R&D Update

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Barracuda Virtual Reactor Users Conference
June 29 – July 1, 2022
Outline

• History of Barracuda Development

• New and ongoing development
  • Multi-GPU
  • Vapor-liquid-solid
Overview

Development, Support, and Training Team

• Software development (Solver, GUI, utilities)
• Numerical research and validation
• Software testing and development of testing framework
• Software support and training
The Evolution of Barracuda Virtual Reactor

- **2007** First Barracuda Release
- **2007** Fluidized bed dryers
- **2010** Chemistry and Heat transfer
- **2010** Polysilicon
- **2012** Multi-component particles
- **2012** Gasification
- **2012** Chemical looping
- **2013** Coal-fired boiler
- **2013** Flue gas desulfurization
- **2013** FCC Regenerator
- **2014** Windows OS
- **2014** Polyolefins
- **2014** FCC Riser
- **2015 - 2019** First GPU release
- **2015 - 2019** Speed and usability
- **2020** Tecplot for Barracuda
- **2020** Gasification
- **2020** FCC Regenerators
- **2021** First Multi-GPU release
- **2022** Multiple-liquids & liquid chemistry
- **2022** Hydrocracking - Ebullated beds
- **2022** Multiple-liquids & liquid chemistry
- **2022** Cement
How simulation time-to-solution has changed over last 10 years...

- Chemical looping reactor model originally developed with NETL in 2011-2012
- Full loop consisting of reactor/riser, cyclone, loop seal, fuel reactor, L-valve
- Ilmenite carrier, methane and coal as fuel source
- Reaction chemistry
  - Oxidation/reduction of ilmenite
  - Coal chemistry: drying, devolatilization, oxidation, water-gas shift, gasification

Improvements in calculation rate over time

Simulation time on readily-available hardware:

- 2012 (v15.0, CPU), 82 days
- 2014 (v16.0, GPU), 16 days
- 2018 (v17.3.1), 4 days
- 2019 (v17.4), 2.5 days
- 2021 (v21.1), under 16 hours
Multi-GPU support in Barracuda

- Changing structures of underlying memory resulted in major speed up
  - Single GPU 2X faster between v20.1 and v21.0
  - Positive scaling up to 4 GPUs
  - Over-subscription of GPU memory is now possible
  - Collaboration with engineers at Nvidia to ensure maximum speed-up

- Work continues to reduce time to solution:
  - Optimizing the “new” GPU bottlenecks to extend scaling to 8 GPUs
  - Gas tracers
  - Chemical reaction solvers

Equal parts hardware and software improvements in speed up

Parker and Larson (2018). Application of Recent CFD Advancements to the Modeling of Chemical Looping Systems
Vapor – Liquid – Solid development

• In v21.1 and earlier
  • Gas-solid (compressible) simulations
    • Droplets Liquid film coating of particles
    • No liquid phase reactions
    • Evaporation model in “beta”
  • Liquid-solid (incompressible) simulations
    • Single incompressible fluid
    • No liquid phase reactions, mass transfer, etc
Development of ebullated bed models

- Three phase model
  - Liquid continuous phase
  - Discrete solid particle phase
  - Discrete gas bubble phase

- Calculate discrete bubbles using CPFD’s underlying platform for fast Lagrangian particle calculations

- New physical models and concepts
- Recently released features
- Upcoming release features
- Future work

Validation of gas holdups in ebullated beds
Demonstration modeling of ebullated bed (LC-FINING)

- Hydrocracker converts vacuum resid into lighter hydrocarbons (VGO, diesel, naphtha, gas) using hydrogen gas
- Dimensions and operation of Syncrude LC-FINING unit obtained/estimated from open literature
  - Isothermal / reacting model
  - 12’ diameter, 120’ tall
  - 11.7 MPa, 440° C
  - Liquid velocity: 0.13 ft/s
  - Gas velocity: 0.13 ft/s
  - Recycle ratio: 5.6
Evolution of a bubble in ebullated bed reactor

Pure H₂ bubble is injected below distributor. H₂ absorbs into the surrounding liquid which is composed of fresh VR and products recycled from top of reactor.

Bubble passes through the distributor, where absorbed H₂ reacts with VR to form lighter components at solid catalyst surface.

Gas (G) diffuses into bubble (gas absorption) and hydrocarbon vapor diffuses into the bubble, changing the size and composition of the bubble. Most bubbles leave at the top of the reactor but some are recycled to the bottom.
Key Development for ebullated beds and VLS applications

- Liquid film chemistry in compressible simulations (v22.0)
- Vapor as phase of matter in Barracuda calculations (v22.0)
- Release / revamp of evaporation model for compressible models (v22.0)
- Multiple liquids & multiple incompressible liquid pressure solver (v22.0)
- Incompressible fluid phase reactions (v22.0)
- Particle/bubble filtering at baffles (v22.0)
- Discrete bubbles (v22.1)
  - Stability improvements for buoyancy-dominated flow (v22.0)
  - Compressibility, surface tension, lift force, virtual mass force (v22.1)
- Bubble / liquid evaporation (v22.1)
- Gas absorption model (v22.1)
- Decoupling of particle / bubble close-pack calculations (v22.1 beta)
VLS Development for Compressible models

- **Chemistry** - Liquid film & droplet chemistry added in v22

- **Evaporation** - In previous versions of Barracuda, evaporation was calculated between a liquid and a *gas*

  - In v22 development, a *vapor* phase is introduced for the calculation of evaporation.
  - A vapor phase is connected to a liquid phase in the material editor
Multiple incompressible liquids / gases – v22.0

- Required rewrite of pressure solver to support incompressible liquids (part of v21.1)
- Incompressible simulations can have **liquids** and **gases** (dissolved) in the fluid phase
- Fluid density is calculated from specified liquid density or gas molar volume

- DEMO: Vacuum resid (L), vacuum gas oil (L), diesel (L), naphtha (G), propane (G), and hydrogen (G) are used
Incompressible liquid reactions – v22.0

• Volume-average chemistry calculated in the incompressible fluid domain
• Reactants / products can be liquids, gases, and solids
• Similar volume-average gas-phase chemistry
• DEMO: Simple chemistry from Stratiev et al (2019) was implemented
Particle filtering – v22.0

- Allow particles, droplets, and bubbles to selectively pass through a baffle
- A positive direction orientation is defined
- Positive and negative direction probabilities are defined
Discrete bubbles – expected in v22.1

• Discrete Lagrangian bubble composed of gases and vapors

• Change in size based on pressure, temperature, surface tension, and composition changes

• Lift force and virtual mass force have significant effect

• Bubble swarm drag models – function of surface tension

• Behave as particles with independent close packing volume fraction*

Validation case of Deen et al (2001)
Gas Absorption Model – expected in v22.1

- Gas dissolves into a surrounding liquid (solvent)
- Equilibrium between gas in liquid and gas in bubble, defined by Henry’s law constant
- Sherwood number using Calderbank and Moo-Young correlation for bubble swarms
- Diffusion coefficient estimated from Wilke-Chang
Particle/Bubble species close-pack volume fraction – (v22 beta)

• Close-pack volume fraction specified for each particle / bubble species

• A local close-pack volume fraction is calculated based mixture of particles/bubbles/droplets that are present

$$\theta_{cp} = \sum_i v_{p,i} / \sum_i \frac{v_{pi}}{\theta_{cpi}}$$
Future work in bubble modeling

- Bubble splitting and coalescence
- Dynamic close-pack / polydispersity modeling
- Bubble and particle interactions
Summary

• Significant and exciting development at CPFD
• Major calculation speed up in recent releases
• Development in support of ebulliated bed and other discrete bubble applications is ongoing
Thank you!