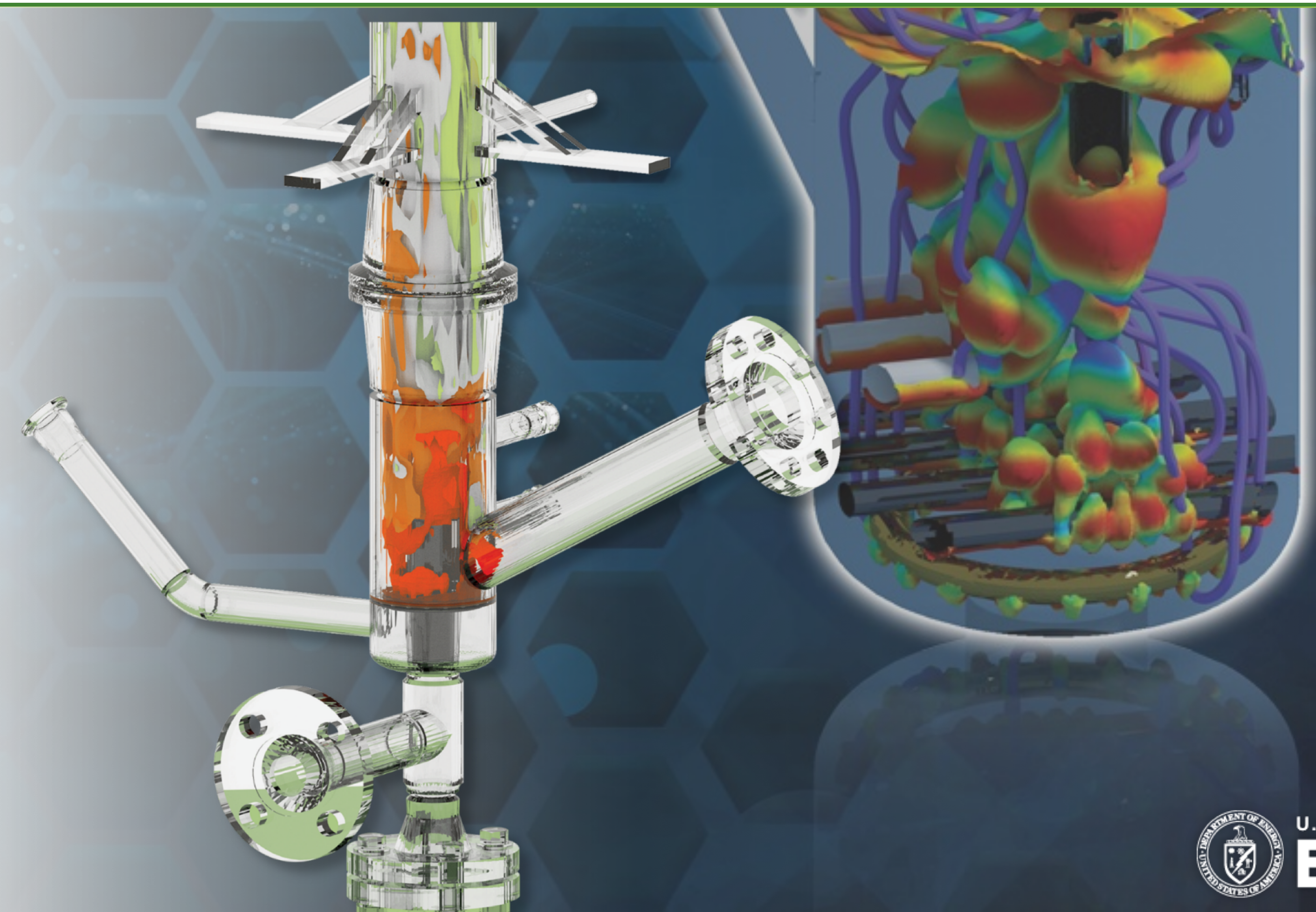
CFD Simulation of Hydrodynamics, Heat Transfer, RTD, and Chemical Reaction in a Pilot-Scale Biomass Pyrolysis Vapor-Phase Upgrading (VPU) Reactor

Xi Gao[1, 2], Tingwen Li[3], William A. Rogers[1], Kristin Smith[4], Katherine Gaston[4]

[1]*National Energy Technology Laboratory, Morgantown, WV 26507, USA*
[2]*Leidos Research Support Team, Morgantown, WV 26507, USA*
[3]*SABIC, Sugar Land, TX 77478, USA*
[4]*National Renewable Energy Laboratory, Golden, CO 80401*

2019 NETL Multiphase Flow Science Workshop, Morgantown, August 7, 2019



NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

Consortium for Computational Physics and Chemistry (CCPC)*

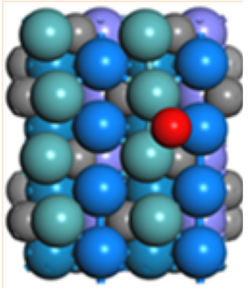
NATIONAL ENERGY TECHNOLOGY LABORATORY

Task 2
Catalysis Modeling at Atomic Scales

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Argonne NATIONAL LABORATORY

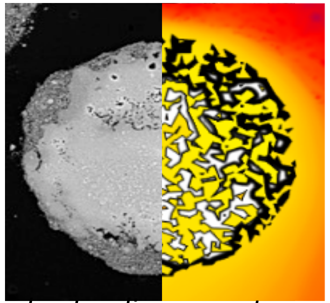
Pacific Northwest NATIONAL LABORATORY



Investigating novel catalyst material combinations and understanding surface chemistry phenomena to guide experimentalists

Task 3
Catalyst Particle Modeling at Meso Scales

NREL NATIONAL RENEWABLE ENERGY LABORATORY



Understanding mass transport of reactants/products, reaction kinetics, and coking and deactivation processes

A multi-scale problem

… A multi-lab solution

CCPC

www.cpcbiomass.org

Task 1
Coordination, Integration, and Industry Outreach

OAK RIDGE National Laboratory

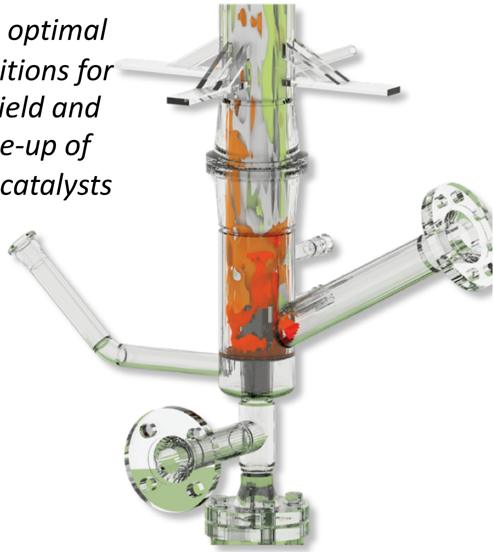
CCPC Industry Advisory Panel
David Dayton (RTI), George Huff (MIT, retired BP), Jack Halow (Separation Design Group), Steve Schmidt (WR Grace), Tom Flynn (Babcock & Wilcox)

Task 4
Conversion Modeling at Process Scales

NATIONAL ENERGY TECHNOLOGY LABORATORY

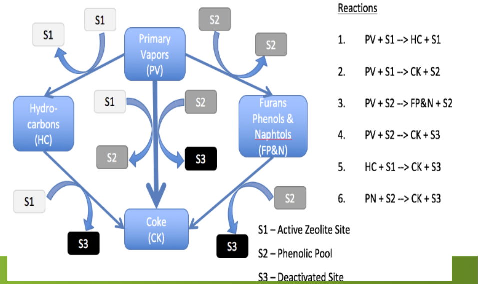
OAK RIDGE National Laboratory

Determining optimal process conditions for maximum yield and enable scale-up of ChemCatBio catalysts



Task 5
Kinetics: Fundamental Reaction Rates for Modeling

Guide efficient technology scale-up, enabling performance gains achieved by ChemCatBio to be maintained at pilot scale



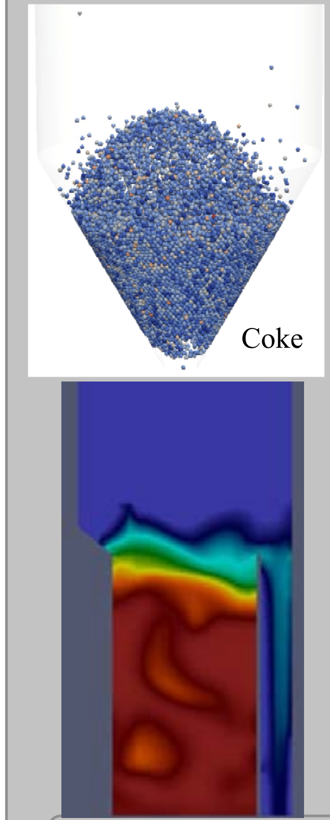
*Adopted from 2019 Peer review

Reactor Models Cover Wide Range of Scale and Type*

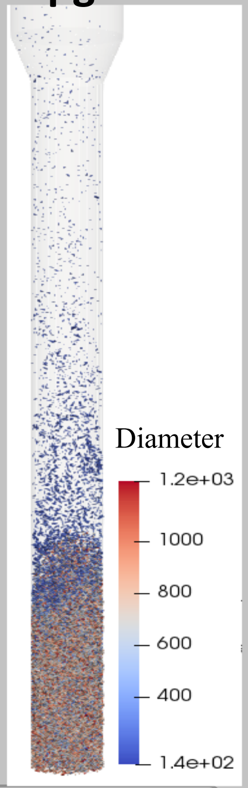
*Adopted from 2019 Peer review

NATIONAL ENERGY TECHNOLOGY LABORATORY

Spouted bed Upgrader (kinetics)



2" Fluidized Bed Pyrolyser and Upgrader

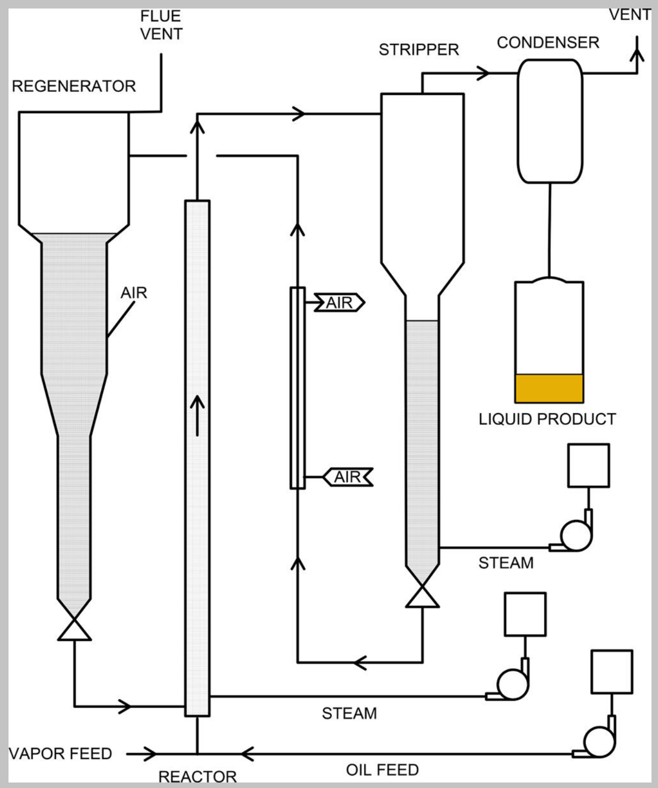


~883 sec residence time

500-900 micron particle

0.5 kg/hr flow rate

Davison Circulating Riser Upgrader

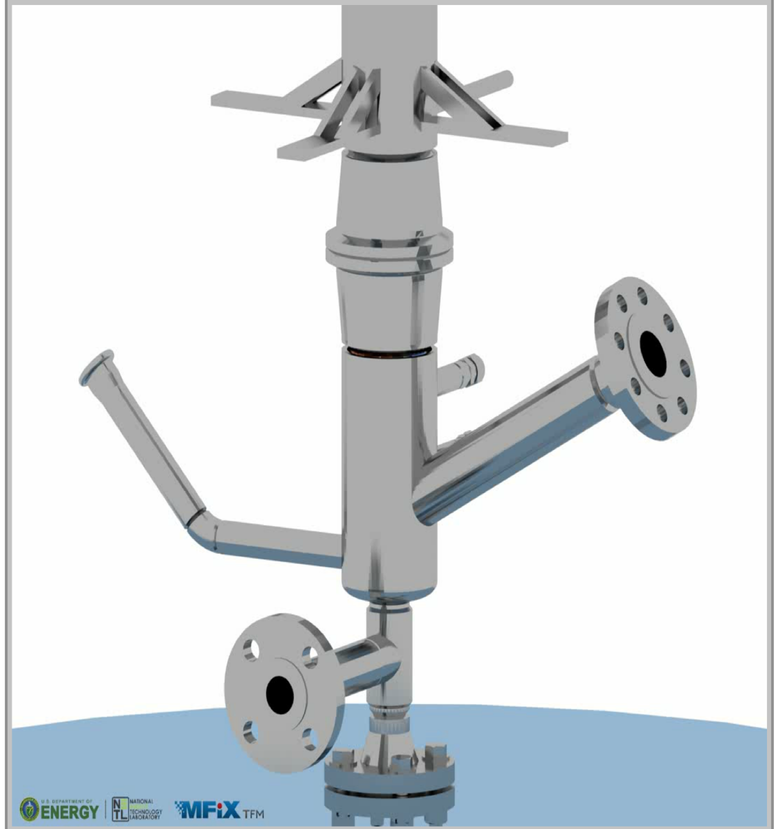


~3 sec residence time

80-100 micron particle

2 kg/hr flow rate

TCPDU R-Cubed riser Upgrader



~10 sec residence time

80-100 micron particle

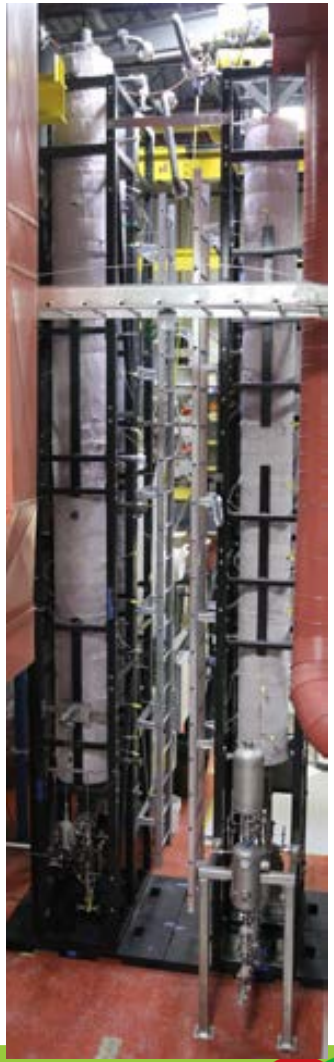
15 kg/hr flow rate

Background and Motivation

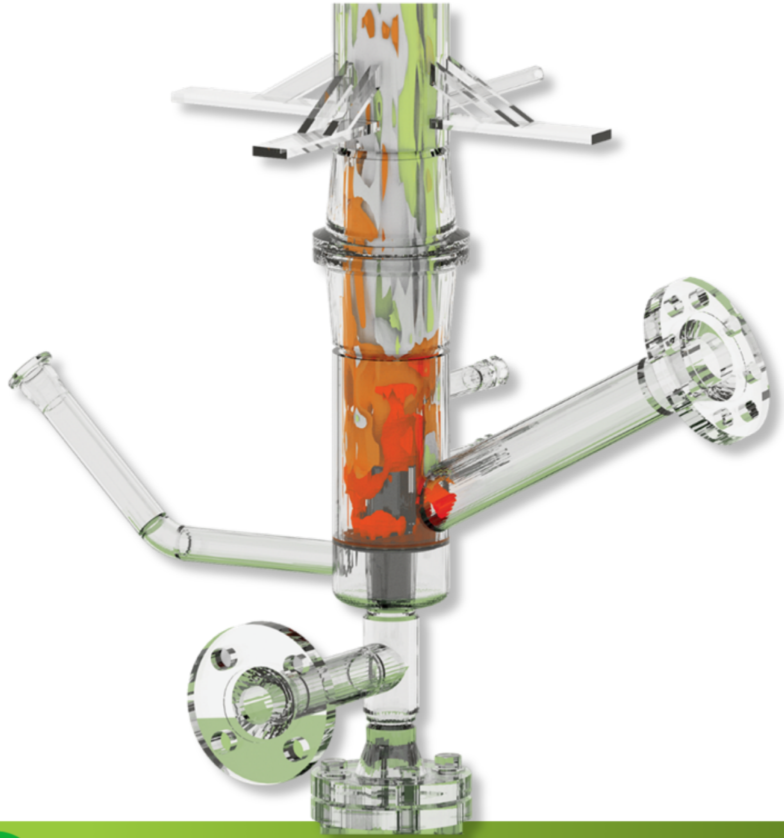
- **Goal of this work**: Use reactor scale multiphase computational fluid dynamics simulations of catalytic upgrading of biomass pyrolysis vapor to provide:
  - Detailed hydrodynamics, RTD, heat transfer and chemistry
  - Model validation using experimental data
  - Gas and catalyst residence time distributions for use in reduced-order reactor models
  - A validated computational tool to support reactor experimentation, design, and optimization

- Models use the NETL MFiX Software Suite
  - MFiX – **M**ultiphase **F**low with **i**nterphase e**X**changes
  - CFD software for reacting, multiphase flow developed and supported by NETL
  - MFiX-TFM, MFiX-DEM, MFiX-PIC, MFiX-Hybrid, MFiX-GUI
  - Open-Source, available to the public

Process Scale Reactor Modeling



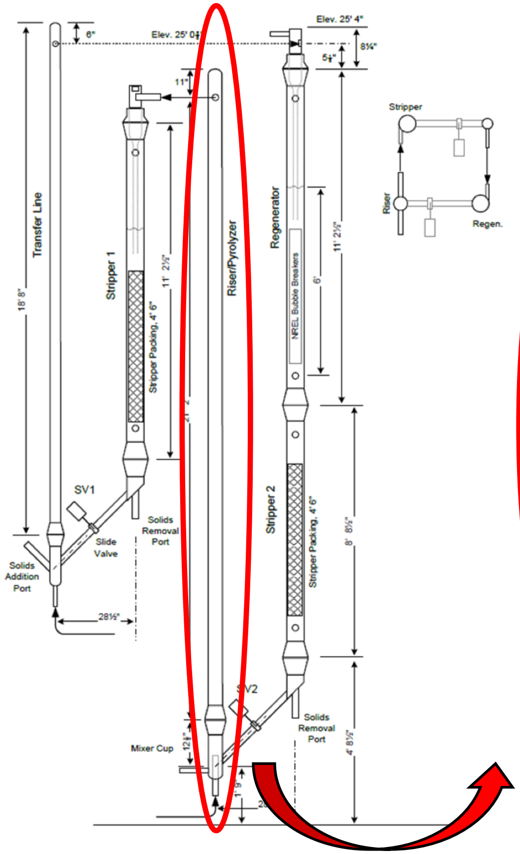
Determining optimal optimal operating conditions for maximum yield and enabling scale-up



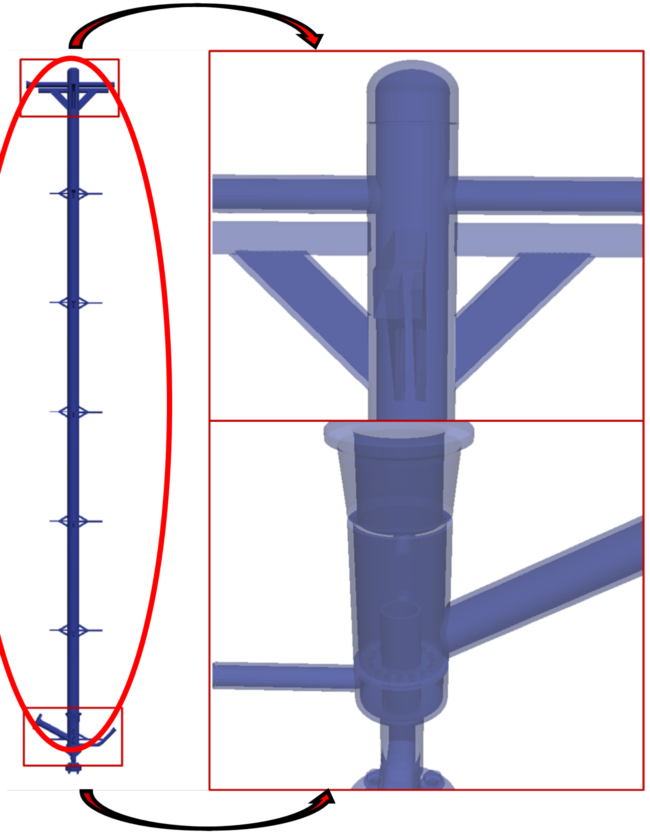
TCPDU R-cubed Reactor

NATIONAL ENERGY TECHNOLOGY LABORATORY

TCPDU Process

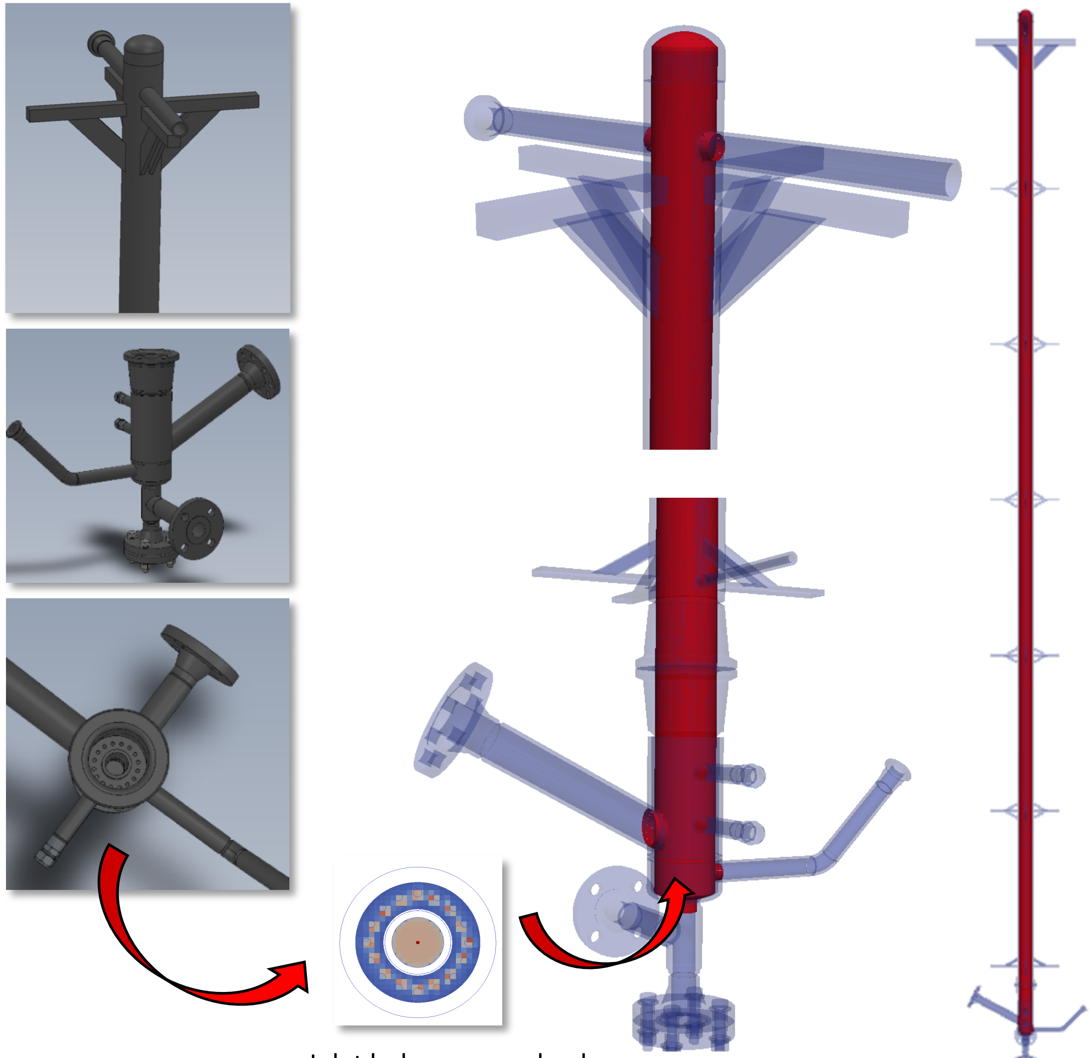


R-cubed riser Geometry



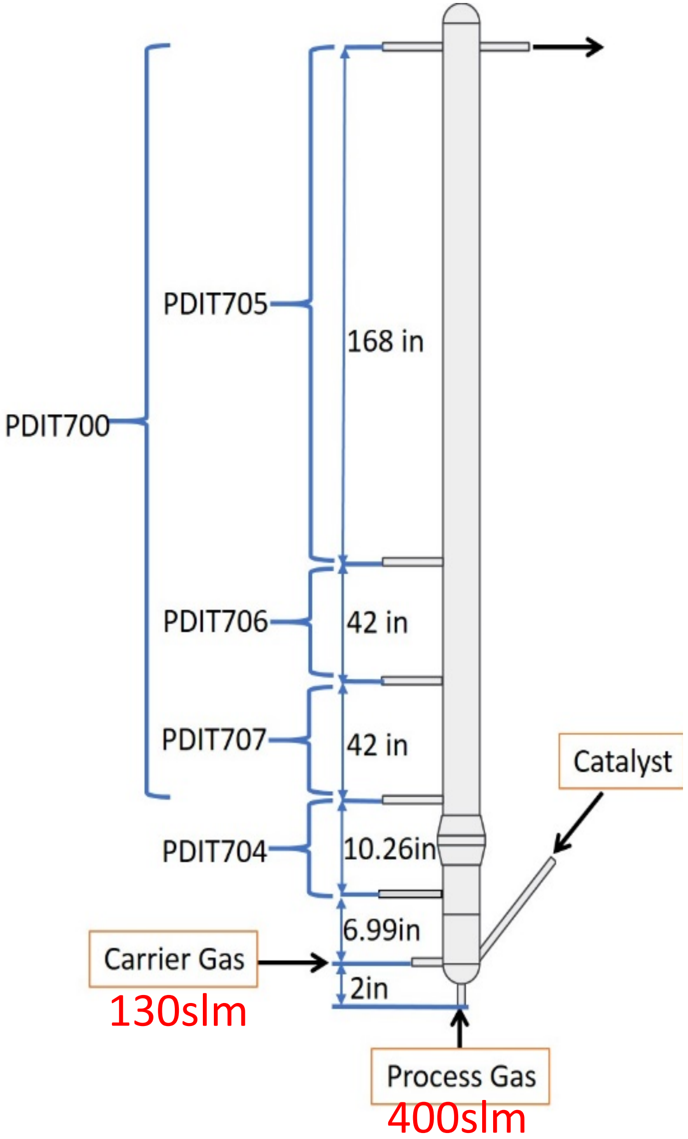
- Riser: Height: 7.05 m, diameter: 0.092 m
- Outlet diameter: 0.038 m
- Solids inlet diameter: 0.049 m
- Pyrolysis vapor inlet diameter: 0.047 m
- Distributor: 16 holes with diameter of 0.00625 m

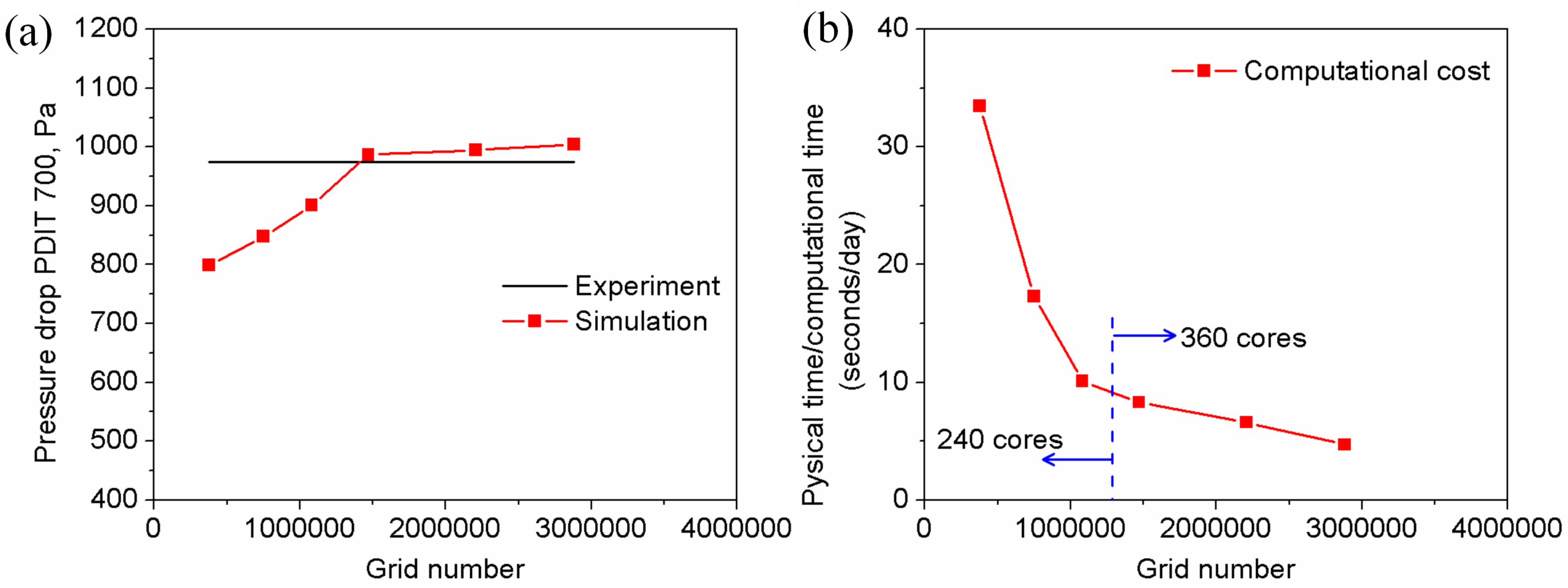
Computational Domain



Inlet holes are resolved

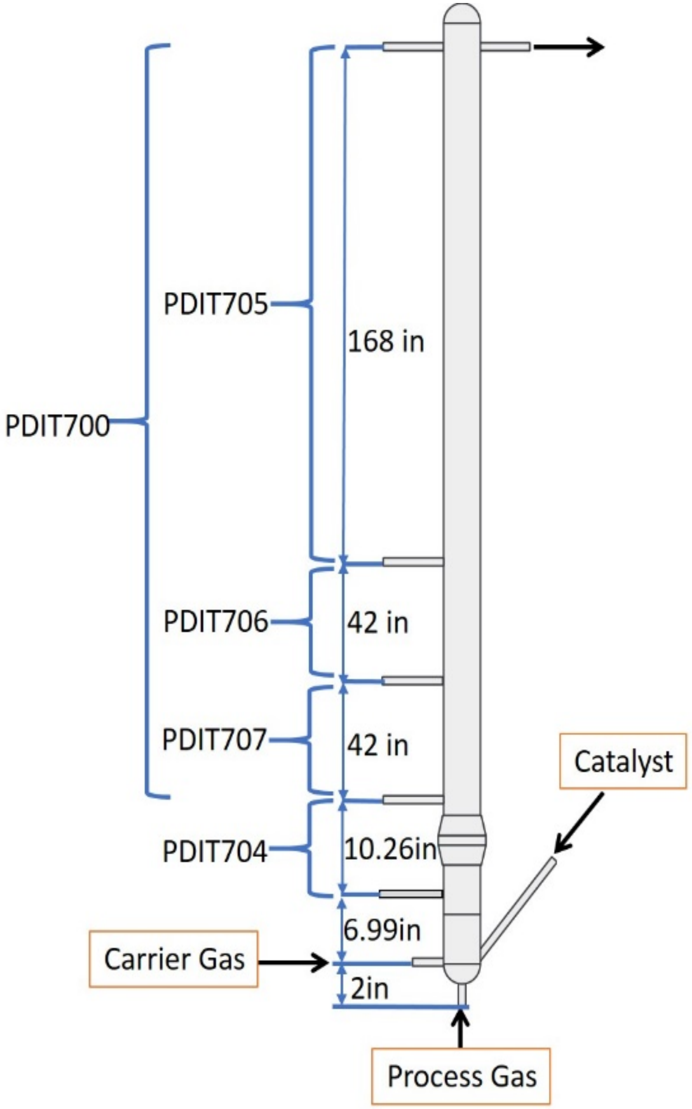
Multiphase Hydrodynamics Simulation in the R-cubed Riser

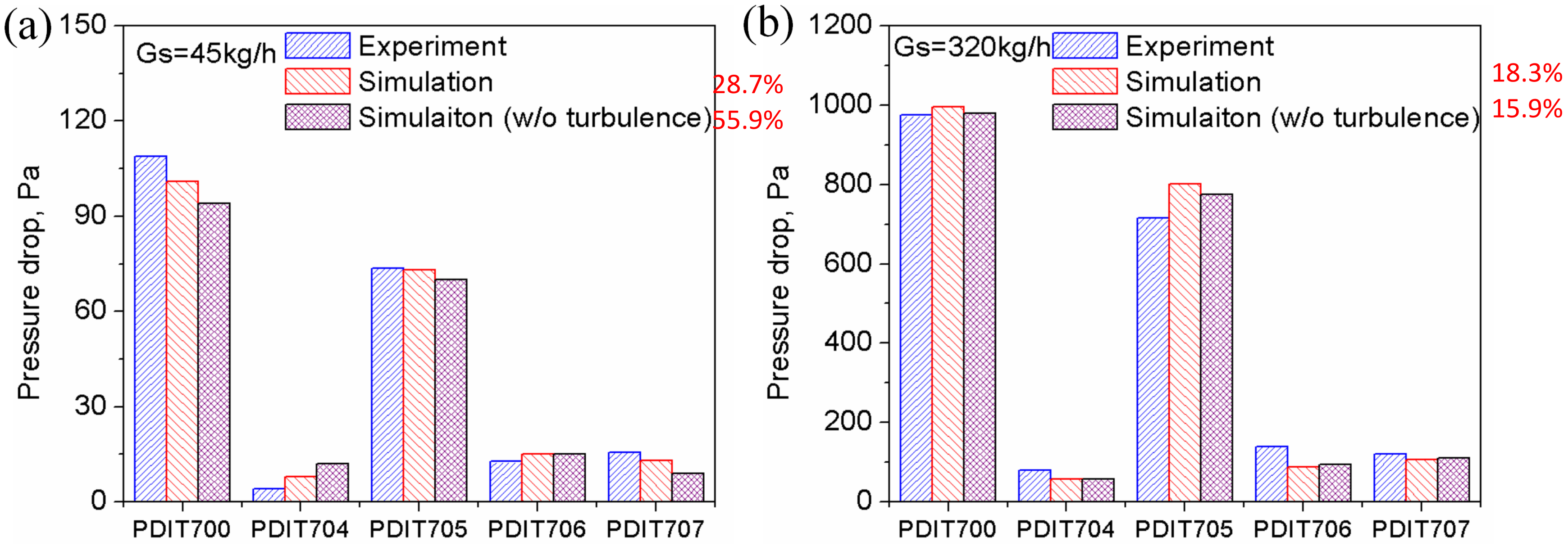




- Pressure drop PDIT 700 increases with the increasing of grid size
- 2.88 million cells (cell~45dp) is enough to get grid independent pressure drop
- Total 40seconds simulation, last 20 seconds used for getting averaged results

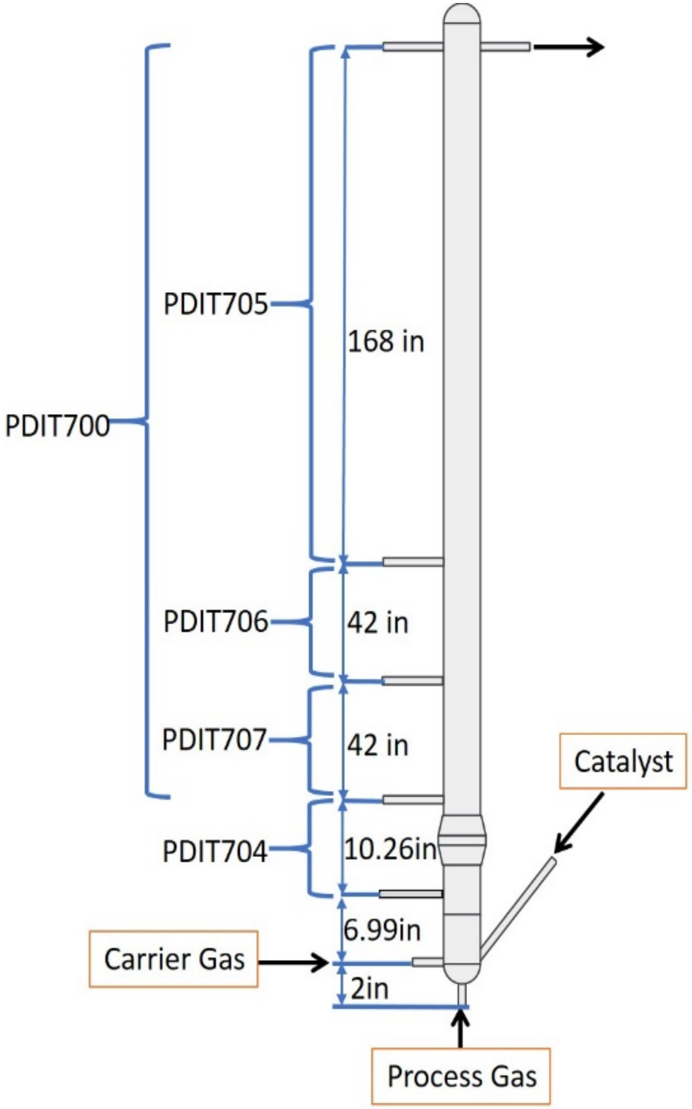
With and without gas phase turbulence model

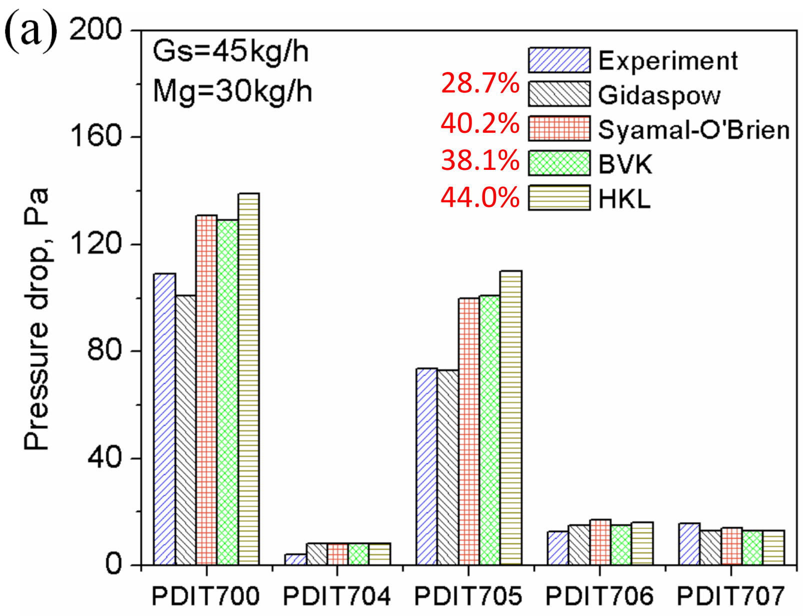


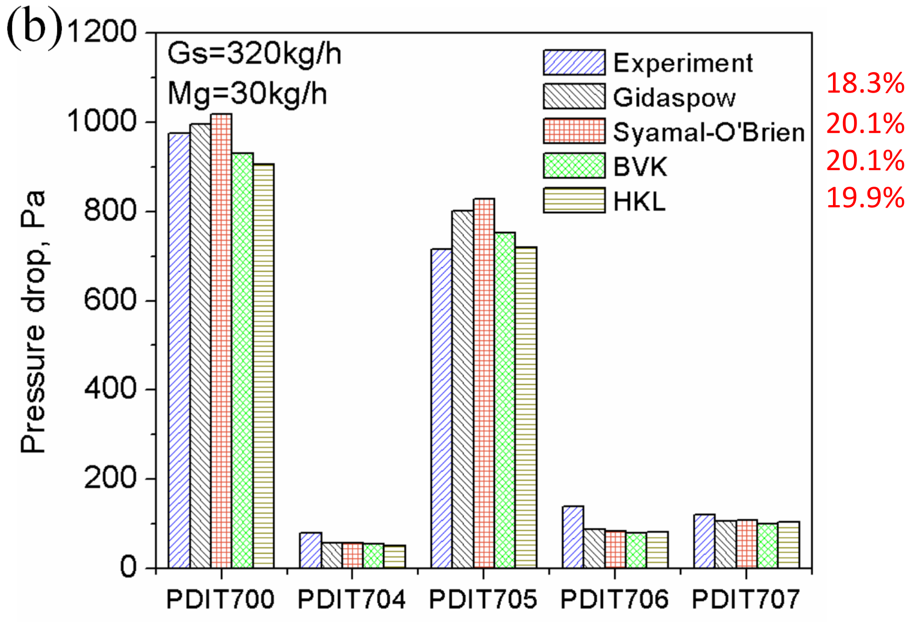


- With turbulence model, the simulation results agree slightly better with experimental data.
- Gas phase turbulence has weak effect.

Determine optimal drag model

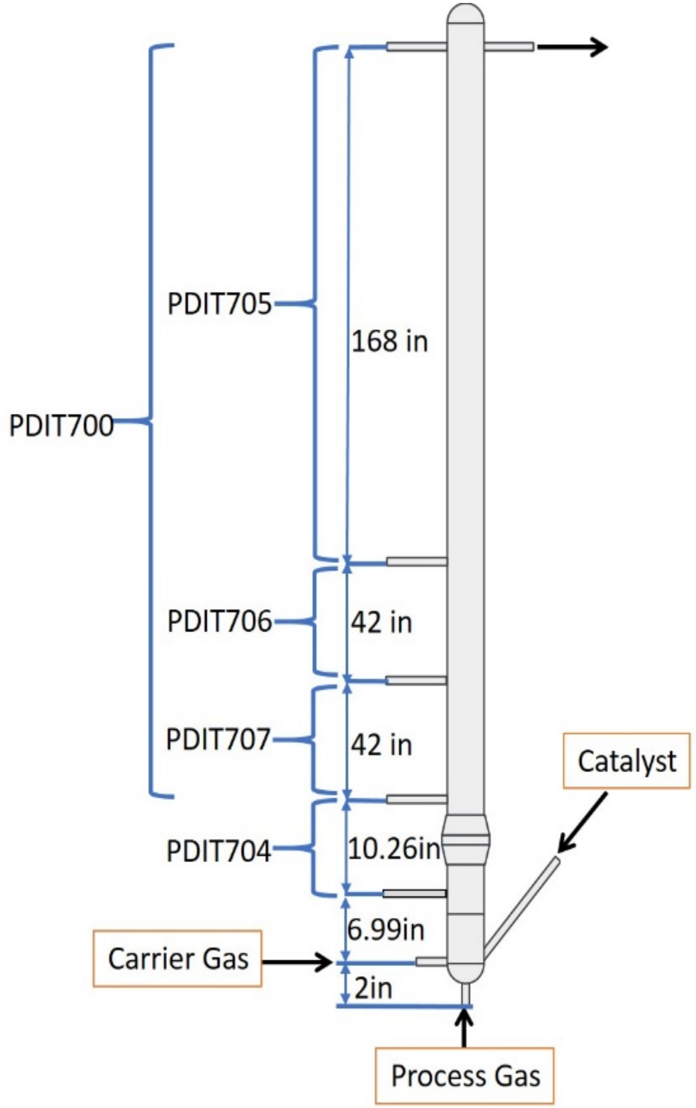


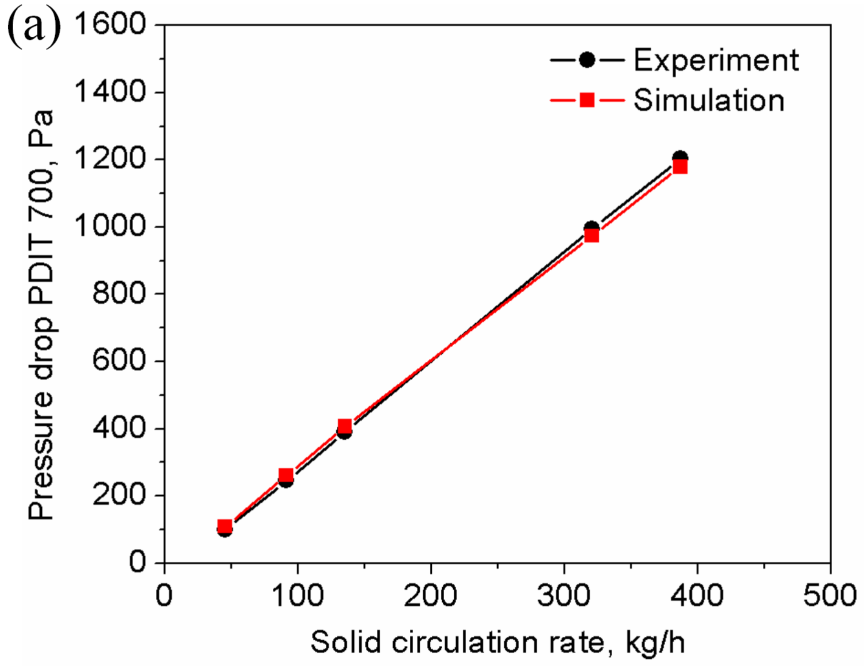


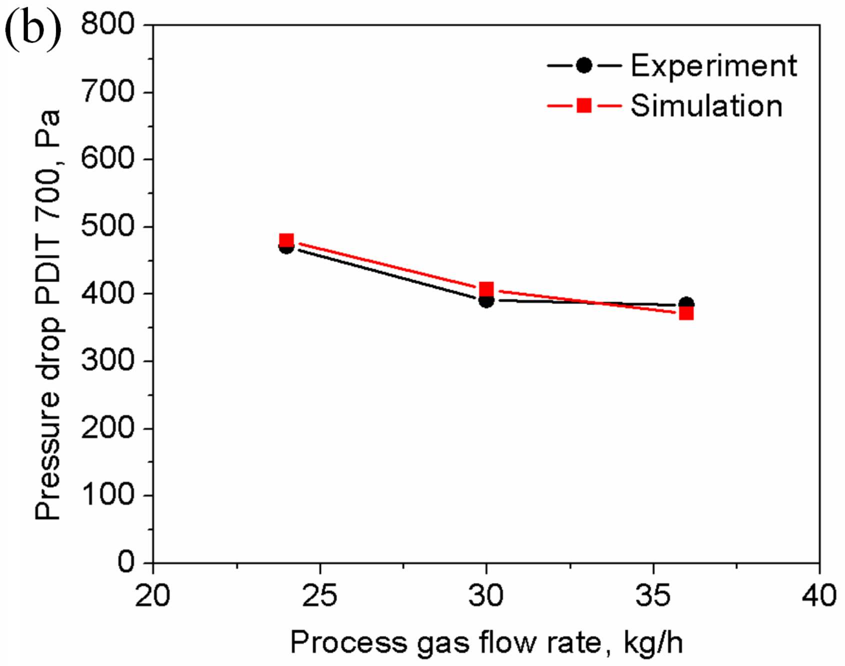


- Four different drag models were compared.
- Gidaspow drag model yields the best agreement with experimental data.

Validation of multiphase hydrodynamics

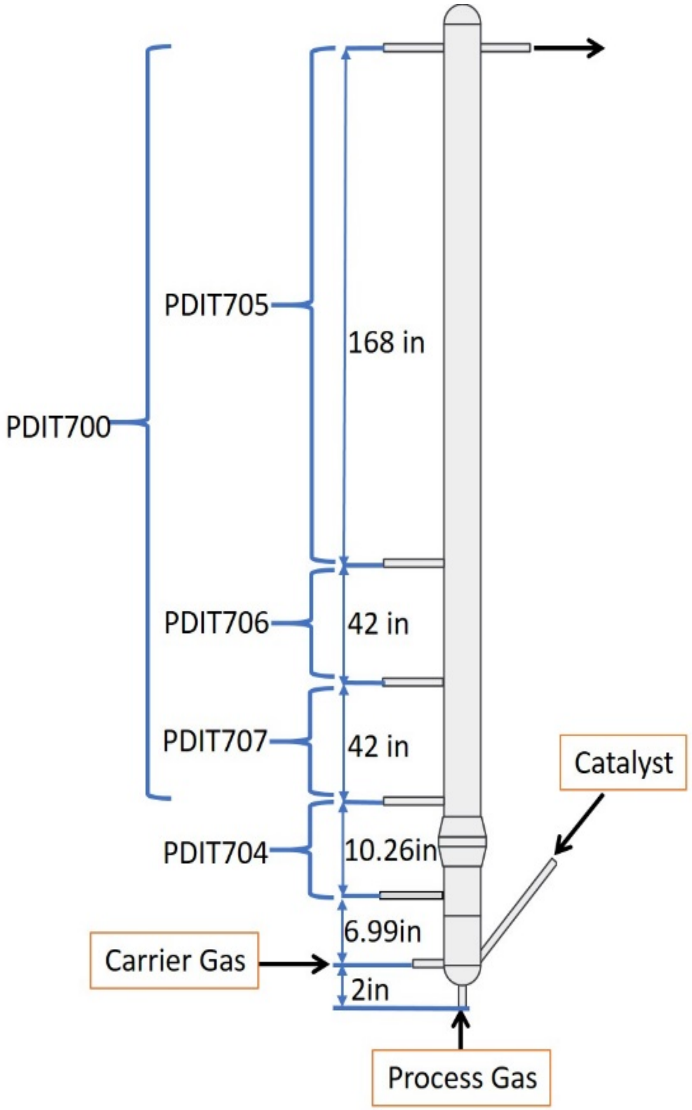


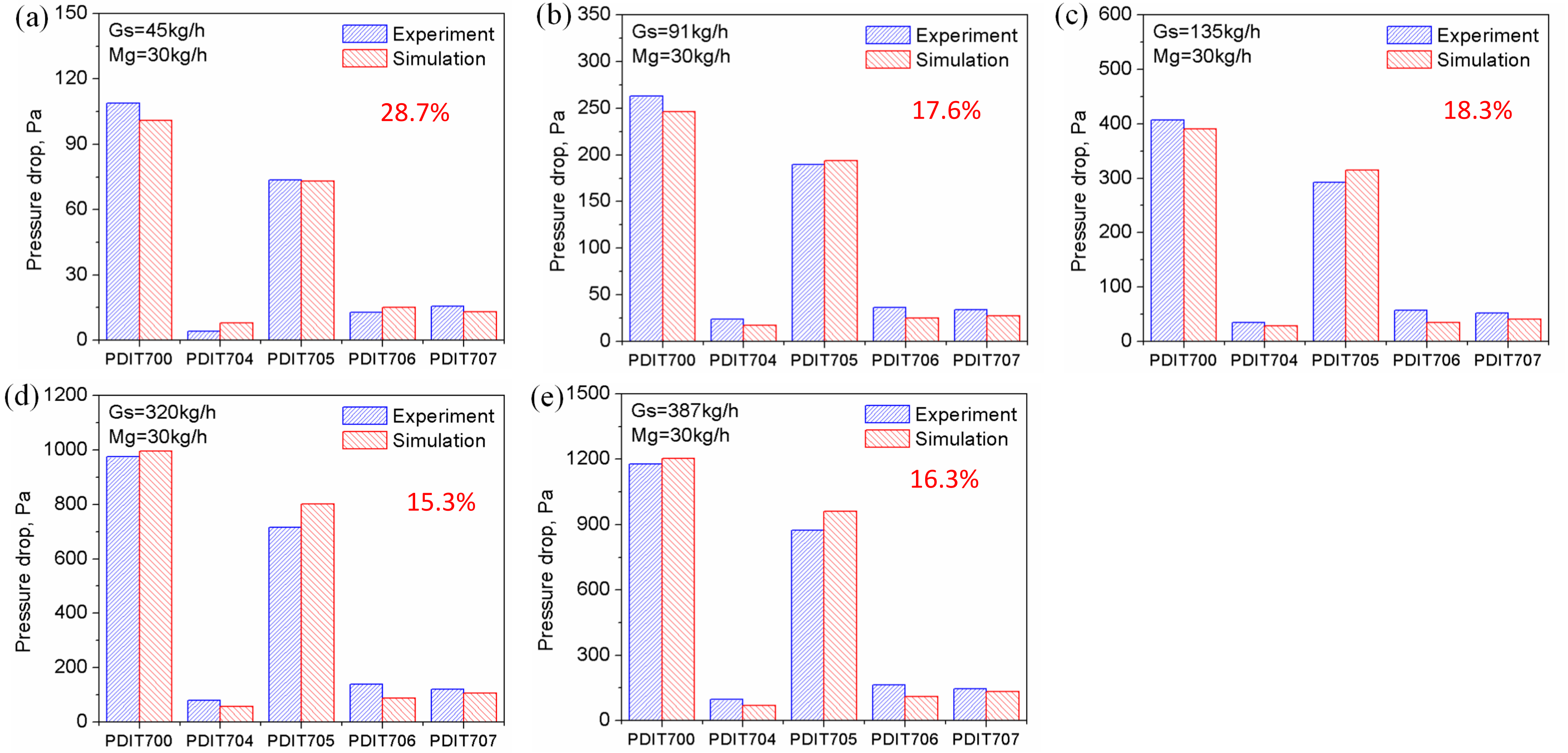




- Pressure drop PDIT 700 almost linearly increase with the solid circulation rate.
- Simulation agree well with experiment data

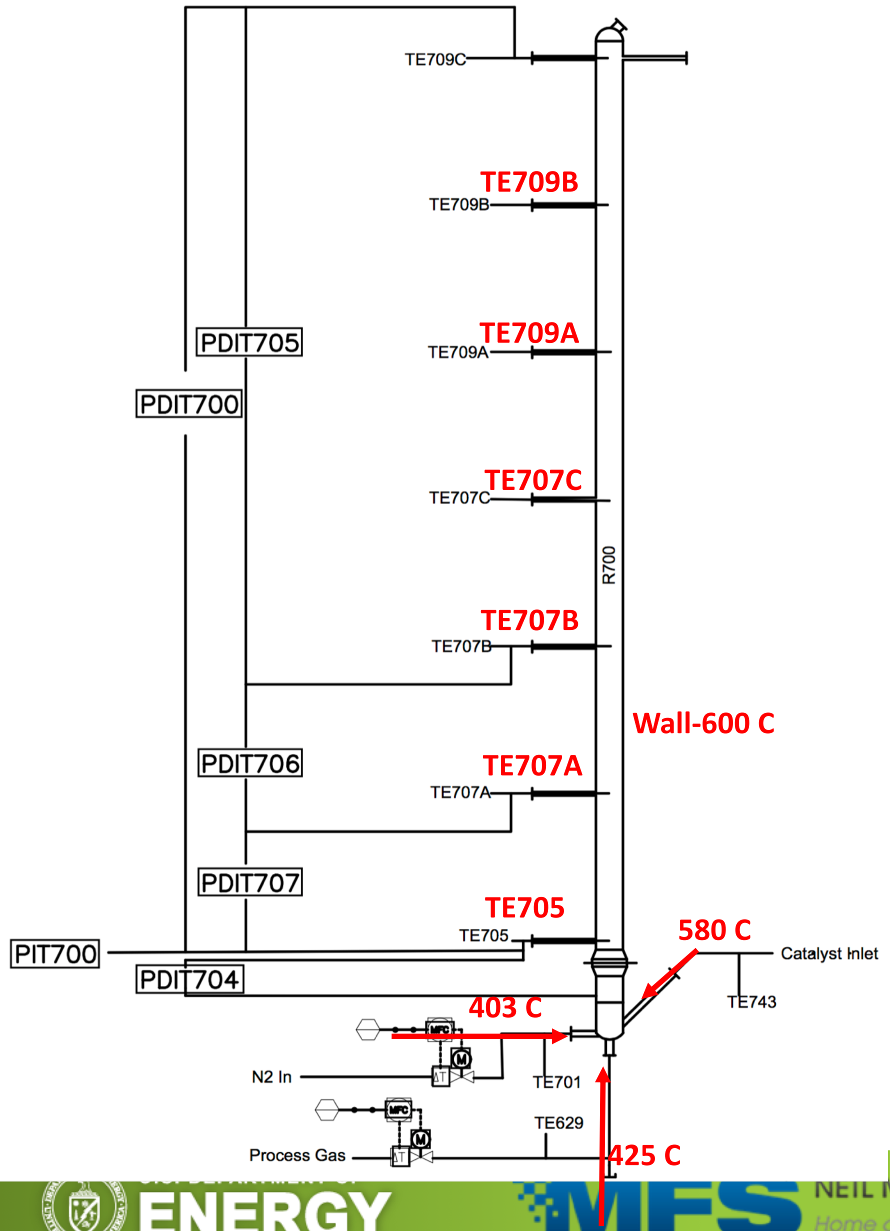
Validation of multiphase hydrodynamics

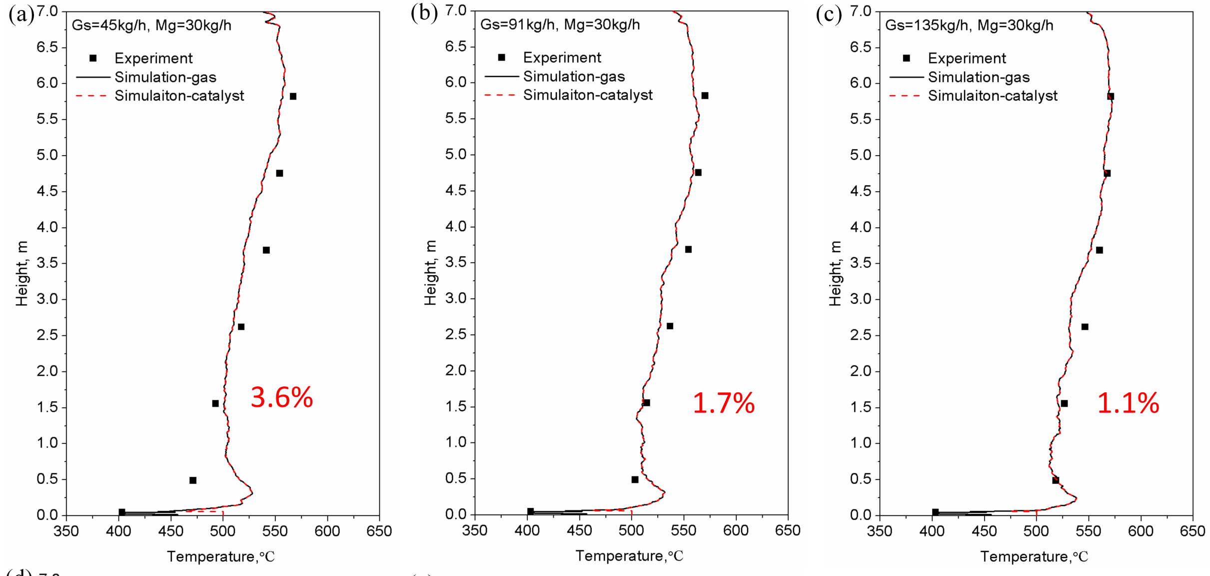


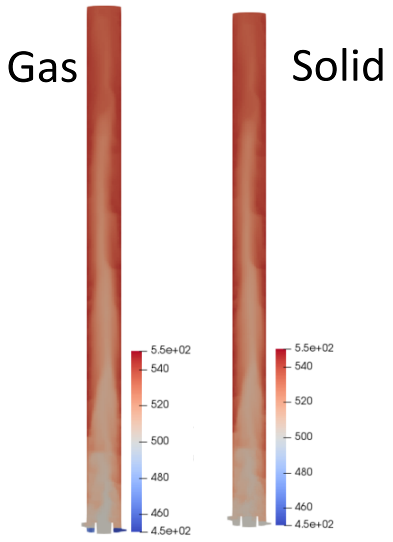


- The absolute errors are around 15-30%.

Validation of heat transfer

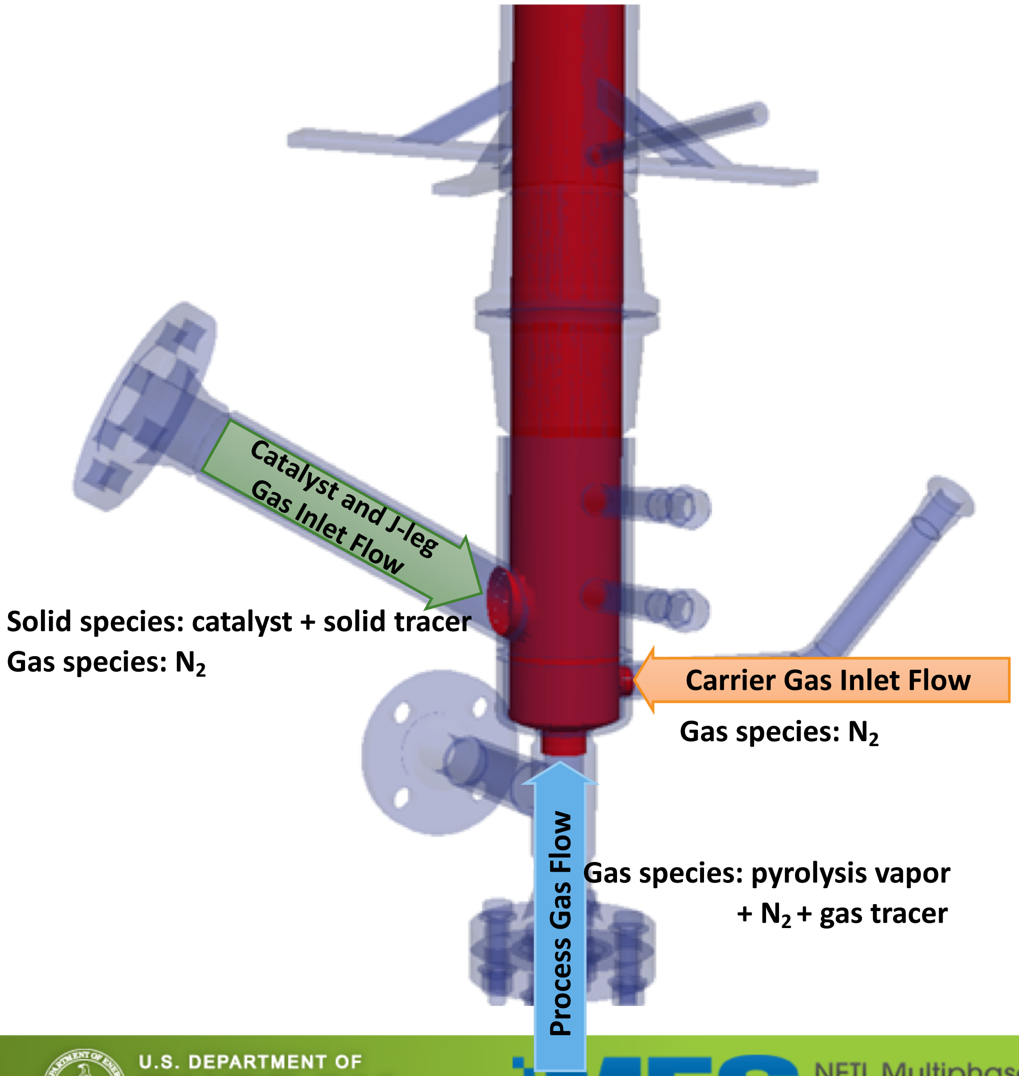




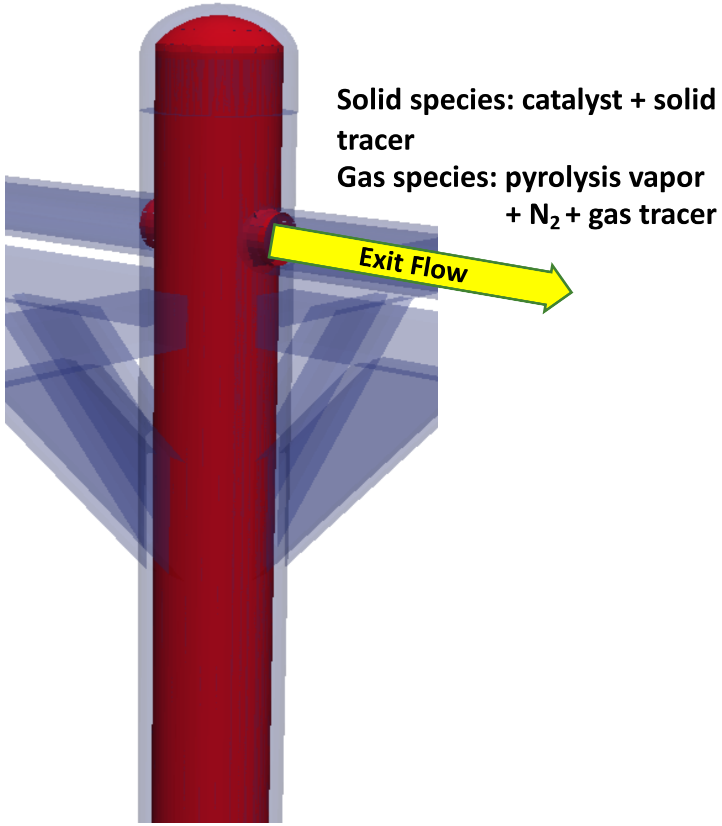


Residence Time Distribution Simulation in the R-cubed Riser

Inlet configuration



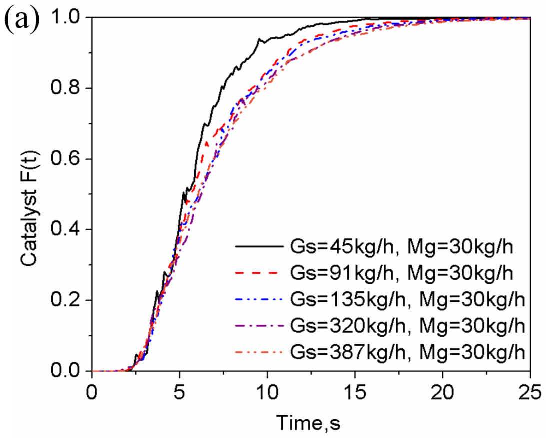
Outlet configuration

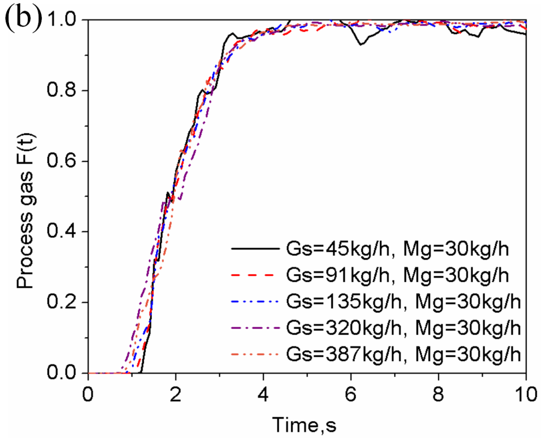


Tracer injection for non-reacting flow RTD

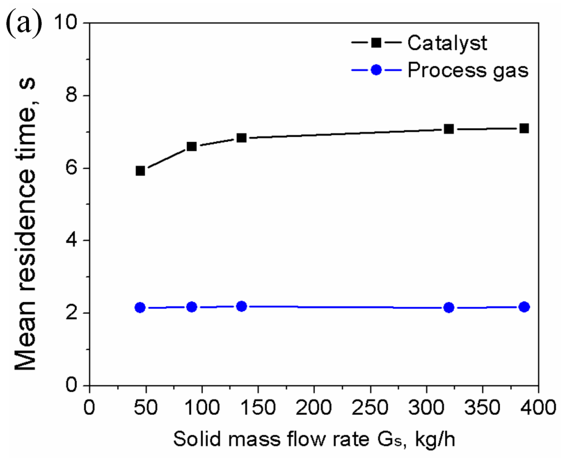
- Continuous tracer injections start at 40s of elapsed time into the simulation
- Gas tracers are given the same properties as process gas and carrier gas
- The solid tracer is given the same properties as the catalyst
- A volume fraction of 5% was used for each tracer
- The tracer outlet concentration is monitored at the top exit

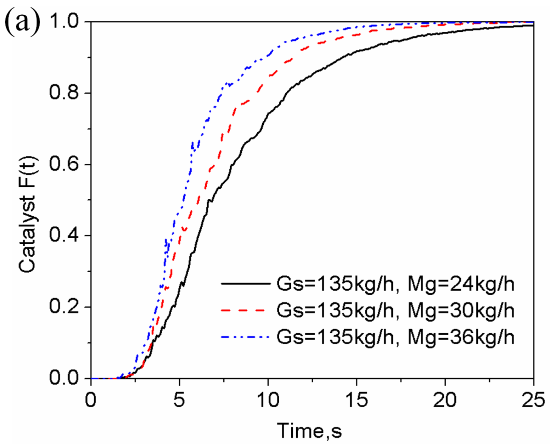
Residence Time Distribution Prediction

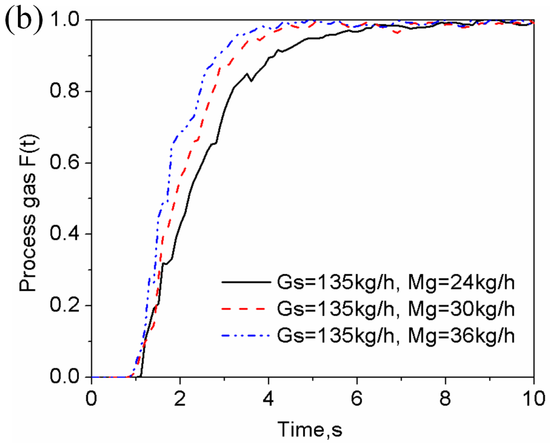




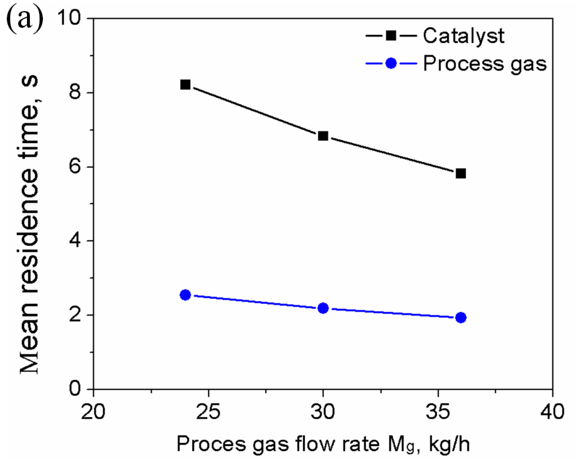
$$t_m = \sum_{i=0}^{N} [1 - F(t_i)] \Delta t_i$$







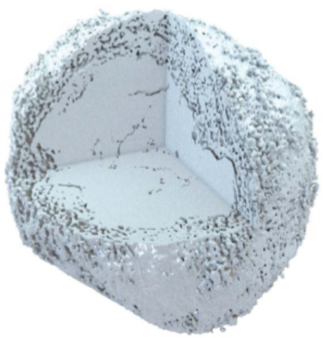
$$t_m = \sum_{i=0}^{N} [1 - F(t_i)] \Delta t_i$$

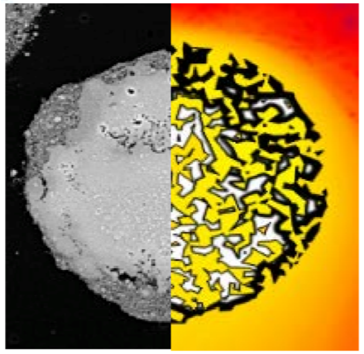


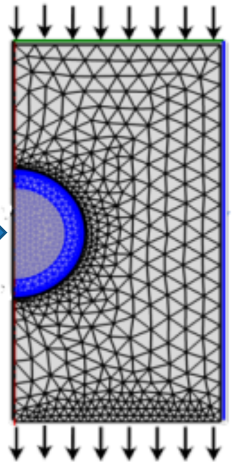
- Solid mean residence time slightly increase with the solid circulation rate, and decrease with process gas flow rate.
- Gas mean residence time keep almost unchanged.

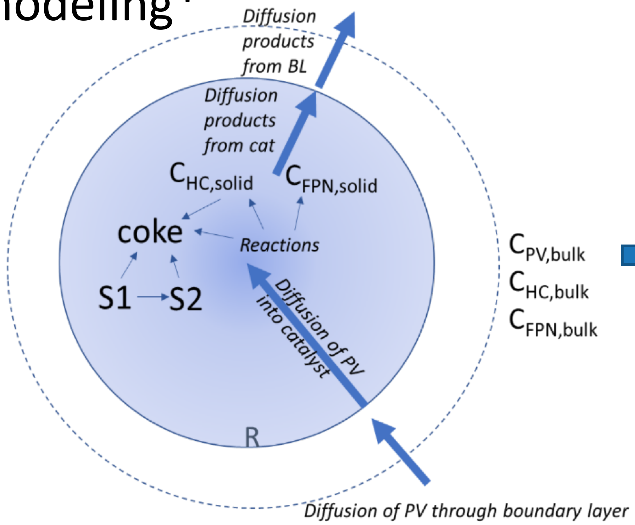
NREL VPU Kinetic Model

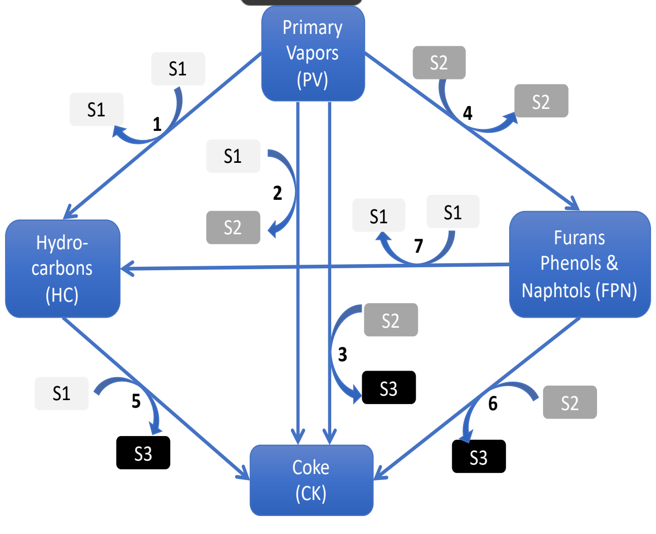
- Kinetics from NREL experiments and mesoscale modeling*





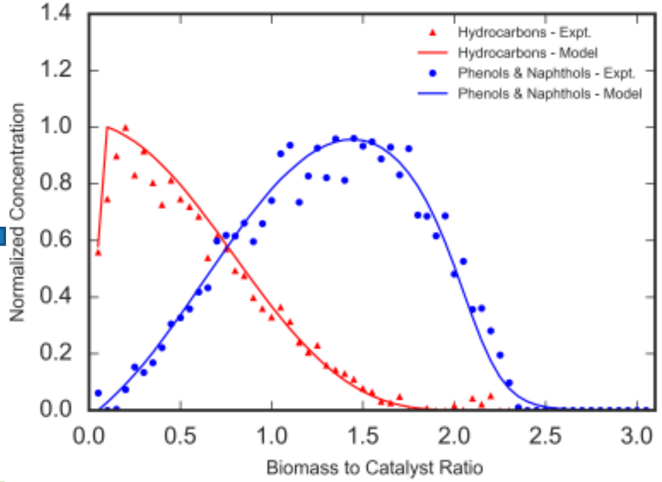






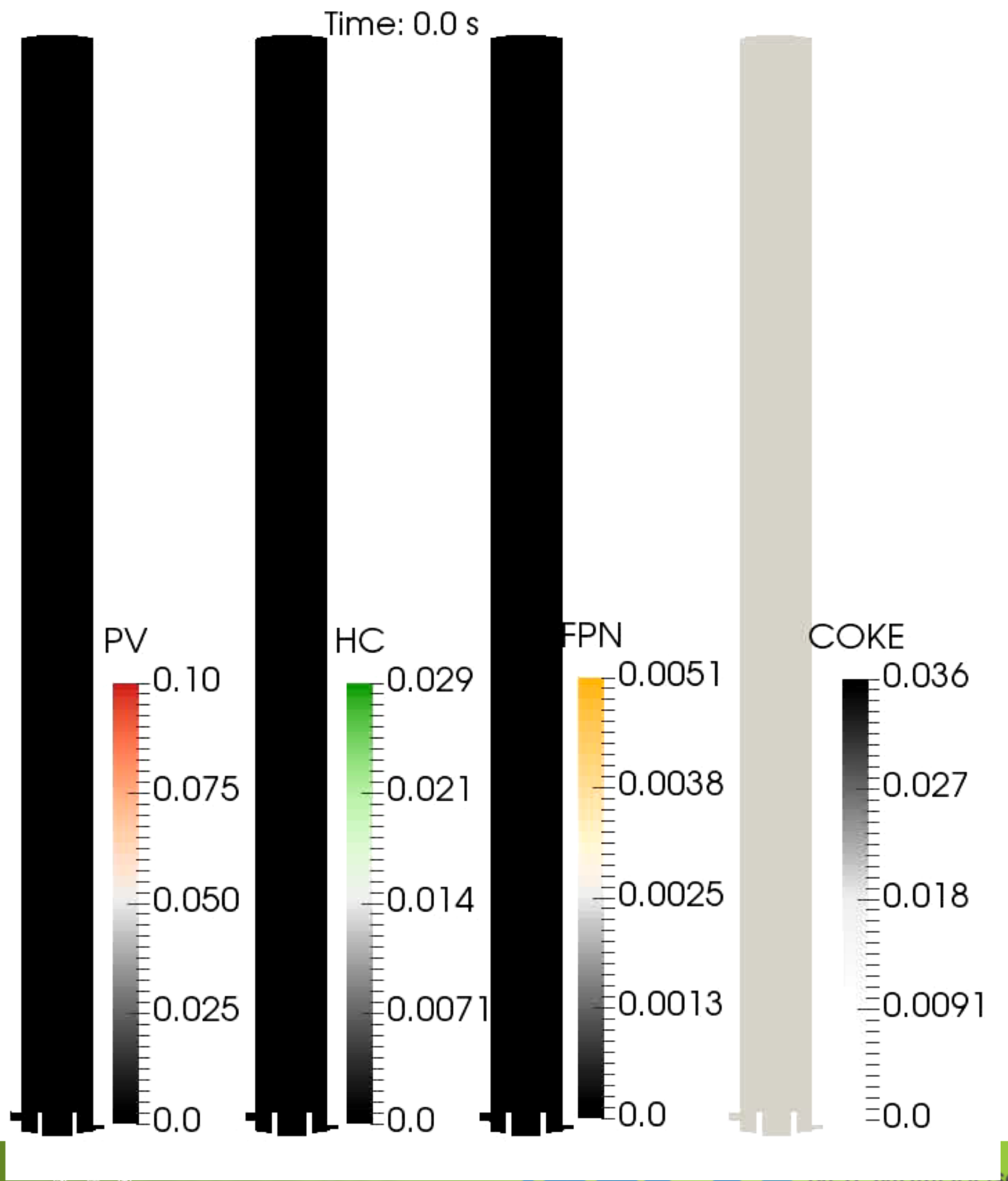
- Catalyst three sites: fresh, intermediate and deactivated sites
- Pyrolysis vapor converts to: Hydrocarbon, FP&N and coke
- Intrinsic kinetics coupled with inter and outer mass transfer limitations

	Reaction	rate constant $k_{i,500\,°C}$ (m³/(mol s))	rate equation (mol/m³ s)
1	PV + S1 → HC_s + S1	2.573	PV S1 $\eta_1 k_1$
2	PV + S1 → CK + S2	0.456	PV S1 $\eta_2 k_2$
3	PV + S2 → CK + S3	0.152	PV S2 $\eta_3 k_3$
4	PV + S2 → FPN_s + S2	2.904	PV S2 $\eta_4 k_4$
5	HC_s + S1 → CK + S3	0.507	HC_s S1 $\eta_5 k_5$
6	FPN_s + S2 → CK+ S3	0.006	FPN_s S2 $\eta_6 k_6$
7	FPN_s + S2 → HC_s + S2	0.051	FPN_s S2 $\eta_7 k_7$
8	FPN_s → FPN	$k_{efflux,FPN}$	$\frac{FPN_s - FPN}{1/k_{BL} + H/k_{diff}}$
9	HC_s → HC	$k_{efflux,HC}$	$\frac{HC_s - HC}{1/k_{BL} + H/k_{diff}}$

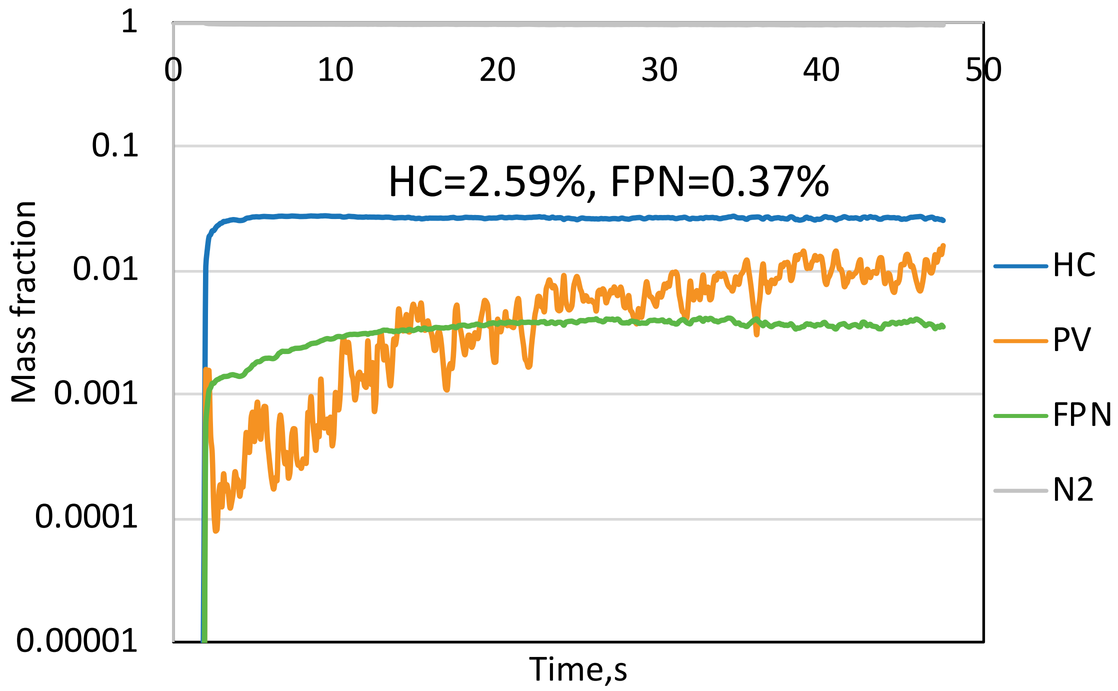


*NREL 2017 Q4 report.

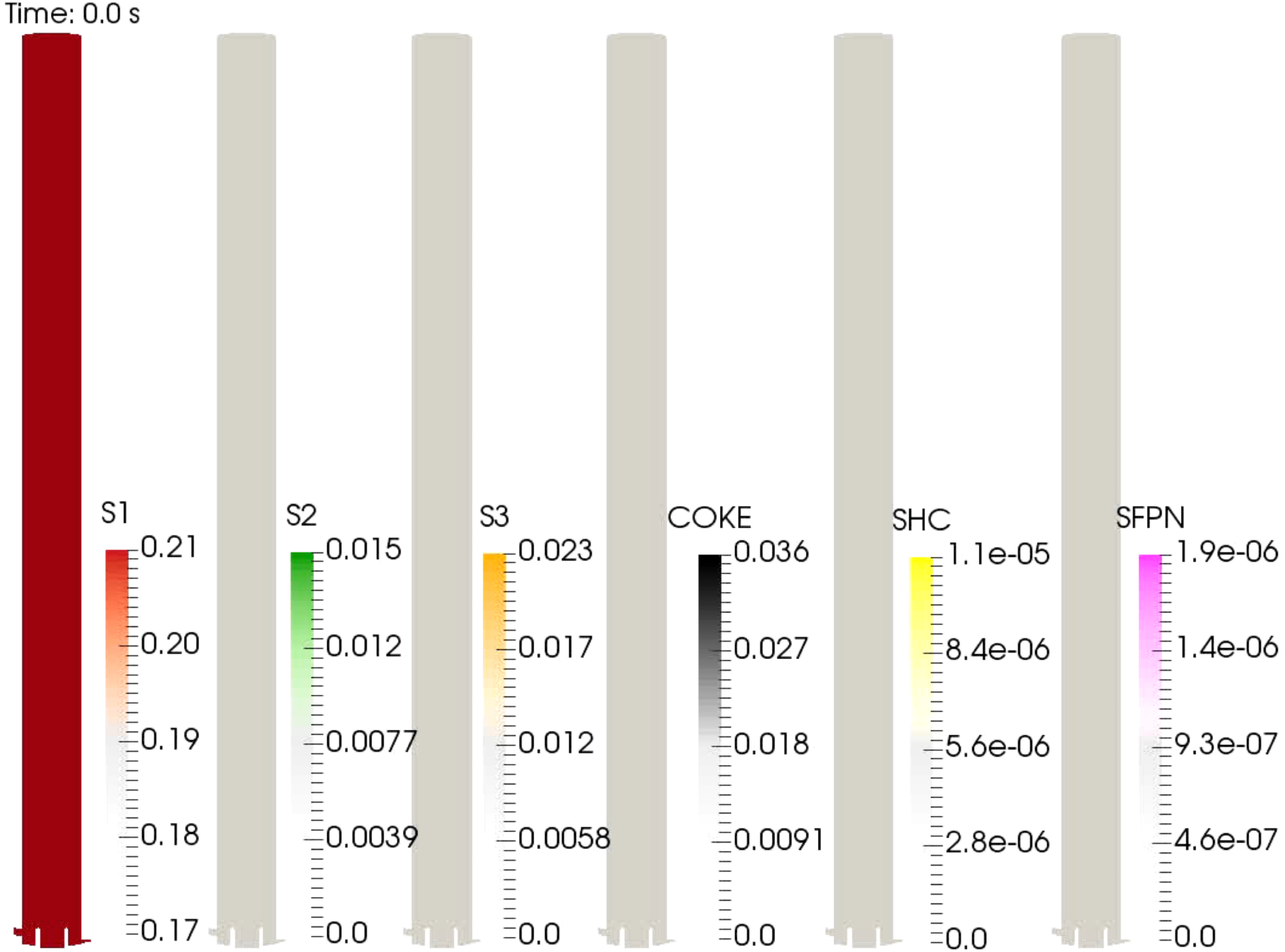
Reaction Simulation in the R-cubed Riser



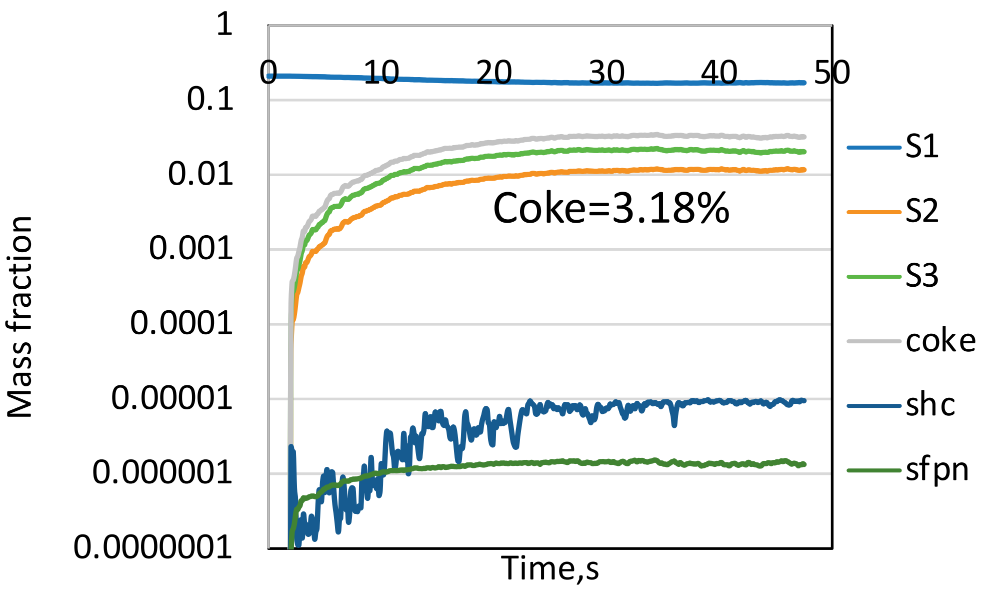
- T= 500 degree C
- P=132 kPa
- process gas: 400SLM, 10% biomass vapor, 90% N2
- Carry gas: 130 SLM, N2
- Solid circulation rate=100lb/hr



Reaction Simulation in the R-cubed Riser



- T= 500 degree C
- P=132 kPa
- process gas: 400SLM, 10% biomass vapor, 90% N2
- Carry gas: 130 SLM, N2
- Solid circulation rate=100lb/hr



Summary of Results

- MFiX simulations were performed to study flow hydrodynamics in the VPU riser and results were compared with the NREL non-reacting flow experimental data.
- MFiX simulations were performed for study heat transfer in the VPU riser and results were compared with the NREL non-reacting flow experimental data.
- Validated CFD model was applied to study the gas/solid RTDs under different operating conditions.
- Reacting flow simulations was conducted with NREL newest VPU kinetics, validation against experimental tests at NREL is undergoing.

Acknowledgements

Special thanks to: Jeremy Leong, Trevor Smith, Kevin Craig, and the DOE Bioenergy Technologies Office

NATIONAL ENERGY TECHNOLOGY LABORATORY

This work was performed in support of the US Department of Energy's EERE **Bioenergy Technologies Office (BETO)** as part of the BETO Consortium for **Computational Physics and Chemistry (CCPC)**. The Research was executed through the NETL Research and Innovation Center's BETO CCPC. Research performed by Leidos Research Support Team staff was conducted under the RSS contract 89243318CFE000003

Oak Ridge National Laboratory

Jim Parks
Gavin Wiggins
Stuart Daw
Emilio Ramirez
Charles Finney
Bruce Adkins
Zach Mills

NREL (National Renewable Energy Laboratory)

David Robichaud
Peter Ciesielski
Seonah Kim
Lintao Bu
Tom Foust
Vassili Vorotnikov
Carrie Farberow
Mark Nimlos
Brandon Knott
Brennan Pecha
Vivek Bharadwaj

Pacific Northwest National Laboratory

Roger Rousseau
Vanda Glezakou
Sneha Akhade
Simuck Yuk
Asanga Padmaperuma

National Energy Technology Laboratory

Xi Gao
Tingwen Li
William Rogers
Madhava Syamlal
Rupen Panday
Cheng Li
Huda Ashfaq
Bryan Hughes
Jia Yu

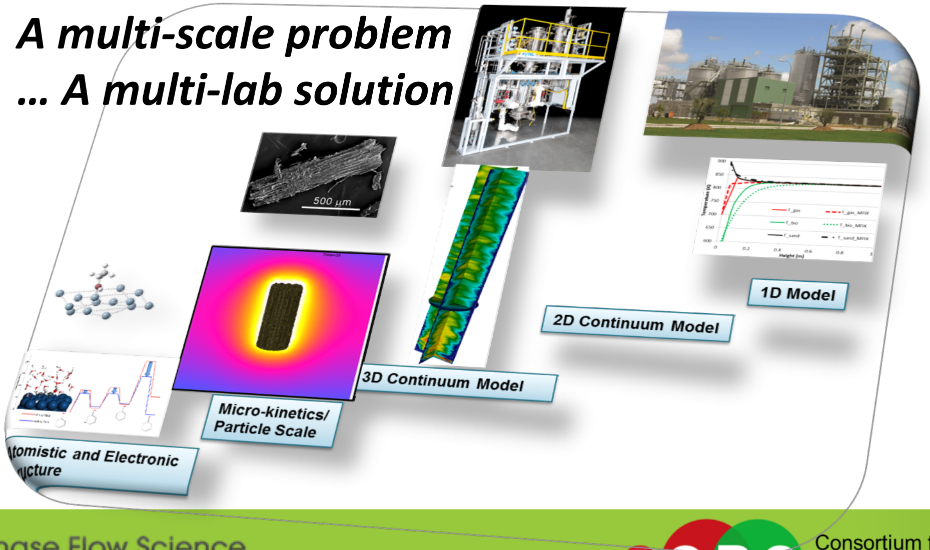
Argonne National Laboratory

Larry Curtiss
Rajeev Assary
Lei Cheng
Cong Liu
Dale Pahls

ChemCatBio
Chemical Catalysis for Bioenergy

CCPC www.cpcbiomass.org

A multi-scale problem
… A multi-lab solution



Thanks!

Questions?

Industry Advisory Panel

David Dayton (RTI), George Huff (MIT, retired BP), Jack Halow (Separation Design Group), Mike Watson (Johnson Matthey), Steve Schmidt (WR Grace), Tom Flynn (Babcock & Wilcox)

Disclaimer

NATIONAL ENERGY TECHNOLOGY LABORATORY

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.