# Modeling Fluidized Bed Gasification with CPFD Barracuda VR® : *Experiences and Challenges*

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# Outline

- Brief overview of GPE catalytic gasification
- Successful validation of experimental data on hydrodynamics and chemistry with CPFD Barracuda VR®
- Simulation of full-scale, continuous flow fluidized bed coal gasifiers with CPFD Barracuda VR®
- Lessons learnt and challenges
- Closing remarks

***GreatPoint Energy has developed the Bluegas™ catalytic hydromethanation process for efficiently converting coal and petroleum coke into clean, low cost natural gas***

# Bluegas™ Technology Overview

**One Catalyst + Three Reactions + One Reactor = Process Intensification**

**Gasification**

$C + H_2O$

↓

$CO + H_2$

Highly Endothermic

+

**Shift**

$CO + H_2O$

↓

$H_2 + CO_2$

Mildly Exothermic

+

**Methanation**

$CO + 3\ H_2$

↓

$CH_4 + H_2O$

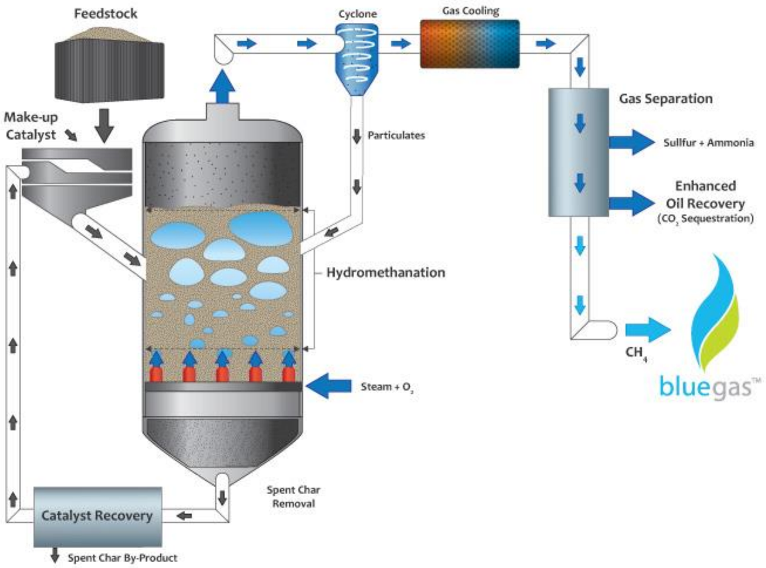
Highly Exothermic

**Overall**

$2\ C + 2\ H_2O \rightarrow CH_4 + CO_2$

Nearly thermally neutral

**Hydromethanation Process Schematic**



# Bluegas™ Technology Highlights

- Step change in the application of gasification for SNG production.
- Coal or petroleum coke reacts with steam in the presence of the hydromethanation catalyst via simultaneous gasification, shift and methanation reactions.
- Catalyst is reactive with coal, petroleum coke, biomass, and refinery bottoms.
- Significantly more efficient than conventional high temperature gasification for SNG.
- In-situ methanation provides most of the heat required for the steam-carbon gasification reaction, greatly reducing oxygen requirements and improving efficiency.
- Near zero-emissions: sulfur, nitrogen, mineral matter and trace metals are all safely removed using commercial processes.
- Capture-ready $CO_2$ is inherent to the process.
- Low water usage per unit of gas produced due to high efficiency and recovery systems.
- 70+ patents pending and issued provides significant competitive technology advantage.

# VALIDATION STUDIES

# Particulate Solid Research, Inc.

- PSRI is an international consortium of companies, each of which pay a yearly membership fee to fund applied research in the fluidization, solids transport, and other fluid-particle areas.
- PSRI focuses its research on large-scale equipment and bridges the gap between fundamental and application-based research in fluidized unit operations.
  - Risers up to 3 ft (0.91 m) ID and 90 ft (27 m) in height
  - Fluidized beds with diameters up to 7 feet (2.2 m)
  - High temperature and pressure (3500 kPa, 800 °C)
  - Cyclones
  - Pneumatic conveying lines
  - Attrition testing: Jet cup, immersed jet and jet impact
  - Specialty probes: $\gamma$-ray, CT, fiber optics, gas and solid tracers, acoustics
- 4201 West 36th Street, Building A, Chicago, IL
- https://www.psri.org/

# List of Experimental Studies Validated with CPFD Barracuda VR®

Non-reactive "cold flow" tests carried out at PSRI, Chicago

- Effect of PSD on fluidization behavior and Geldart regime
  - **Minimum fluidization, transition to bubbling mode, deaeration rate**
- Determination of Geldart A/B boundary for blends with wide PSD
- Hydrodynamics of deep fluidized beds with Geldart A and B-particles
  - **Bed density**
  - **Bubble size, radial distribution, voidage**
  - **Entrainment**
  - **Solid mixing and RTD with NaCl tracer**
  - **Gas mixing and RTD with He tracer**
- Effect of absolute pressure on fluidization
- Concept of drag force equivalence in "cold-flow" tests
- Effect of bed internals on fluidization

# List of Experimental Studies Validated with CPFD Barracuda VR® (Contd.)

Chemistry:

- Lab-scale fixed bed catalytic gasification
  - chemistry validation
  - carbon conversion profile
  - gas profiles
  - heat release/energy balance
- Lab-scale fluidized bed catalytic gasification
- Pilot scale gasification

- All validation studies have been performed without adjusting any internal parameters in CPFD to reconcile differences between experiments and CPFD predictions *except*:
  - We have had most of our success only with the EMMS drag model.
  - The number of computational particles has to be empirically set to balance accuracy and simulation time.

- Otherwise, experimental conditions and parameters have been entered on the user-interface and the code has been run “straight-out-of-the-box”.

# Validation Example:

## 36” PSRI Cold Flow Unit

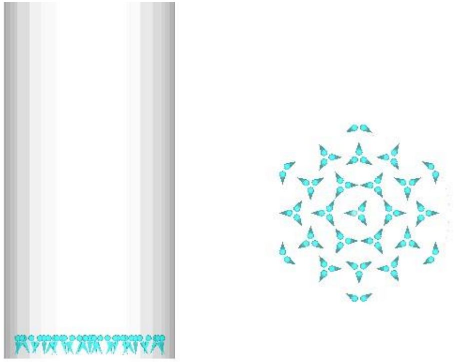
Outlet

Cyclone Return

Salt Injection

Centerline Helium Injection

Bottom Air Inlet



69 individual nozzles included as separate fluid injections

Overall geometry

35.25 inch inside diameter

91 ft tall from bottom plate to outlet

Flexicoke

Geldart B particles

Pressure profile

Bed density

Entrainment rate

Particle segregation

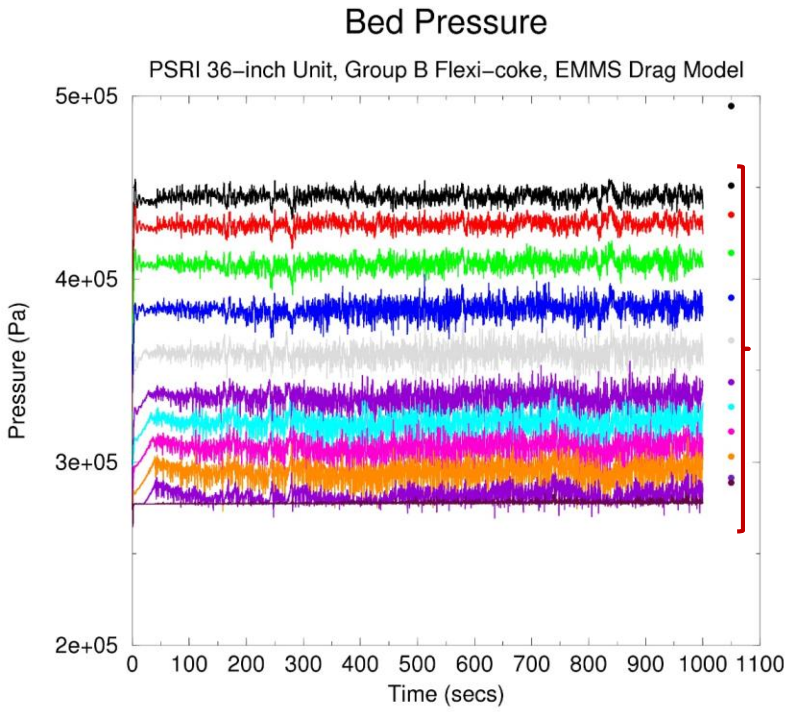
Gas mixing/RTD: He tracer

Solids mixing/RTD: NaCl tracer

Effect of bed internals

# PSRI 3-ft ID Unit Tests with Geldart B Particles:

## Pressure Profile Validation



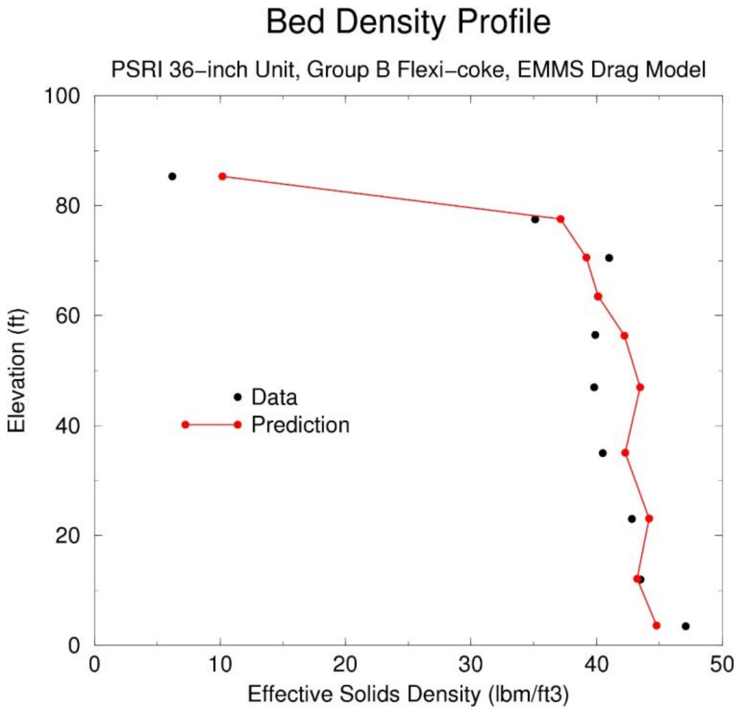
Plenum

Data in bed
from PSRI
experiments

- Pressure profile is in excellent agreement with PSRI experimental data

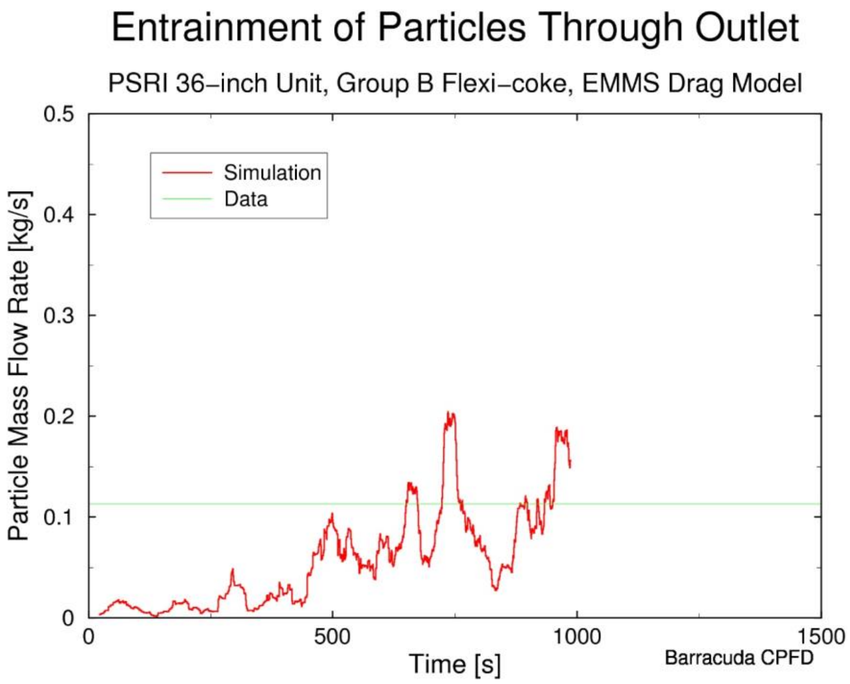
# PSRI 3-ft ID Unit Tests with Geldart B Particles:

# Bed Density Validation



- Bed density profile compares favorably with measured PSRI experimental data
- Bed height tracked accurately

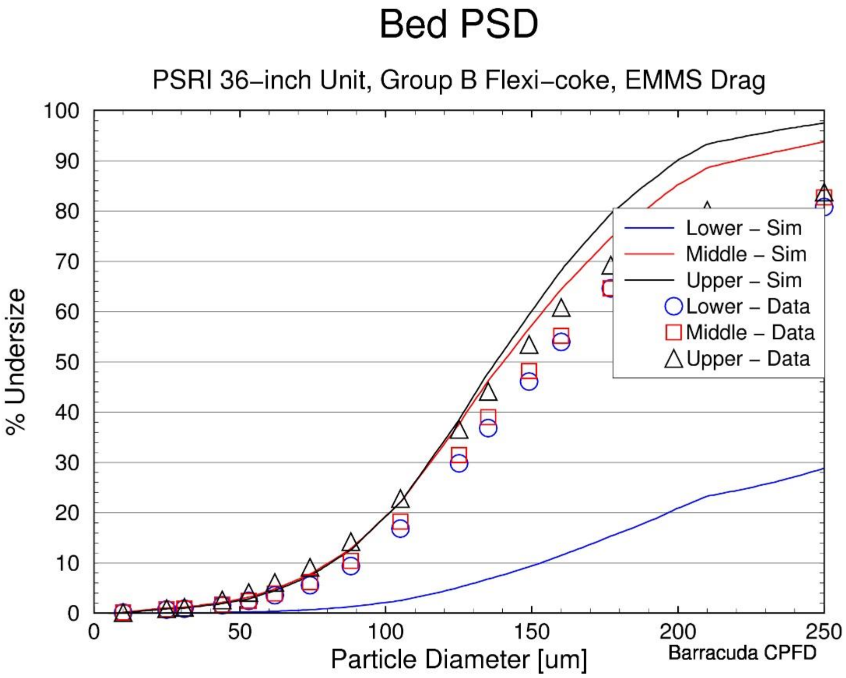
# PSRI 3-ft ID Unit Tests with Geldart B Particles: Entrainment Rate Validation



- Average entrainment of ~0.10 kg/s from simulation
- Experimental data = ~0.11 kg/s
- Excellent agreement

# PSRI 3-ft ID Unit Tests with Geldart B Particles:

## Validation of particle segregation

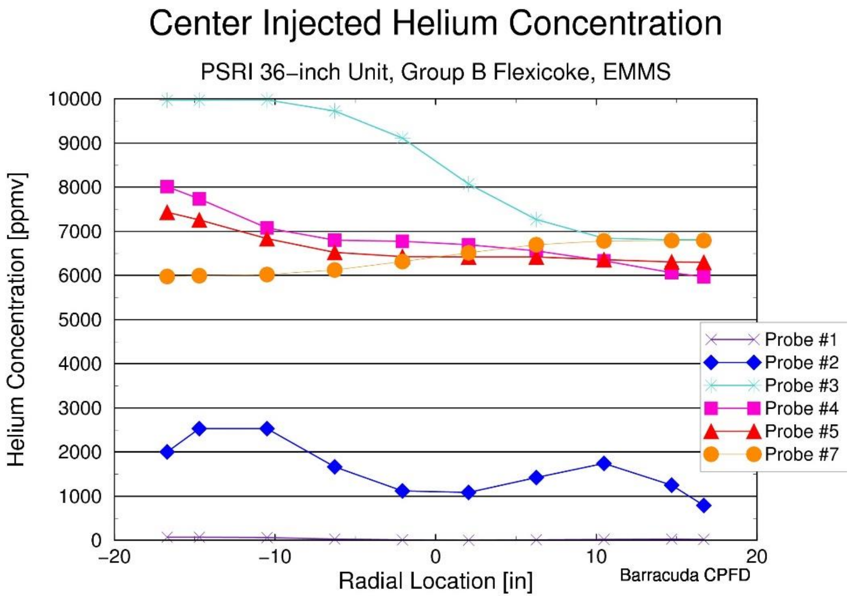


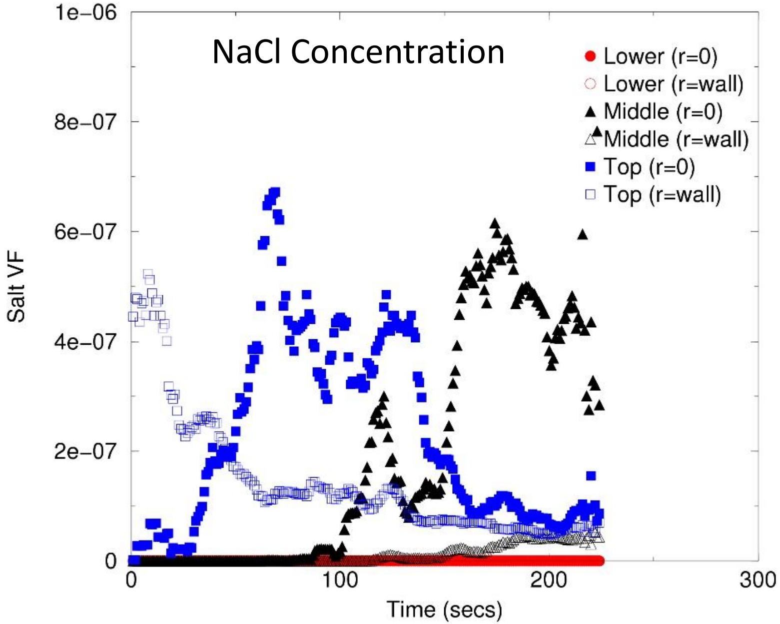
- Predictions of PSD with elevation compare favorably with measurements in the upper and middle portions of bed
- PSD data at lower levels not in good agreement

# PSRI 3-ft ID Unit Tests with Geldart B Particles:

## Gas-phase and solid-phase mixing/RTD

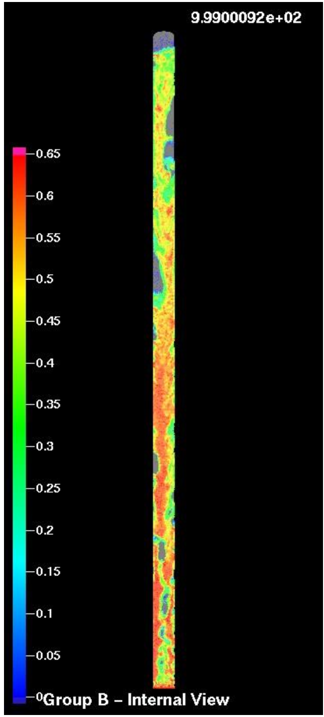
Good agreement for He and NaCl tracer tests. Slightly longer solids mixing time.

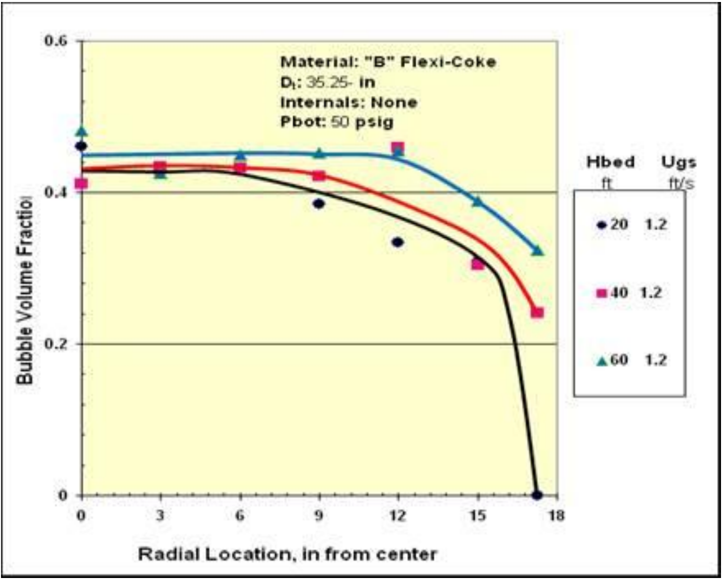




# PSRI 3-ft ID Unit Tests with Geldart B Particles:

## Bubble characterization





Experimental data shows bubbles in the center of the vessel

CPFD simulation results:

- In lower region, gas bubbles migrate upward in center
- In upper region, gas bubbles migrate upward along wall, not in center

Similar discrepancy observed for Group A particles.

We are studying in further detail whether this is an optical illusion created by the videos.

# Keys to Success for Experimental Validation

- Ensure that the pedigree of data is good, which has been ascertained in the case of the GPE/PSRI tests.
- Accuracy of particle size distribution and particle density
  - Particle and skeletal densities should be measured with porosimetry. Inferred particle densities and close-pack volume fractions based on bulk density measurements and assumed void fractions can be largely in error.
  - PSD techniques: sieve, dry laser, wet laser, coulter counter
  - All give sufficiently different results to throw CFD simulations off
  - Need to accurately account for $d_{p,50}$, $d_{sv}$ and $F_{44}$
- Must plan experiments with CPFD Barracuda VR ® specifications in mind
  - Important data that was not measured cannot be retrieved
  - Start-up procedure of experiment must be incorporated into CPFD Barracuda simulation to improve performance of CPFD code
  - Does the data scan ensure a period of steady operation?
- Is the "experimental" quantity truly measured?
  - e.g. Bubble size and bed density may be calculated from other measurements and involve assumptions such as no wall drag or a probe factor
- Cross-check separate experimental measurements against each other to ensure consistency.

# FULL-SCALE SIMULATIONS OF CONTINUOUS COAL GASIFIERS

# Full-Scale Modeling Experience

- GPE has successfully modeled catalytic gasification with CPFD Barracuda VR® for the proposed design of the full-scale reactor
- Detailed catalytic gasification chemistry modeled
  - Drying, devolatilization, partial oxidation also included
- Thermal mode
- Details of steam/oxygen grid injection captured with point source boundary conditions
- Multi-particle physics and PSD included.
- Good match of bed density, bed expansion, entrainment rate, thermal profile and gas composition profile with expected values
- Consistent with PSRI hydrodynamic tests and GPE lab kinetics measurements

# Simulation Time:

## PSRI reactors, 3-D, isothermal flow, chemistry off

### 6” unit (2015 simulations)

- GPU version
- 10,000 cells
- 55,000 computational particles
- 1 second of real time = 19 s of simulation time (10 min = 3.2 h)
- Relatively simple problem
- Correctly predicts experiment
- Has provided excellent guidance on validating experimental work

### 36” unit (2014 simulations)

- GPU version
- 100,000 cells
- 2 MM computational particles
- 1 sec of real time = 30 min CPU time
- 30 min wall time = 21 days CPU time

# Simulation Time:

## Full-scale reactor (3-D), thermal flow, chemistry on

### 2008

- CPU version
- No oxygen chemistry.
- 2 sec of real time = 1 day of CPU time
- 1 h = 4.5 years!

### 2015

- GPU version
- Full oxygen chemistry
- 150,000 cells
- 11 MM computational particles
- 80 sec of real time = 1 day of CPU time
- 1 h = 45 days
- 40X improvement in simulation time on more difficult problem
- Chemistry not parallelized. Kinetically-controlled operational regime does not benefit from GPU acceleration.
- CFL-based step-size control not active: low CFL, low step-size

# Keys to Success for Coal Gasification Simulations:
## Importance of 1.5-D model

- GPE has internally developed a 1.5-D model to simulate the steady-state and transient behavior of the gasifier.
- Results from the 1.5-D model are needed to specify and initialize CPFD solver.
  - Overall flows of gas and solid streams, initial PSD, initial composition profile must all be initialized to consistent values (as given by the 1.5-D model).
  - Without such an initialization, the code may encounter several numerical difficulties either preventing or slowing down convergence.
  - Certain aspects of reacting coal particle behavior are not directly available in CPFD such as changes in particle composition and size distribution with time.
- Residence time distribution of gas and solids occurs on very different time scales. In our experience, we cannot simulate bed turnover in a reasonable CPU time.
- Default structure of user interface is not consistent with rate expressions and particle properties. The 1.5-D model is used to “regress parameters” for the CPFD default models.
- Many of the above features strengthen the call for user-defined functions.

# LOOKING AHEAD:
# CHALLENGES & WISH LIST

# Wish List of Features

- User-defined functions
  - Important for chemistry and drag laws
- Easily accessible variables in conventional use:
  - bubble size, bed height, bed density
- Parallelization of chemistry
- Pre-processing feature: all GUI inputs can be imported from an ASCII file
- Post-processing feature:
  - tools catered to Microsoft Windows™ environment
- Option to customize the interface to use and display properties of choice everywhere:
  - diameter rather than radius on interface
  - display gas void fraction
- Fully-documented validation cases

# The Issue of Validation

- GPE works with several entities to design its proprietary hydromethanation technology.
- We are often questioned on the ability of computational fluid dynamics to be able to accurately describe experimental data on fluidization.
- To address these concerns, we have carried out several fundamental studies to successfully validate the CPFD model against experimental hydrodynamics and chemistry data.
- Areas for improvement of predictions are also identified.

# Closing Remarks

- GreatPoint Energy has successfully employed CPFD Barracuda VR® software in-house to study its proprietary fluidized bed reactors for gasification of coal and petroleum coke.
- Experimental studies have been carried out for various scales ranging from small-scale lab to large pilot plants.
- A majority of the experiments carried out at PSRI and GPE labs have been validated with CPFD software.
- CPFD Barracuda VR® has proven to be a powerful tool for GreatPoint Energy that we hope will be further improved for the simulation of large-scale coal gasifiers.

# Acknowledgements

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- CPFD Team *quick start program, consulting, support*
  - Sam Clark, Steve Webb
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