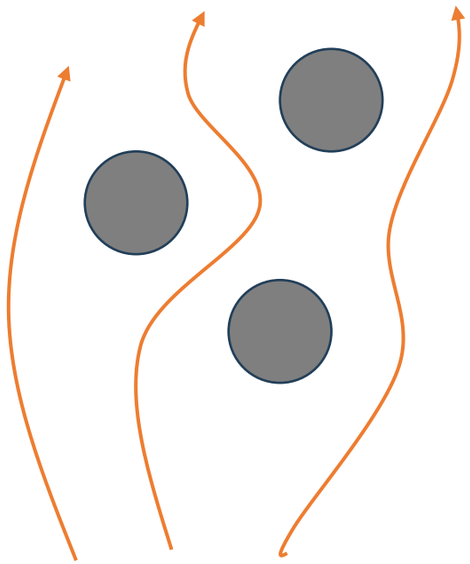
- Expanding application areas
- Increasing calculation speed & domain sizes
- Improving usability

Particle and bubble physics is central Barracuda Virtual Reactor simulations

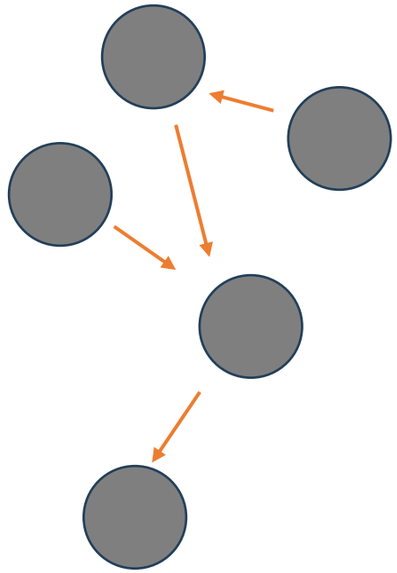
- Drag models – validation and recommendations
- Particle-particle models
- Bubble breakup and coalescence



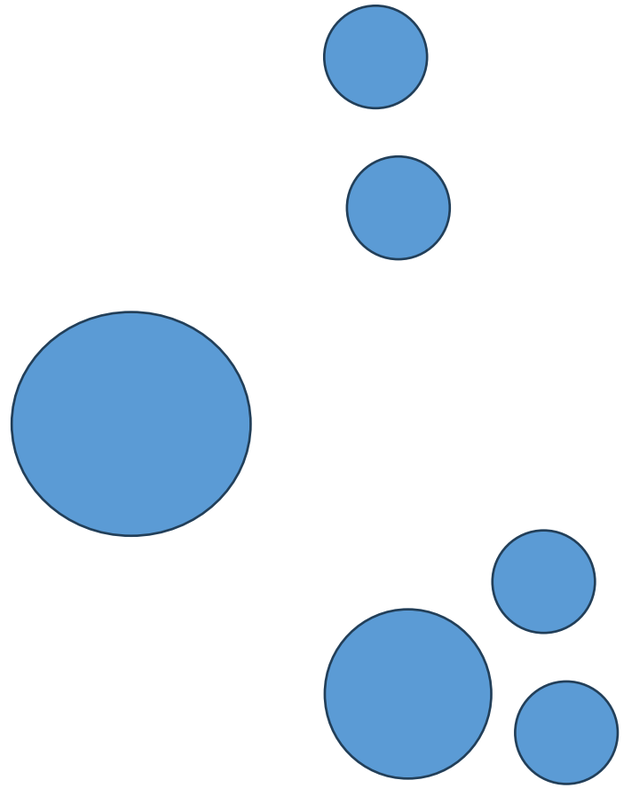
Particle / Bubble Physics



Particle drag



Particle-particle interactions



Bubble coalescence / breakup

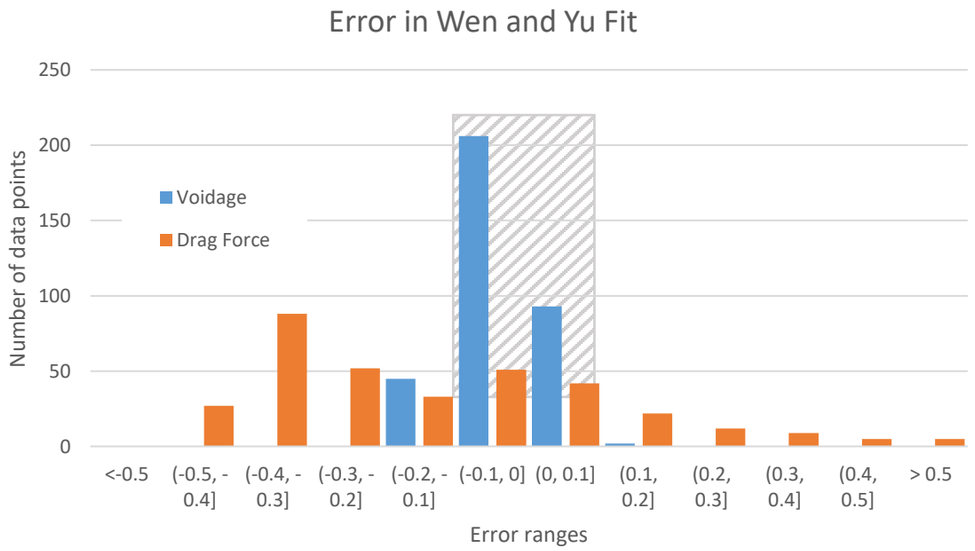
Spherical drag model validation

Assembled the data sets used by Wen and Yu (1966) plus data of Jottrand (1952)

- Particle diameters: 20 um to 6.35 mm
- Voidage: 0.36 to 0.95

Voidage error consistent with +/- 10% reported by Wen and Yu

Drag force errors are significantly higher



Re-creation of Wen & Yu Fig 3

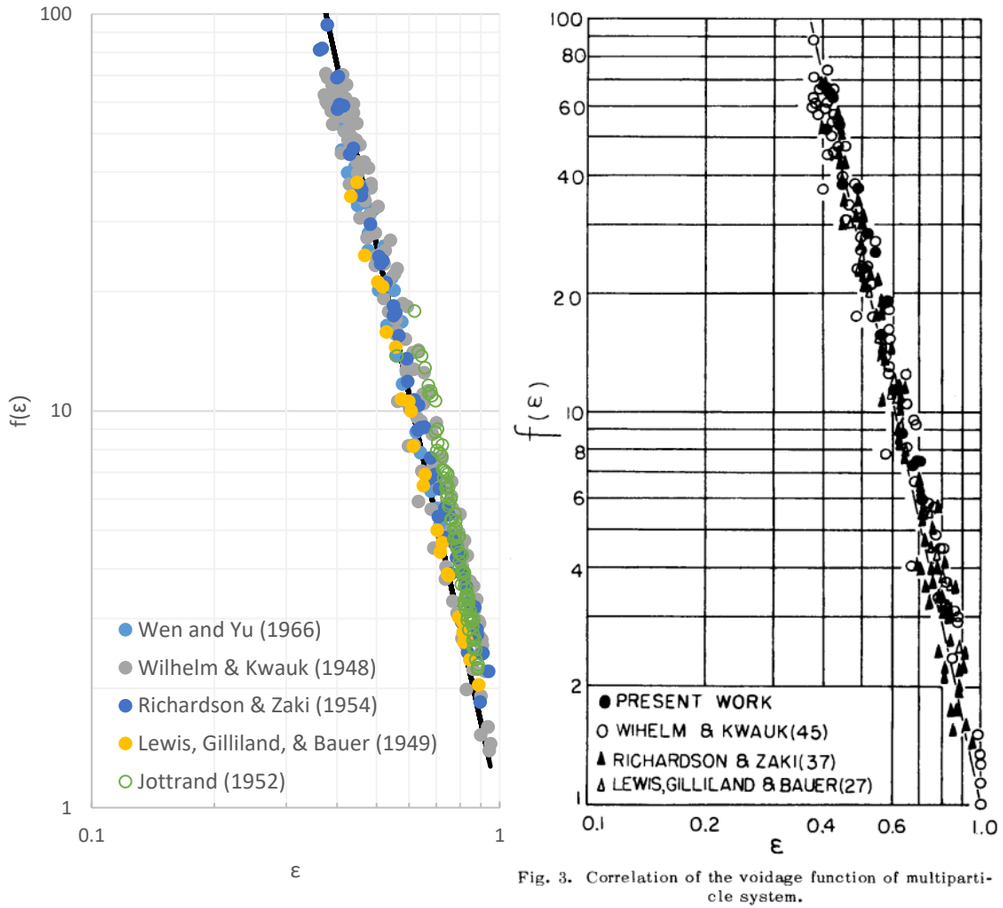


Fig. 3. Correlation of the voidage function of multiparticle system.

$$F_{WY}/F_{Stokes} = \left(1 + 0.15\,\mathrm{Re}^{0.687}\right)\varepsilon^{-3.65}$$

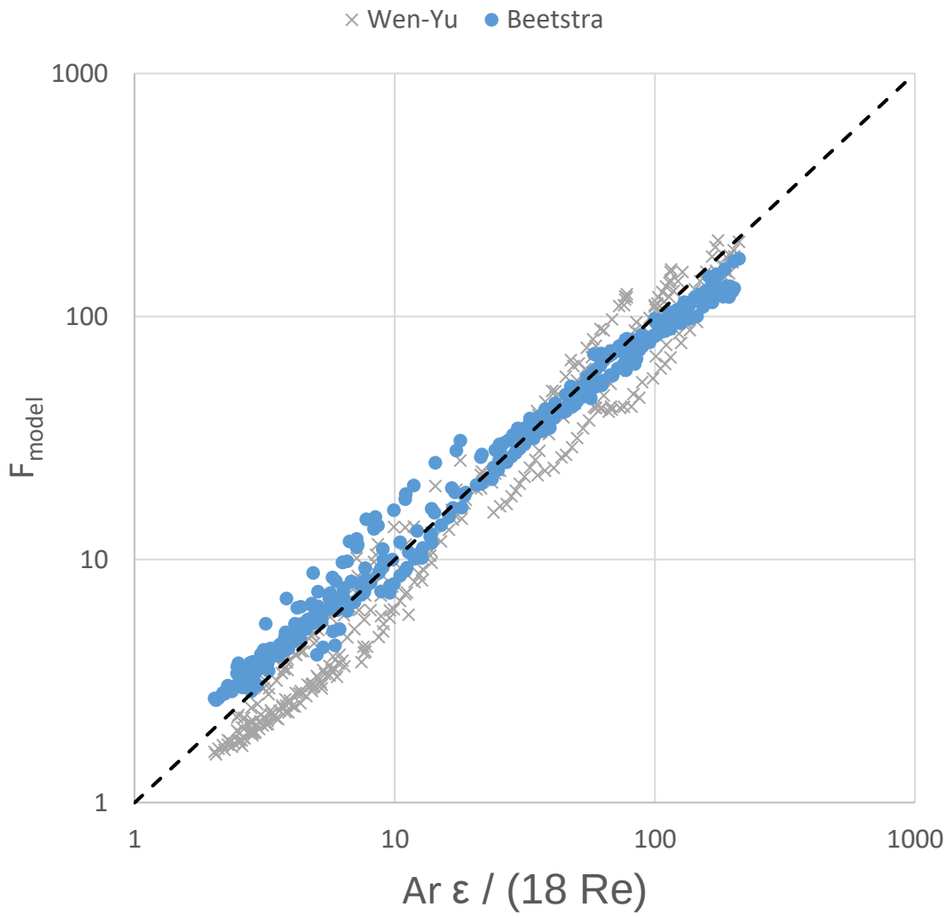
Spherical Model Results

Tuning dataset contains defluidized pressure / velocity data in addition to expansion data

Beetstra drag model has low overall error

Improvement to models possible by tuning to data

Drag model	Tuning Dataset		Full Dataset	
	Avg. Err.	*Max. Err.*	*Avg. Err.*	*Max. Err.*
New model - Tuned	*8.9%*	*23.3%*	-	-
New Model - Untuned (A=180, B=1.8)	*11.6%*	*32.3%*	*17.6%*	*47.2%*
Beetstra et al (2007)	**15.5%**	**37.6%**	**25.2%**	**88.6%**
Di Felice (1994)	20.9%	33.9%	24.5%	49.0%
Wen-Yu / Ergun Blend (A=180, B=1.8)	22.6%	47.6%	26.3%	77.1%
Wen and Yu (1966)	26.6%	58.6%	26.9%	58.6%
Gidaspow (1986)	31.2%	98.9%	27.5%	98.9%
Tang (2015)	32.1%	53.9%	34.5%	89.6%
Tenneti (2011)	36.3%	54.3%	31.7%	73.1%
Ergun (1949)	57.7%	230.3%	42.7%	230.3%



Non-spherical modeling

Work with Molten Industries on modeling their decarbonization technologies

Separation of carbon particles from hydrogen in cyclone

Based sphericity on the bulk density measurements and Sphericity vs voidage curve from Wen and Yu (1966)

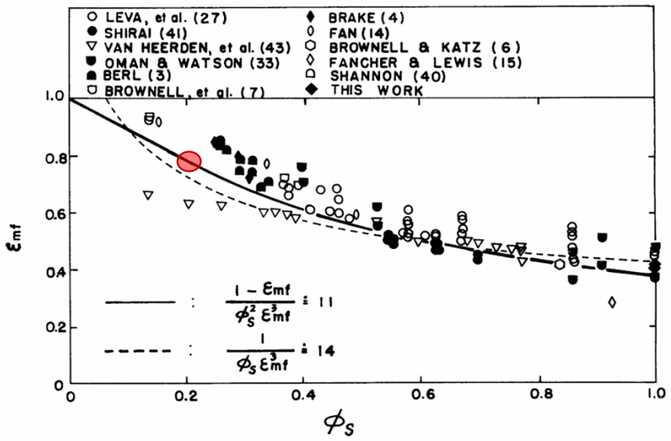
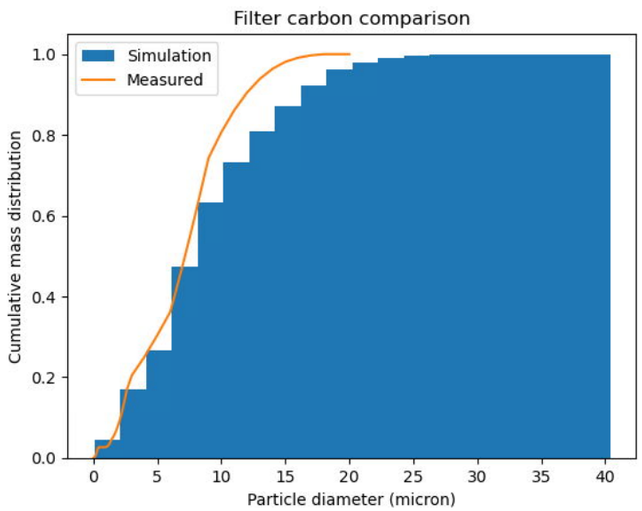


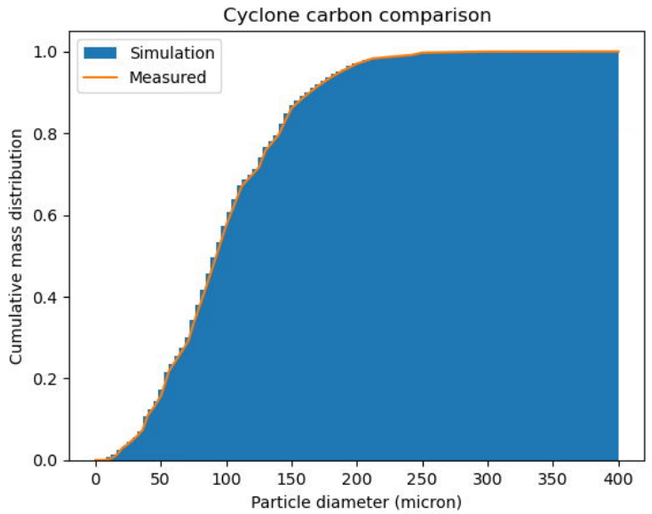
Fig. 8. Relation between ε_{mf} and ϕ_s.

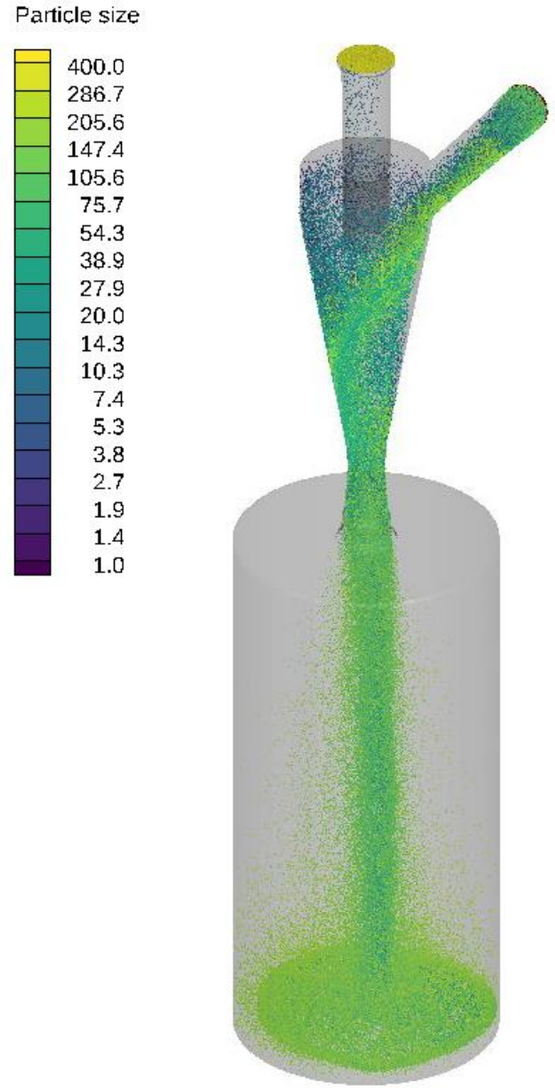
Non-spherical modeling

Simulated efficiency matched the measured efficiency exactly

Very close match with measured size distributions







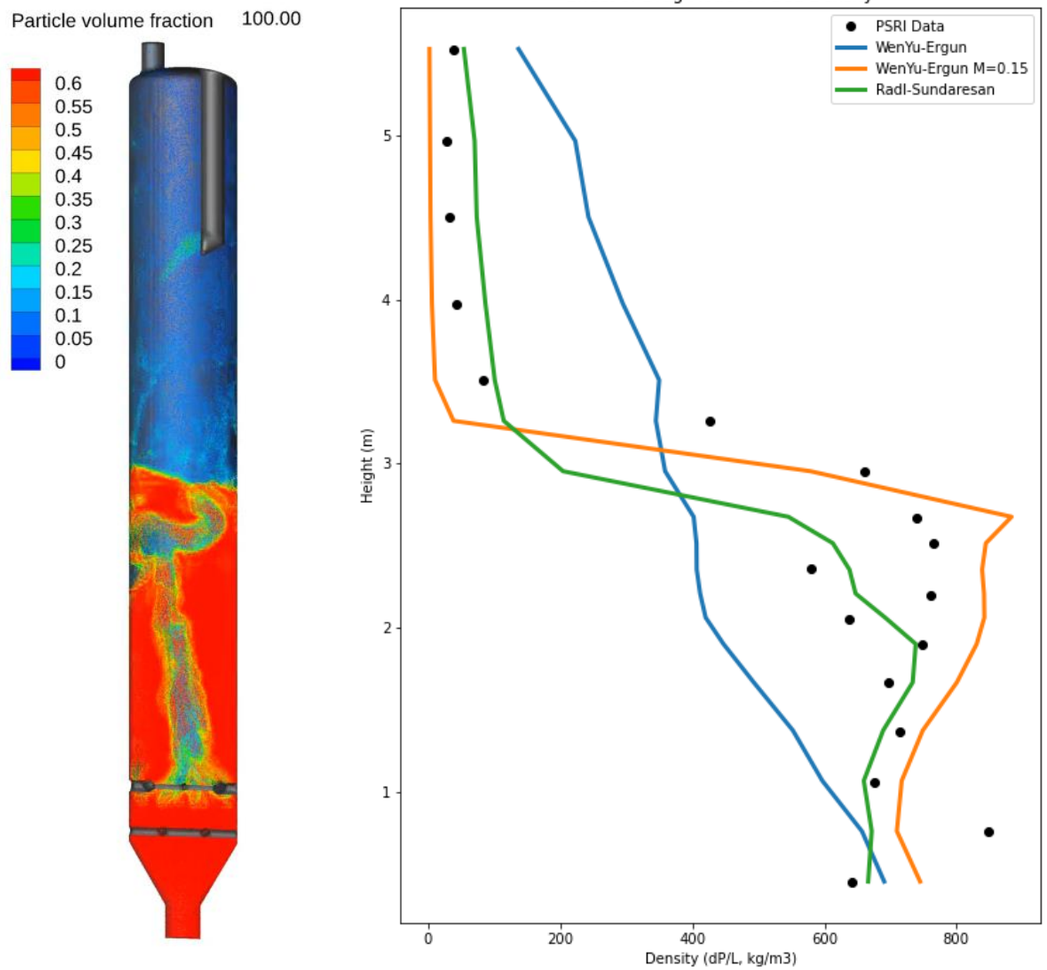
Subgrid modeling

Radl-Sundaresan subgrid drag model shows significant improvement for modeling of large systems

Based on Beetstra drag model

Accounts for hydrodynamic clustering of particles occurring at the subgrid scale

Accumulation of solids on crossovers



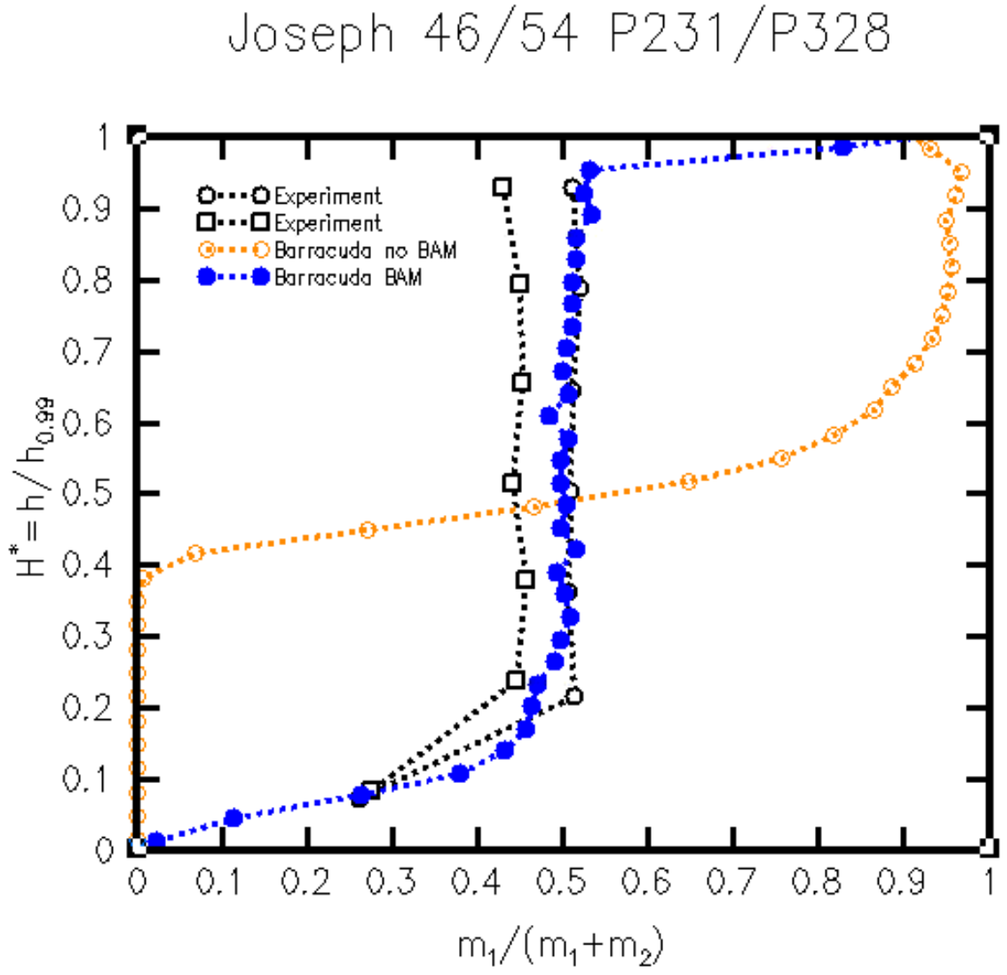
2010 PSRI Challenge problem case – 8 ft bed

Particle-particle models

Blended acceleration model

Simulates the common acceleration of particles that would occur due to particle-particle contacts

Improves particle segregation predictions when size or density differences are present

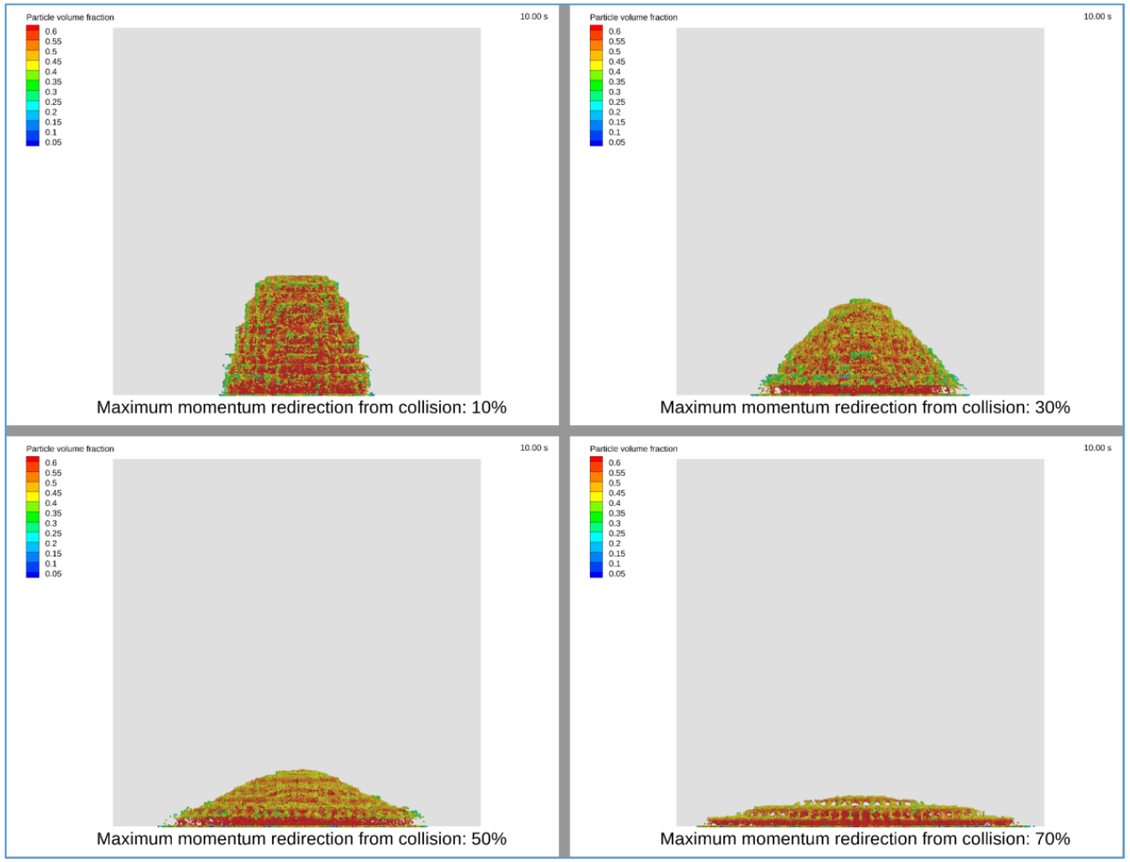


Particle-particle models

Directional momentum redirection

Simulates the effect of particle-particle collision due to stress model

- Replaces random-scatter approach
- Improved participation of particles in bed
- Angle of repose predictions



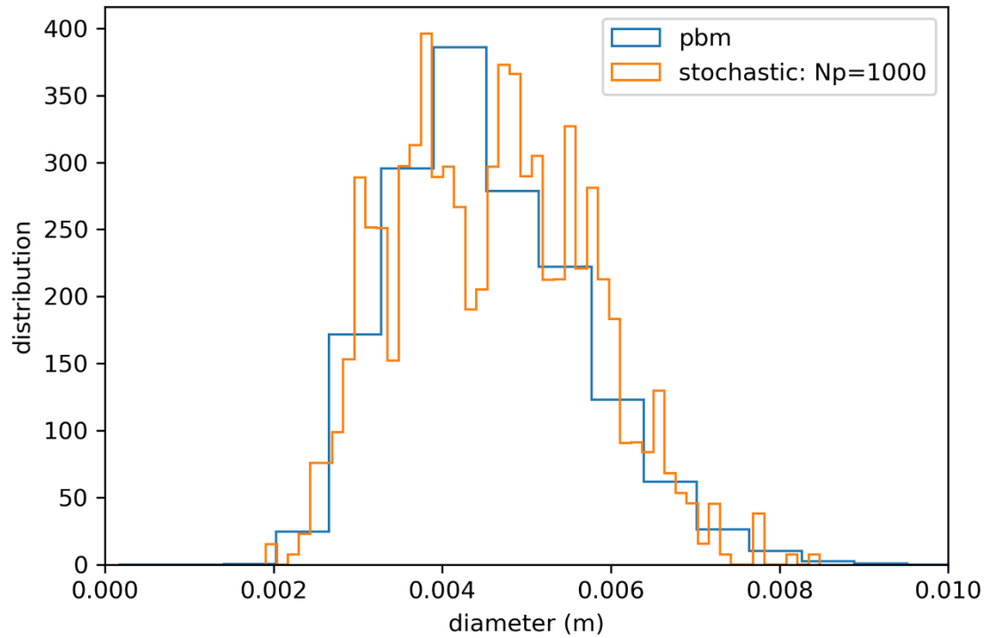
1 – sin(Angle of repose) = Momentum redirection

Bubble Breakup and Coalescence

Bubble breakup / coalescence is critical for determining the evolution of bubble size within a simulation

Stochastic implementation of the bubble breakup and coalescence model of Lehr (2002)

Reduced calculation complexity from N^2 to N through some simplifying assumptions



Product Updates

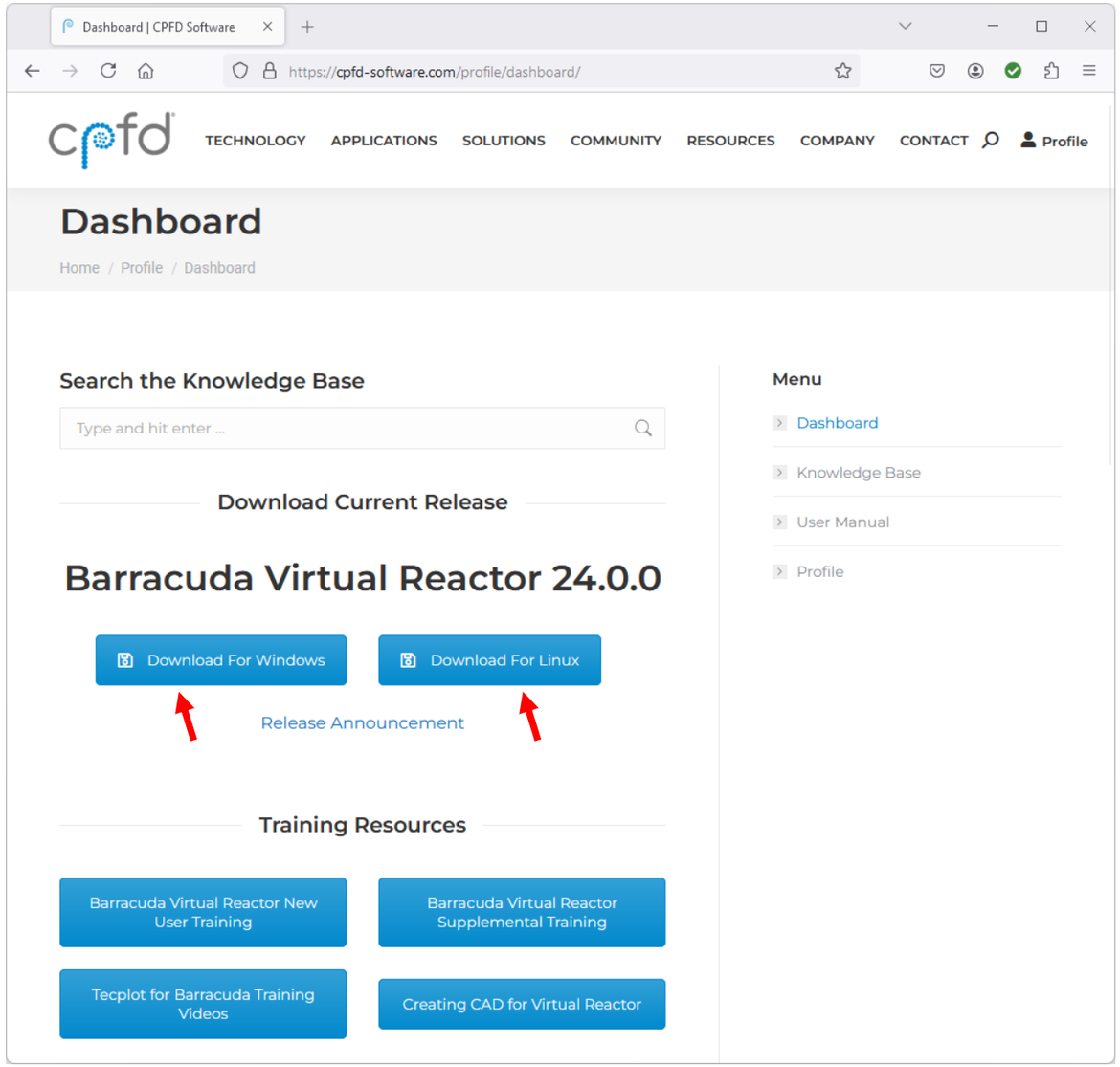
Two releases per year

- April/October release schedule
- Latest release can always be downloaded on the Dashboard of the CPFD support site

Substantial physics improvements

Improved usability

Maintained GPU acceleration benefits



Barracuda Virtual Reactor 22.1 Release

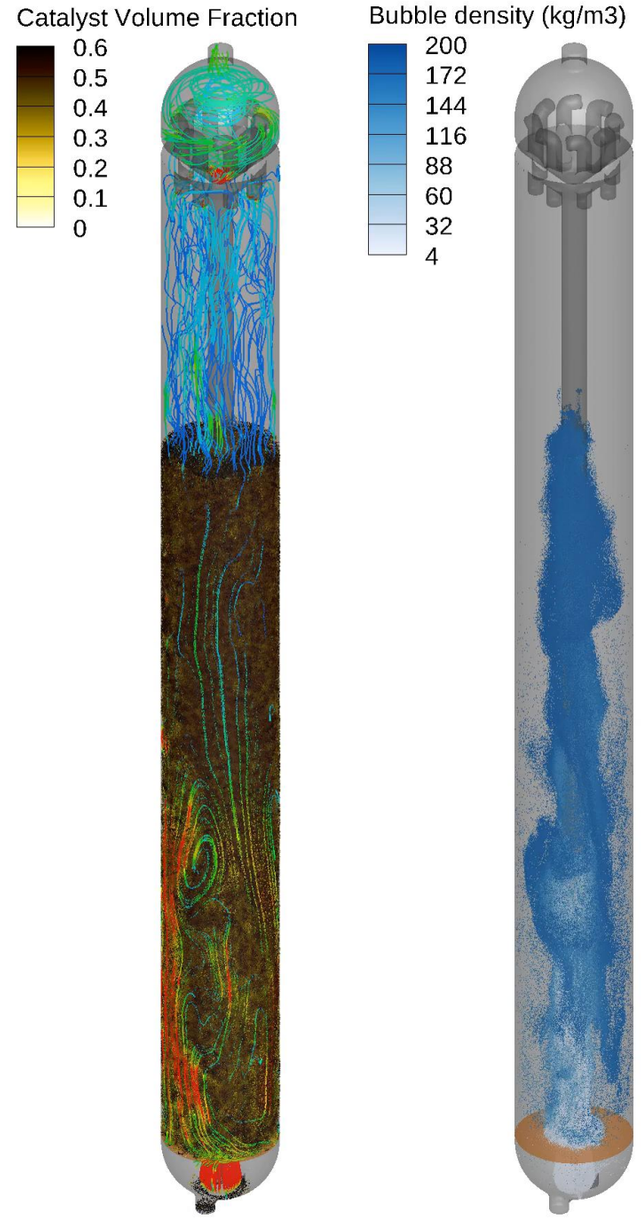
Bubbles

- Gas absorption models
- Bubble condensation/evaporation
- Compressibility
- Bubble drag models

Tracers Improvements

GUI BC Dialog Redesign

batch_movie Improvements



Barracuda Virtual Reactor 23.0 Release

Drag model updates

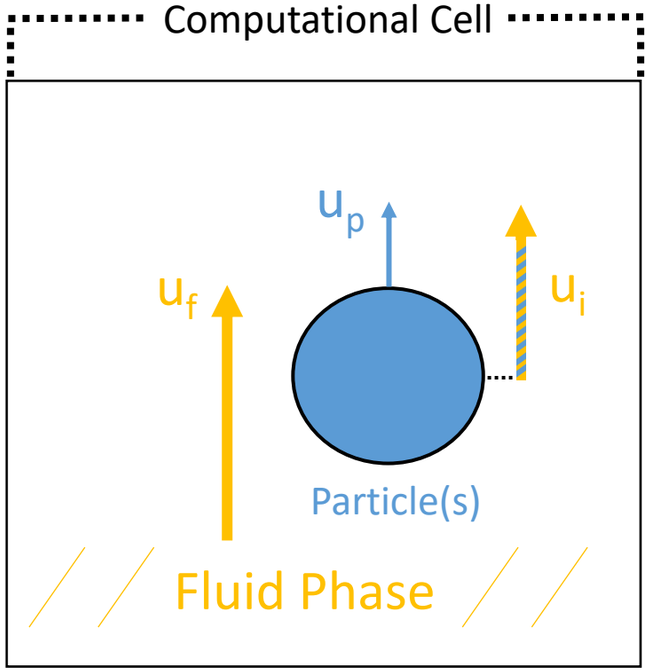
- Beetstra
- Tenneti
- Tang
- Syamlal-O'Brien

Temperature-dependent material densities

Secondary Feeds GUI redesign

Time-averaged fluid velocity fluctuations

New utility script: pid_controller.py



Interstitial Velocity $u_i = u_f - u_p$

Superficial Velocity $U = \theta_f(u_f - u_p)$

θ_f: Fluid Volume Fraction

Barracuda Virtual Reactor 23.1 Release

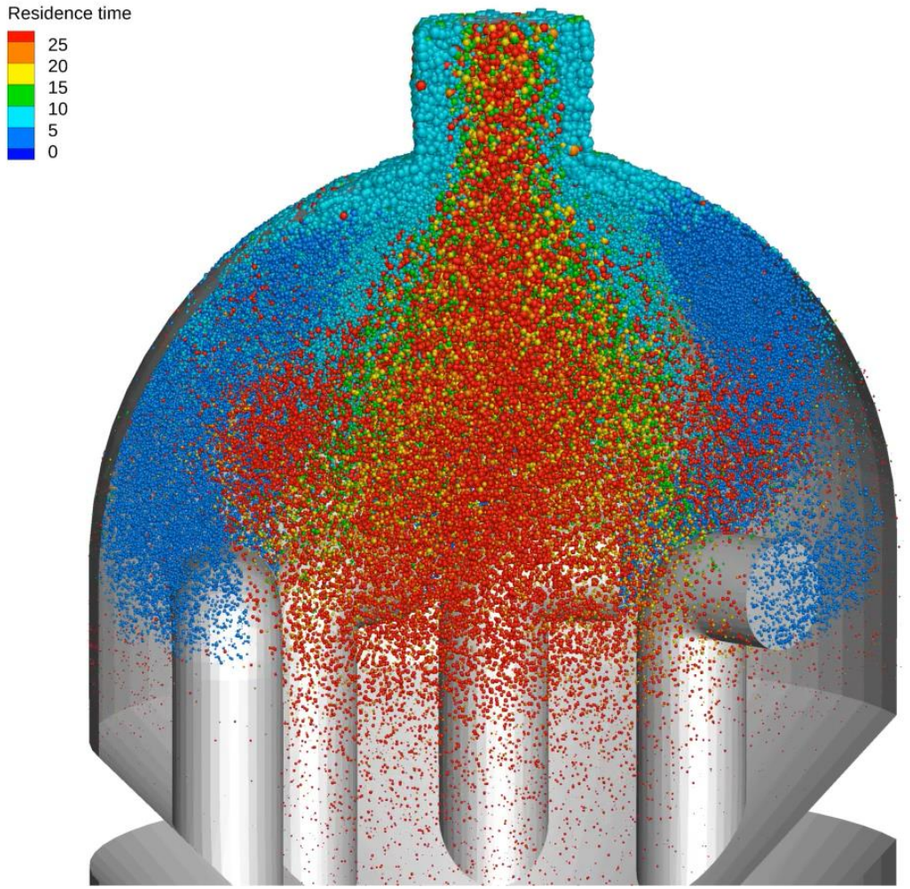
Bubble coalescence and breakup

Radl-Sundaresan drag model

Per-species close pack volume fraction

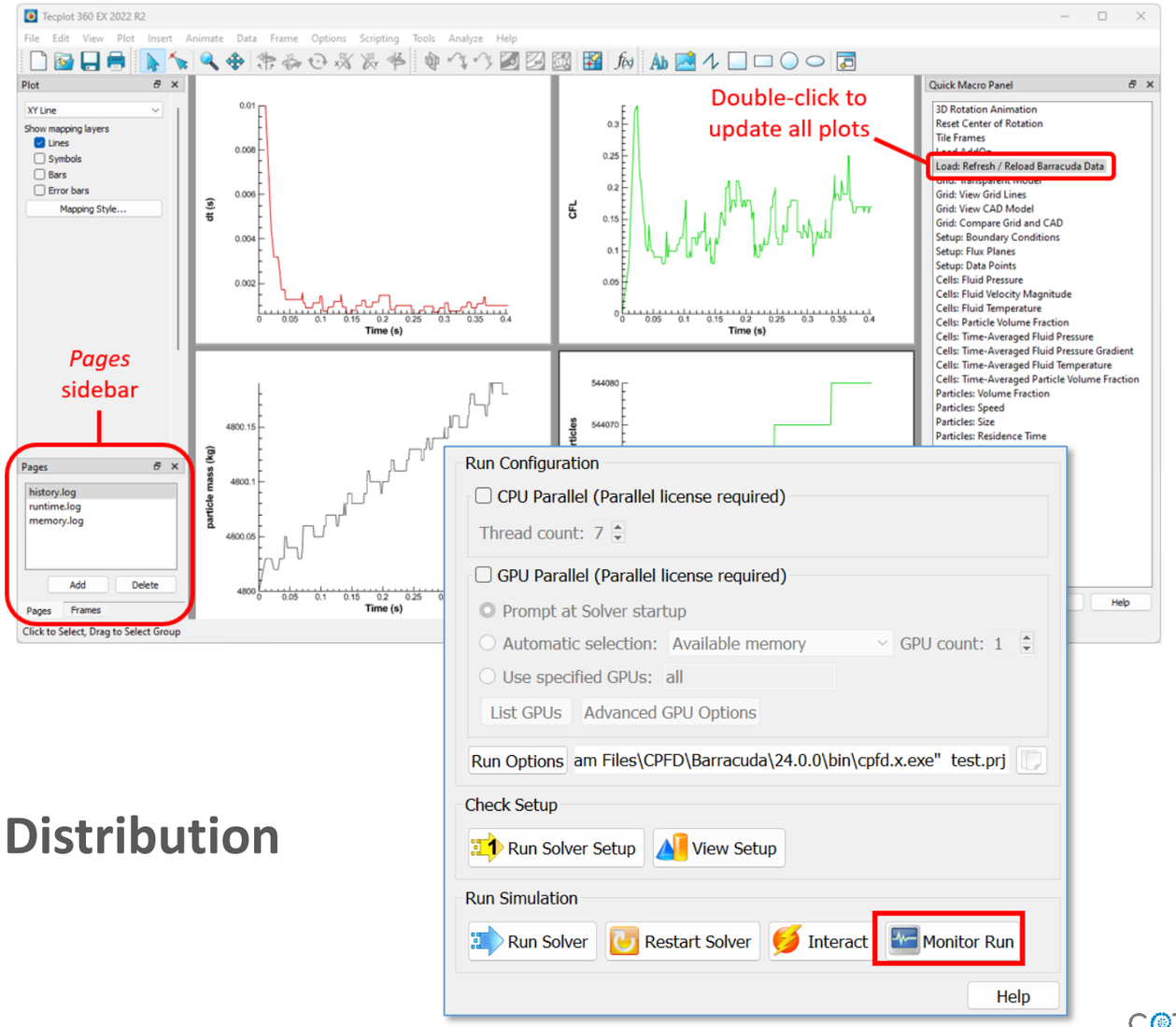
Output improvements

- New output files: mass.log and energy.log
- Time-varying visualization output data
- New data output: chemical reaction rates



Barracuda Virtual Reactor 24.0 Release

- Monitor Run Automated Plots
- SFF Option to Disable Interpolation
- Time-Varying Gravity
- Particle-particle Thermal Conduction
- Evaporation Model Stability Improvements
- Directional Momentum Redirection
- BC Connector Pressure Feedback
- Volume-Average Chemistry Heat of Reaction Distribution



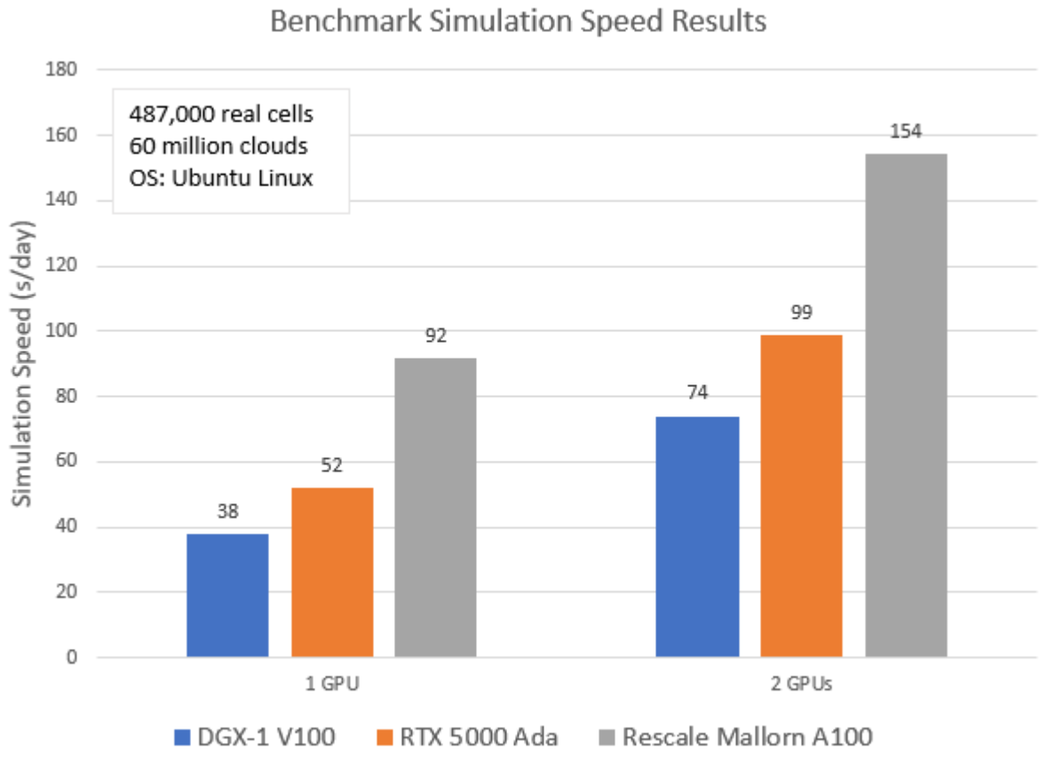
NVIDIA GPU Hardware Advancements

Latest-generation NVIDIA GPU cards give impressive speed boosts for Virtual Reactor simulations

For users with on-premise hardware:

- If you are currently running on a computer and/or GPU card more than 5 years old, we recommend upgrading to new hardware

Running Barracuda on the cloud allows users to access latest-generation GPU cards



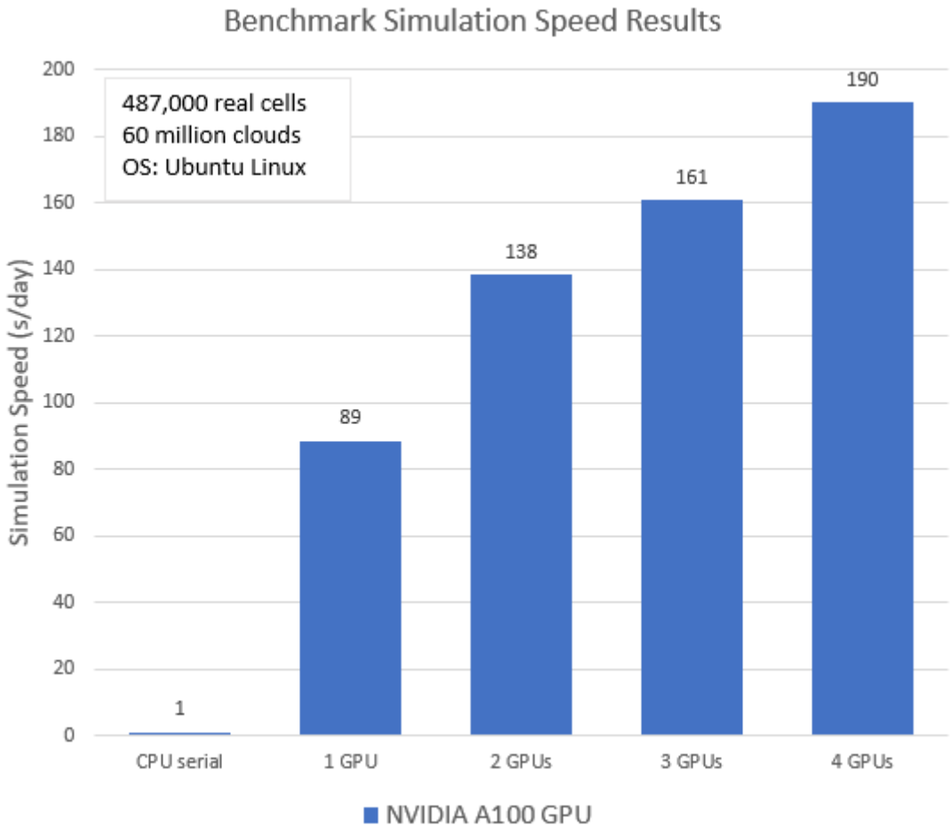
Virtual Reactor Multi-GPU Speedup

Multi-GPU acceleration enables fastest possible simulation speeds

- Only supported on Linux
- 1 GPU license required for each GPU card used

Metered licensing is supported

- Choose single- or multiple-GPU acceleration based on your needs
- Pairs well with cloud-based HPC

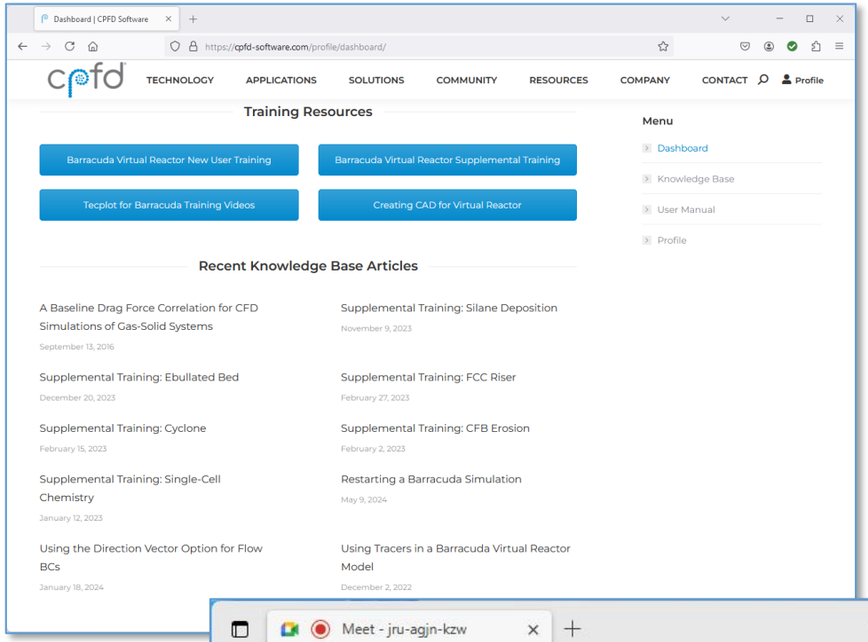


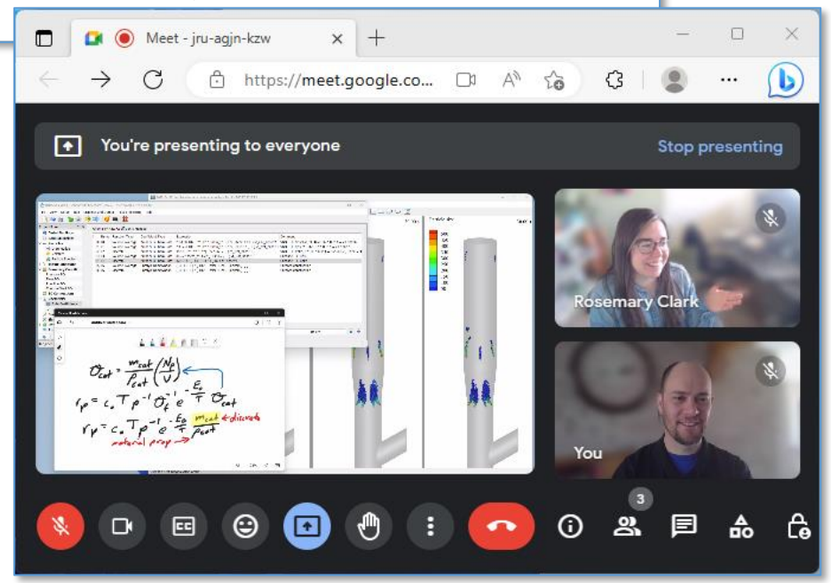
Support and Training Updates

CPFD's support team strives to provide excellent support to Barracuda Virtual Reactor users worldwide

Best way to contact us is via email: support@cpfd-software.com

- We might have an answer already documented on our support site
- If live screen-sharing is helpful to help you solve a problem, we're happy to schedule web meetings



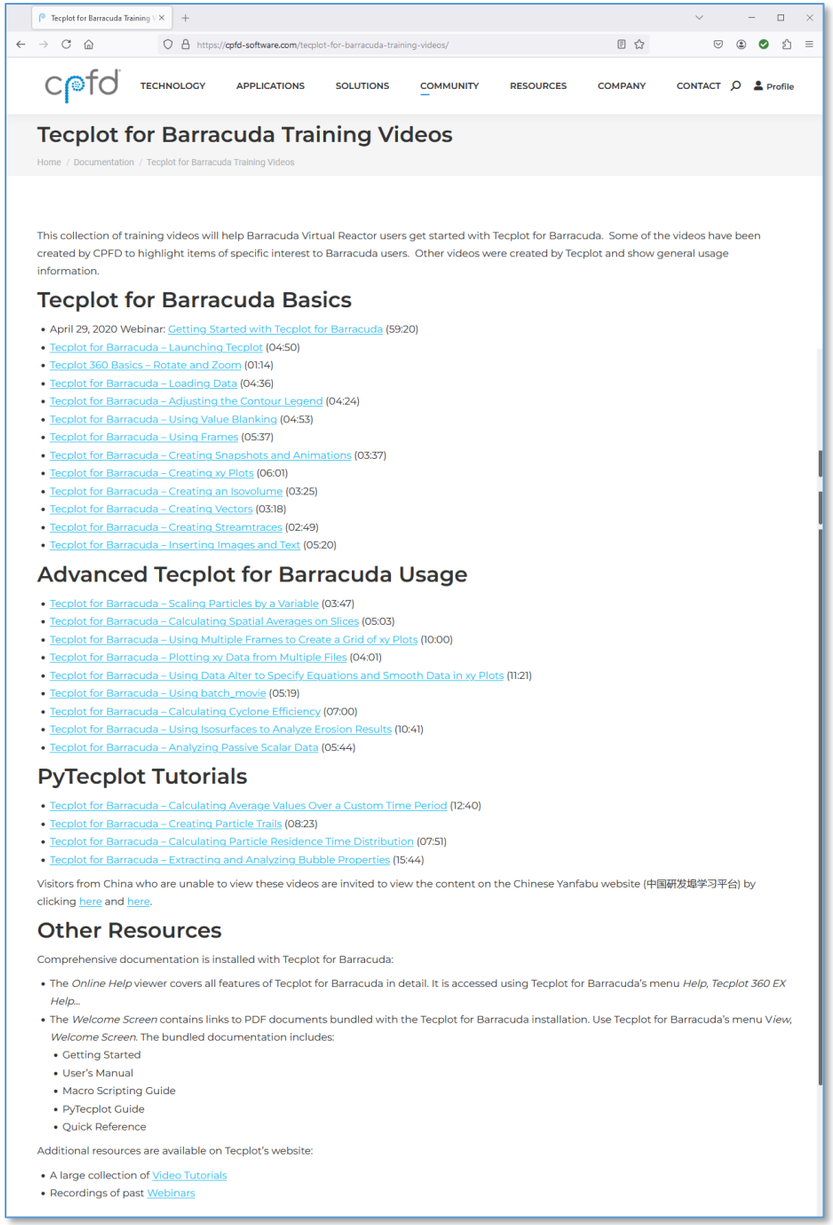


Tecplot for Barracuda Training Videos

Large collection of how-to videos on the CPFD support site for post-processing Barracuda Virtual Reactor simulations

- Most videos are < 10 minutes
- Range from basic to advanced usage

Let us know if there's a specific topic you'd like us to make a video about

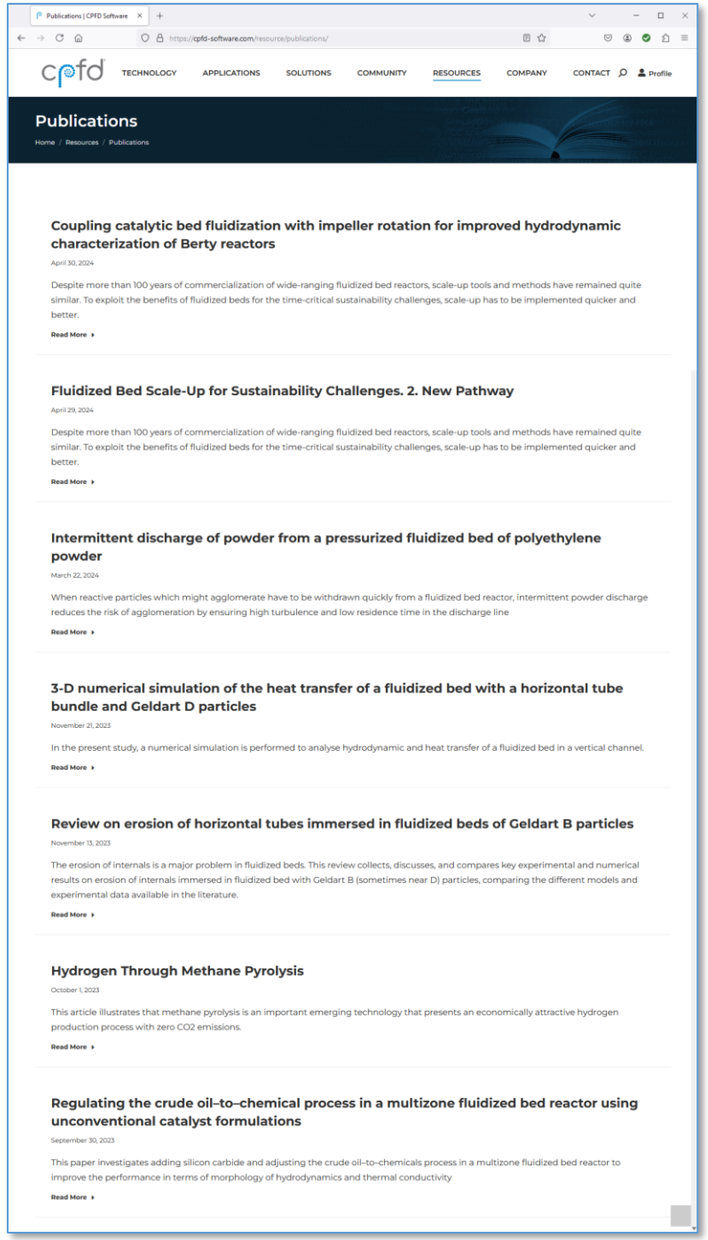


Publications on CPFD's Website

Search our website's Publications list to find published papers and articles about a wide range of topics related to particle technology and simulation

- If CPFD holds the copyright, you will often be able to download the material directly
- If not, there will be a link to the original publisher's website

Contact us if you have publications you'd like us to include in our list!

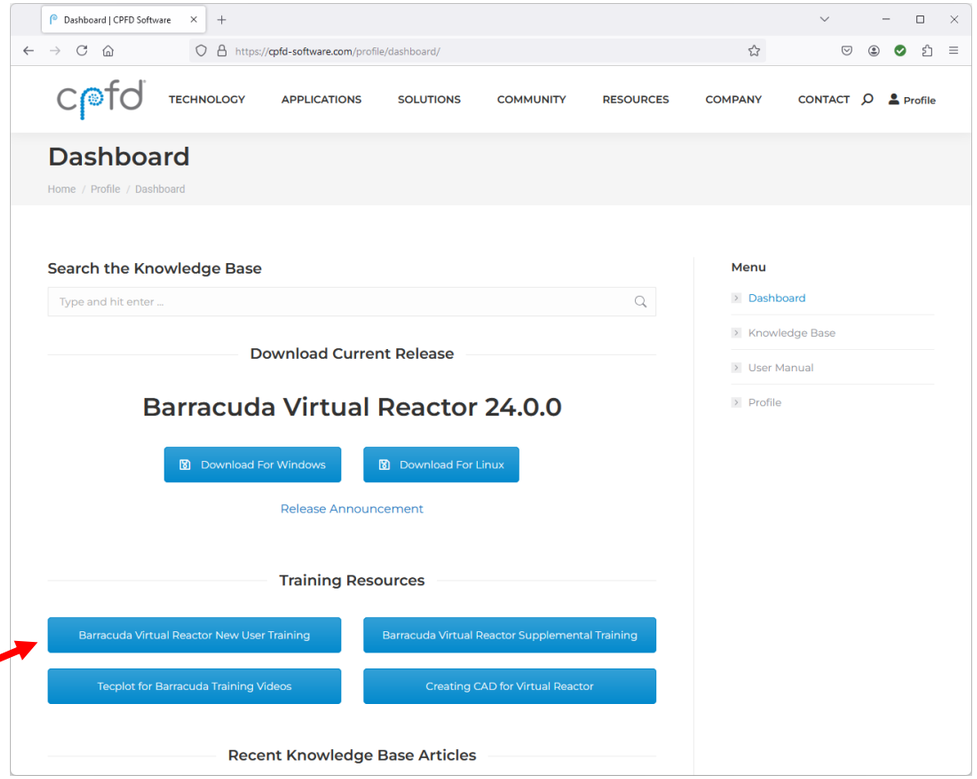


Barracuda Virtual Reactor New User Training

The Barracuda Virtual Reactor New User Training course is always available on our support site

- Can be completed as either:
  - A web-based, CPFD-led training class
  - A self-led, independent course
- Updated with each version release

Great resource for new employees who will be using Barracuda Virtual Reactor

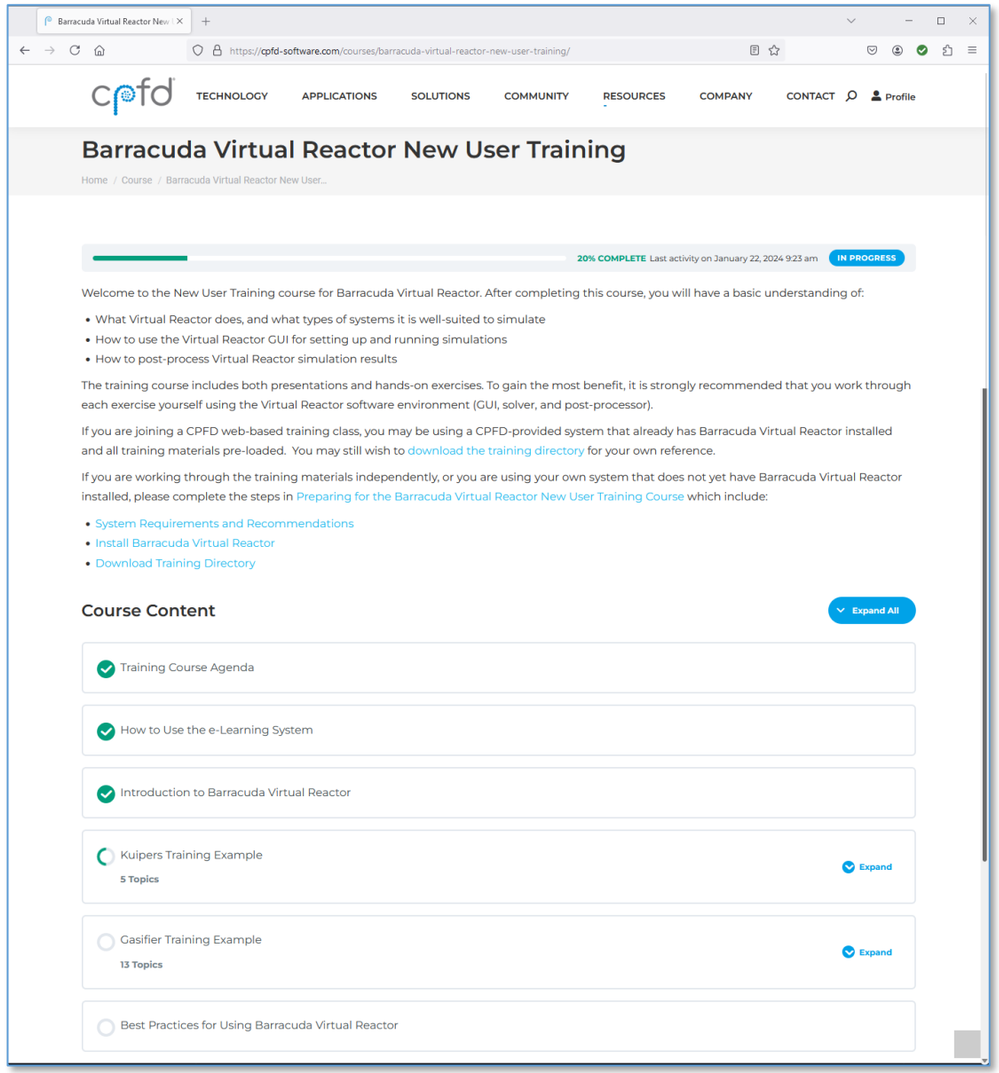


2024 New User Web-Based Training Class Schedule

Web-based, CPFD-led training classes for the remainder of 2024:

- July 15-19
- August 19-23
- September 23-27
- October 21-25
- December 9-13

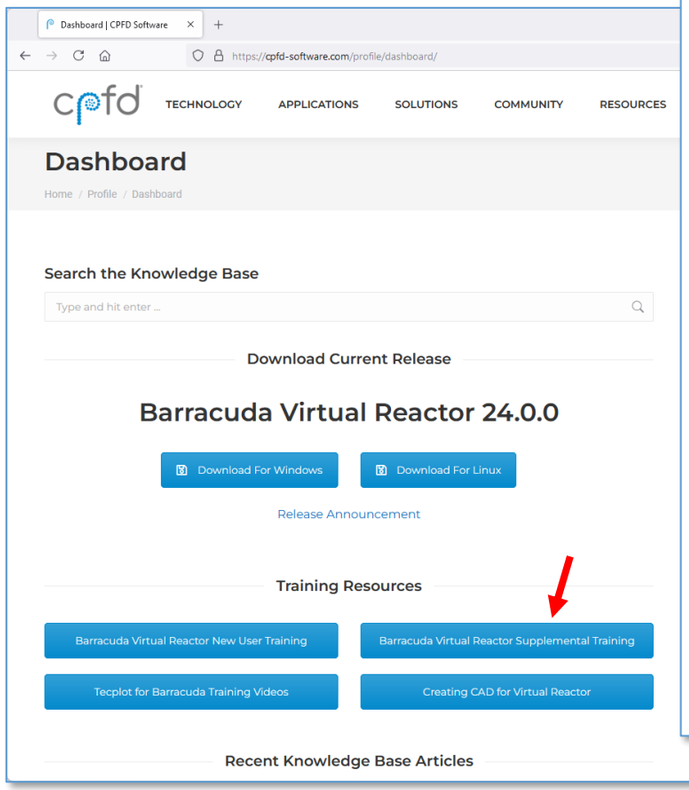
Contact us if you would like to participate in one of these classes!

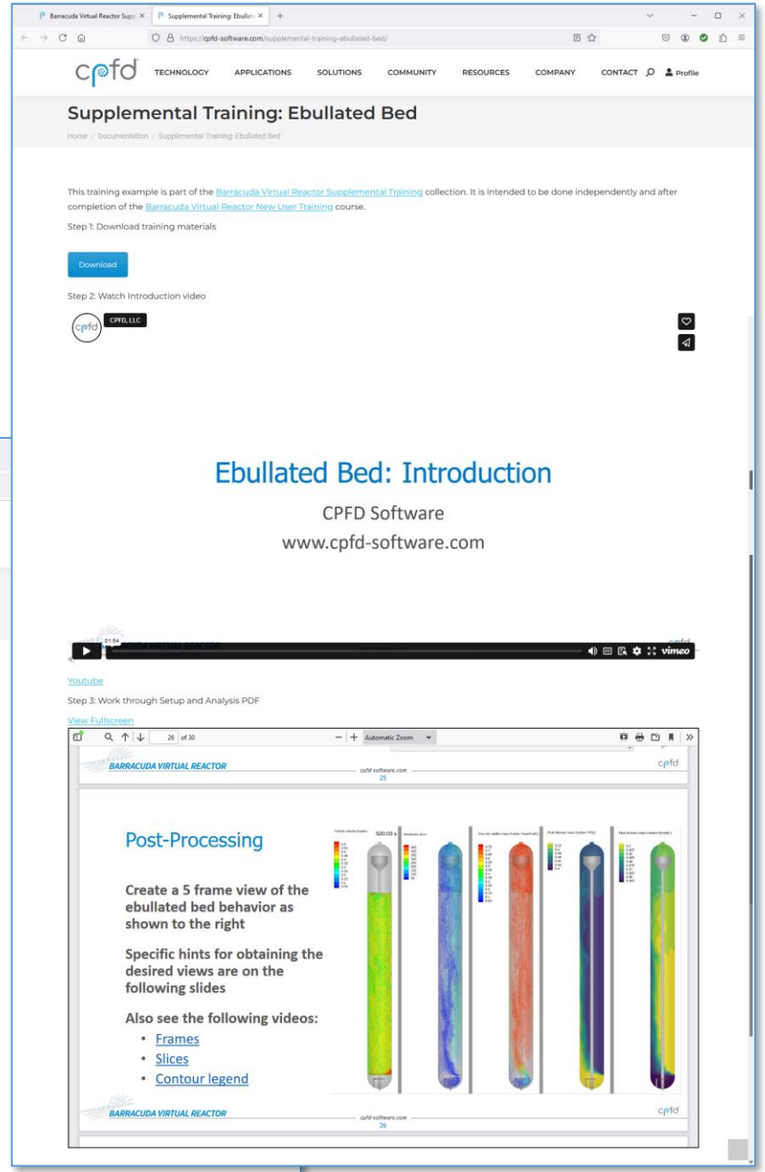


Supplemental Training Examples

Barracuda Virtual Reactor Supplemental Training

- Available to all customers with support site accounts
- Useful for those who have attended New User Training class and want to learn more advanced topics
- Cyclone, FCC Riser, Single-Cell Chemistry, CFB Erosion, Ebullated Bed, Silane Deposition





Q&A

We welcome your questions

For more information

- Visit our website: https://cpfd-software.com
- Follow CPFD on LinkedIn: https://www.linkedin.com/company/cpfd-software/
- Email: info@cpfd-software.com
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