

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 Li³, William A. Rogers¹, Kristin Smith⁴, Katherine Gaston⁴

¹National Energy Technology Laboratory, 3610 Collins Ferry Road, Morgantown, WV 26507, USA

²Leidos Research Support Team, 3610 Collins Ferry Road, Morgantown, WV 26507, USA

³SABIC, Sugar Land, TX 77478, USA

⁴National Renewable Energy Laboratory, Golden, CO 80401

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



Solutions for Today | Options for Tomorrow



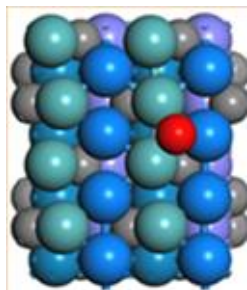
- Background and motivation
- Multiphase hydrodynamics simulation in the R-cubed VPU riser
- Residence time distribution (RTD) simulation in the R-cubed VPU riser
- Heat transfer simulation in the R-cubed VPU riser
- Vapor phase upgrading (VPU) reaction simulation in the R-cubed Riser
- Summary of results and next steps

Consortium for Computational Physics and Chemistry (CCPC)*



Task 2

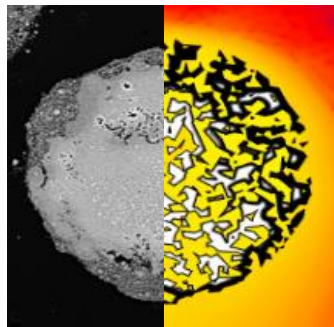
Catalysis Modeling at Atomic Scales



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

Task 3

Catalyst Particle Modeling at Meso Scales

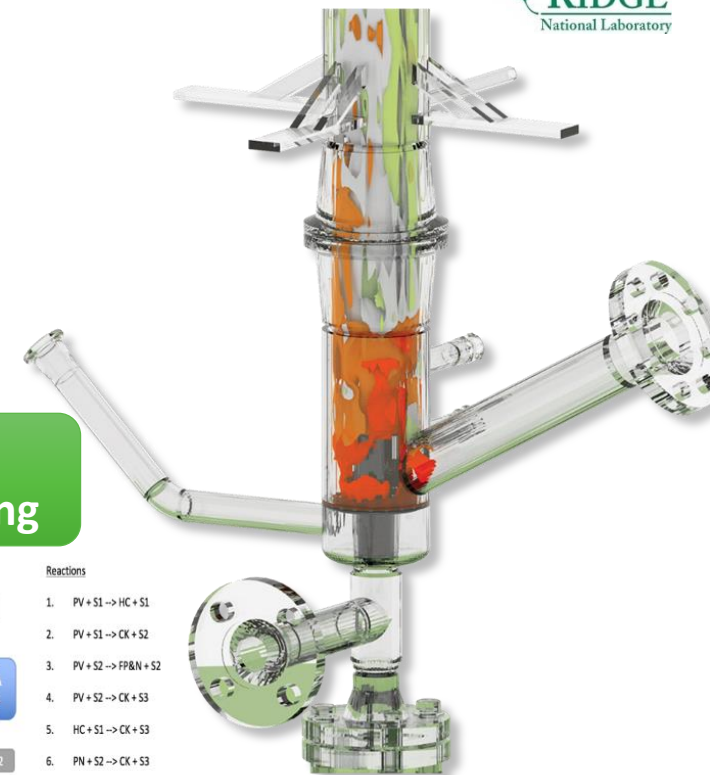


Understanding mass transport of reactants/products, reaction kinetics, and coking and deactivation processes

Task 4

Conversion Modeling at Process Scales

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



Task 1

Coordination, Integration, and Industry Outreach



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)

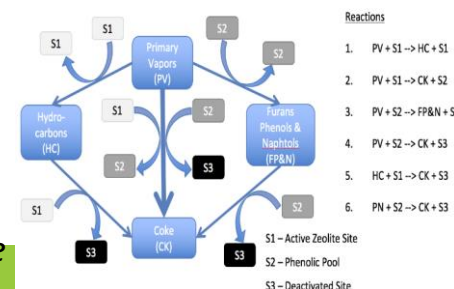


www.cpcbmass.org

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



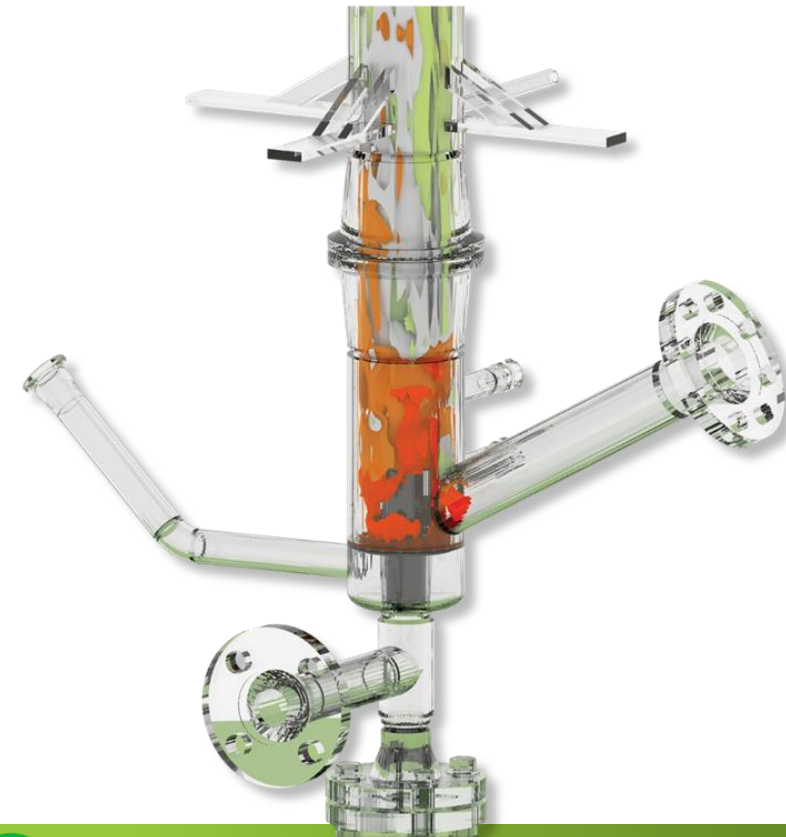
*Adopted from 2019 Peer review

- **Goal of this work:** Use reactor scale multiphase computational fluid dynamics simulations of catalytic upgrading of biomass pyrolysis vapor to provide:
 - Detailed modeling of 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 interphase **eX**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



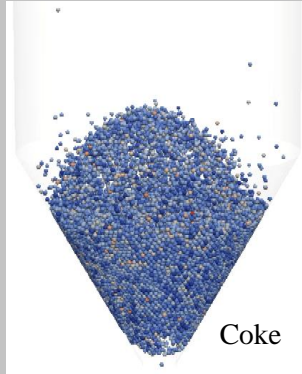
*Determining optimal
optimal operating
conditions for maximum
yield and enabling scale-up*



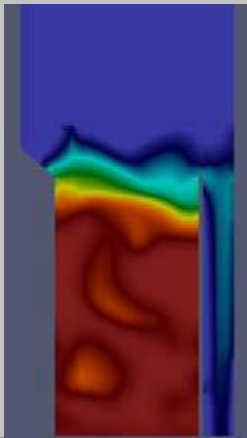
Reactor Models Cover Wide Range of Scale and Type*

*Adopted from 2019 Peer review

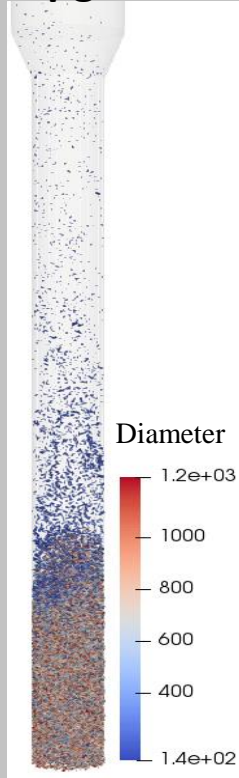
Spouted bed Upgrader (kinetics)



Coke



2" Fluidized Bed Pyrolyser and Upgrader

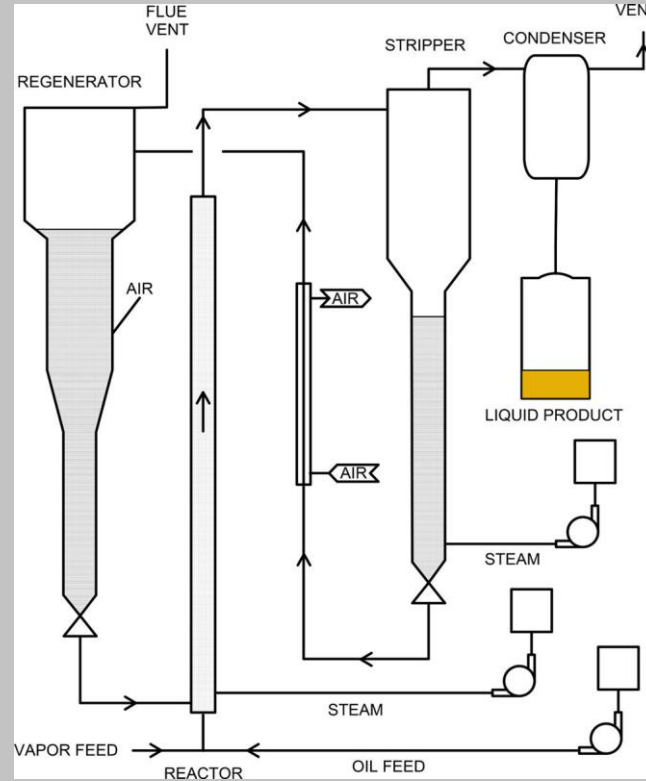


~883 sec residence time

500-900 micron particle

0.5 kg/hr flow rate

Davison Circulating Riser Upgrader

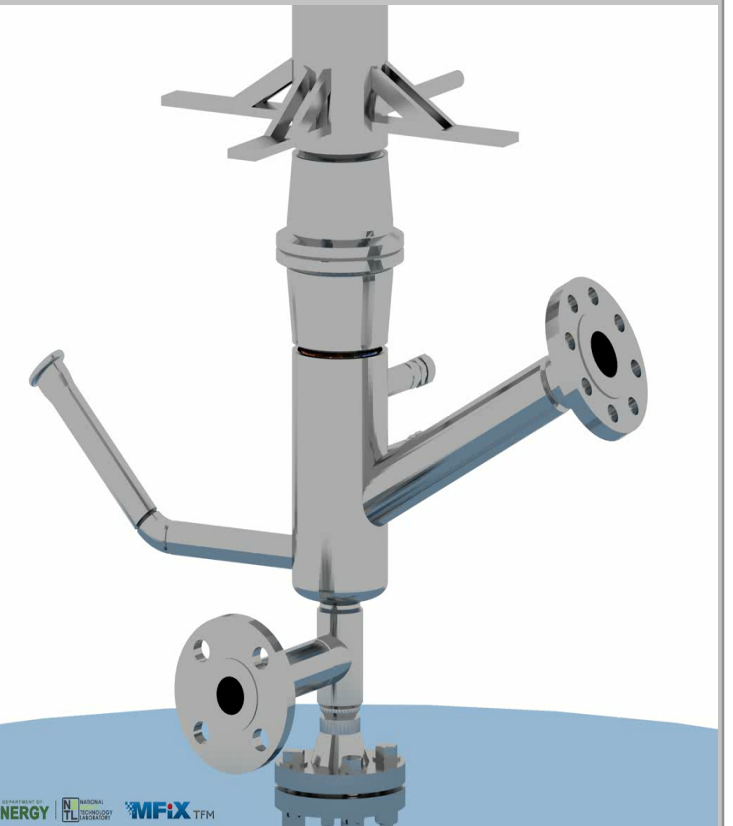


~3 sec residence time

80-100 micron particle

2 kg/hr flow rate

TCPDU R-Cubed riser Upgrader



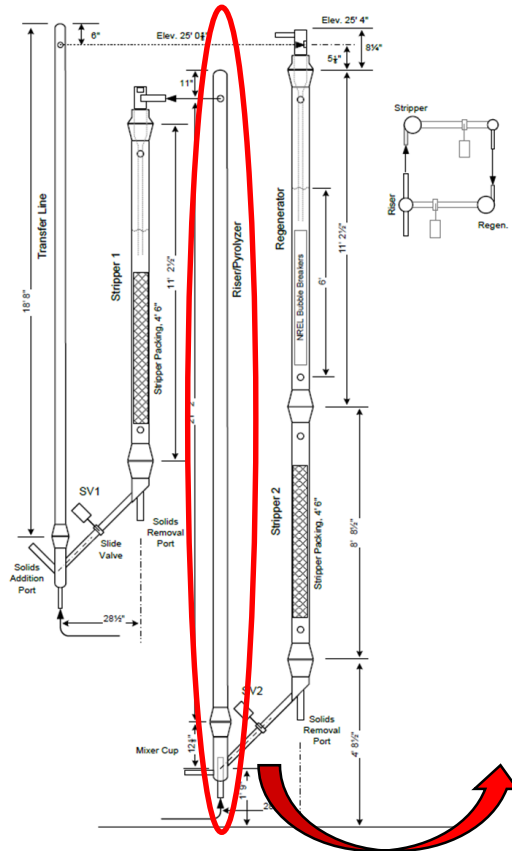
~10 sec residence time

80-100 micron particle

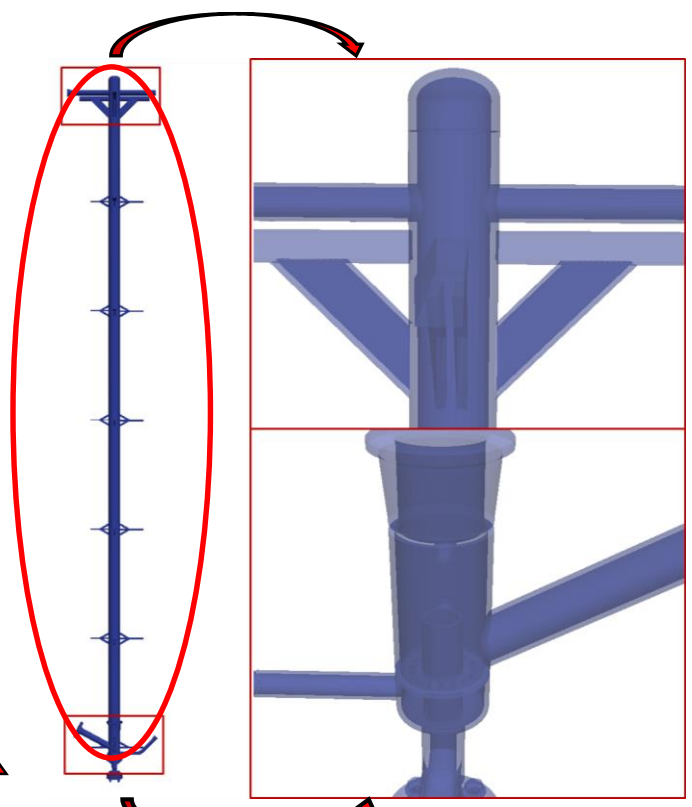
15 kg/hr flow rate

TCPDU R-cubed Reactor

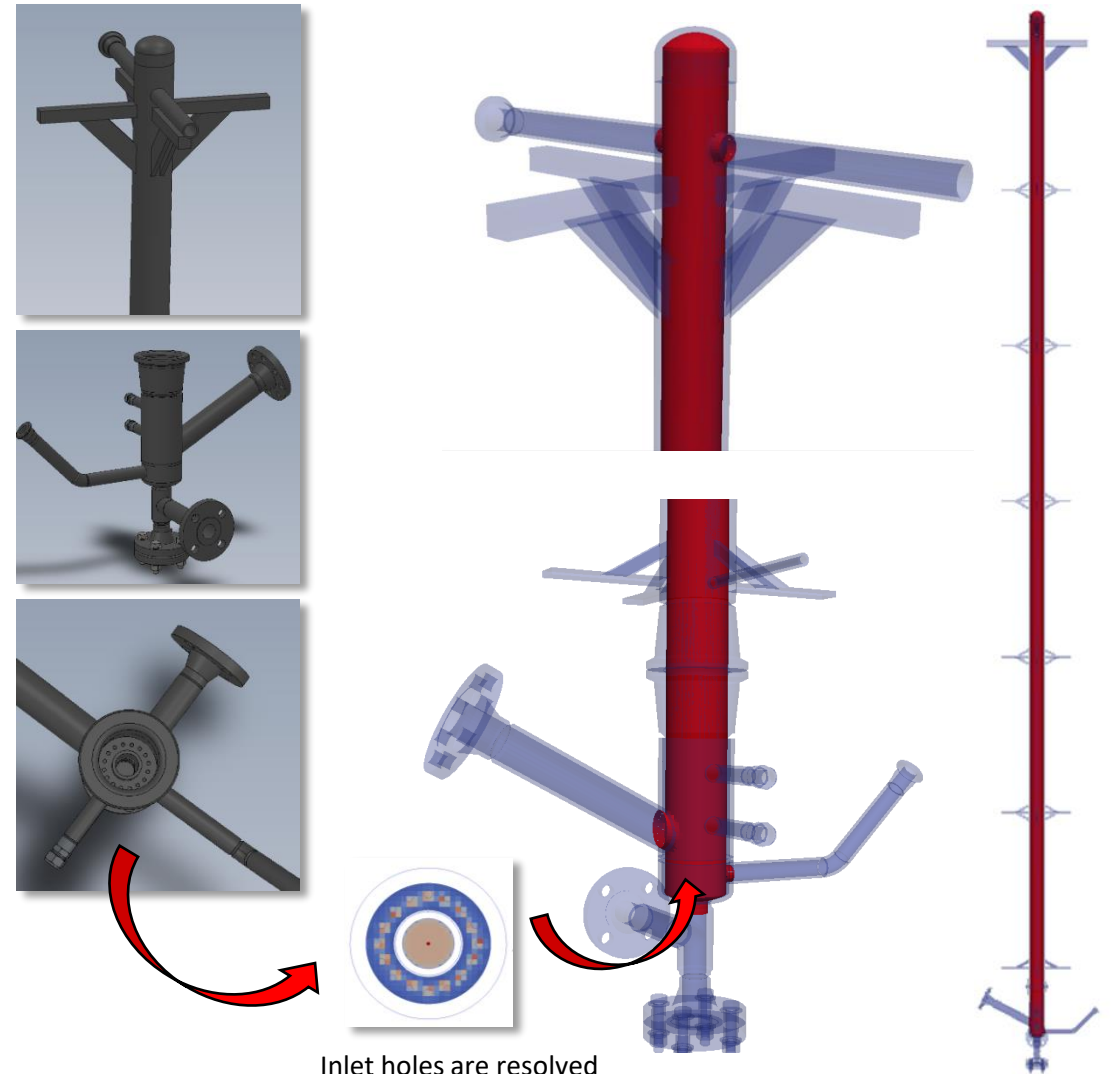
TCPDU Process



R-cubed riser Geometry

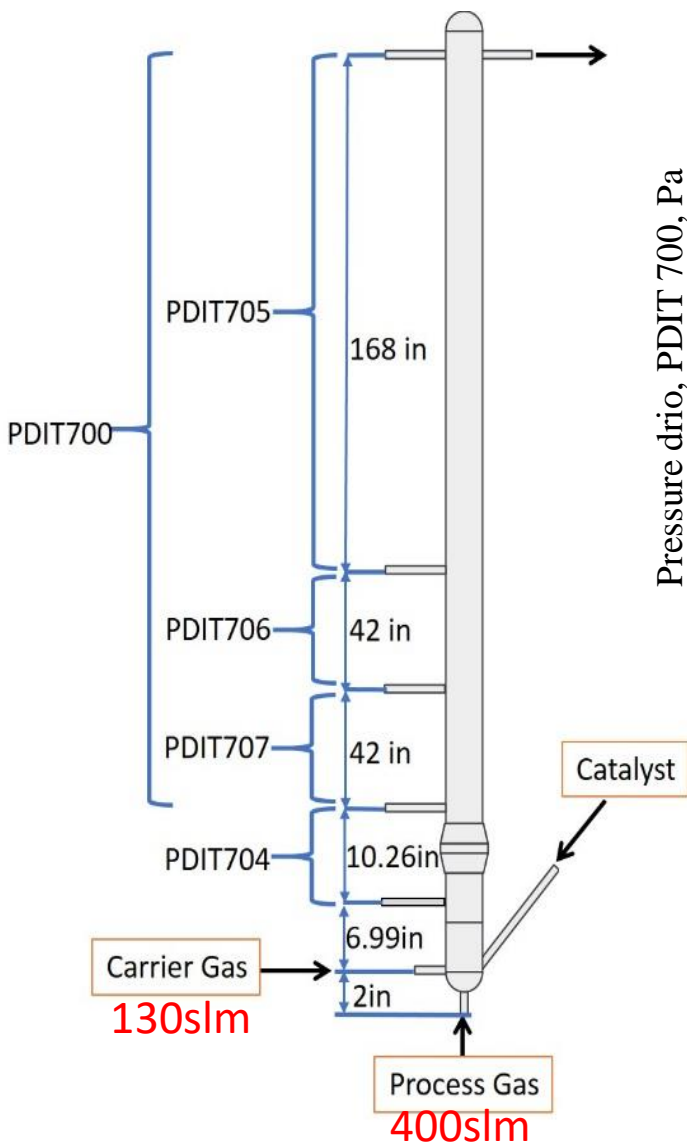


Computational Domain

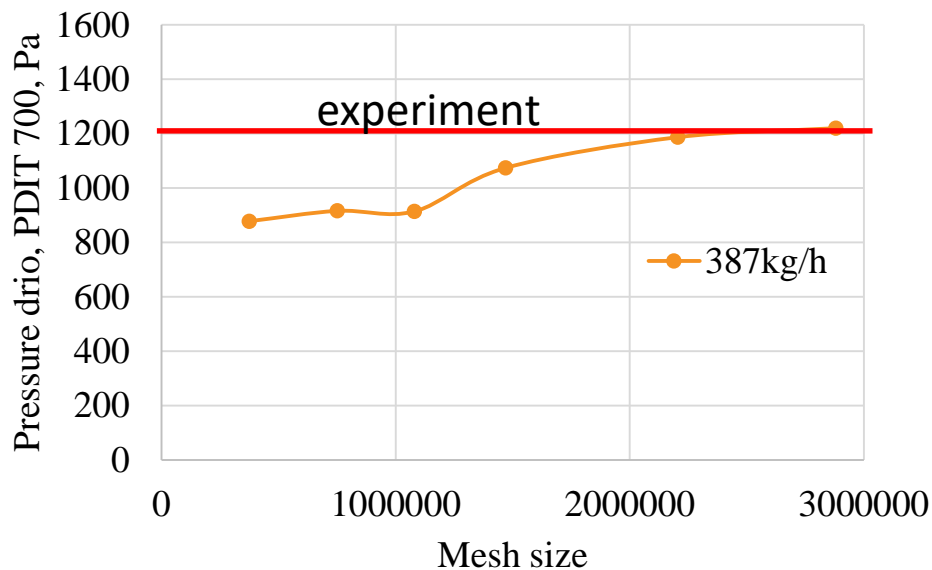


- Riser: Height: 7.05 m, diameter: 0.092 m
- Outlet diameter: 0.038 m
- Solids inlet diameter: 0.049 m
- Pyrolysis vapor inlet diameter: 0.047 m
- Distributor: 16 holes with diameter of 0.00625 m

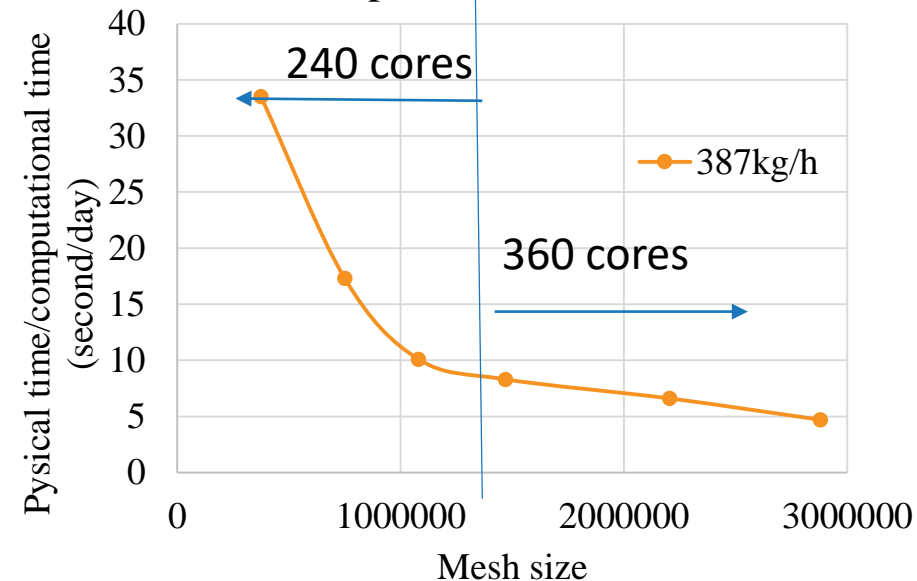
Multiphase Hydrodynamics Simulation in the R-cubed Riser



Mesh independence study

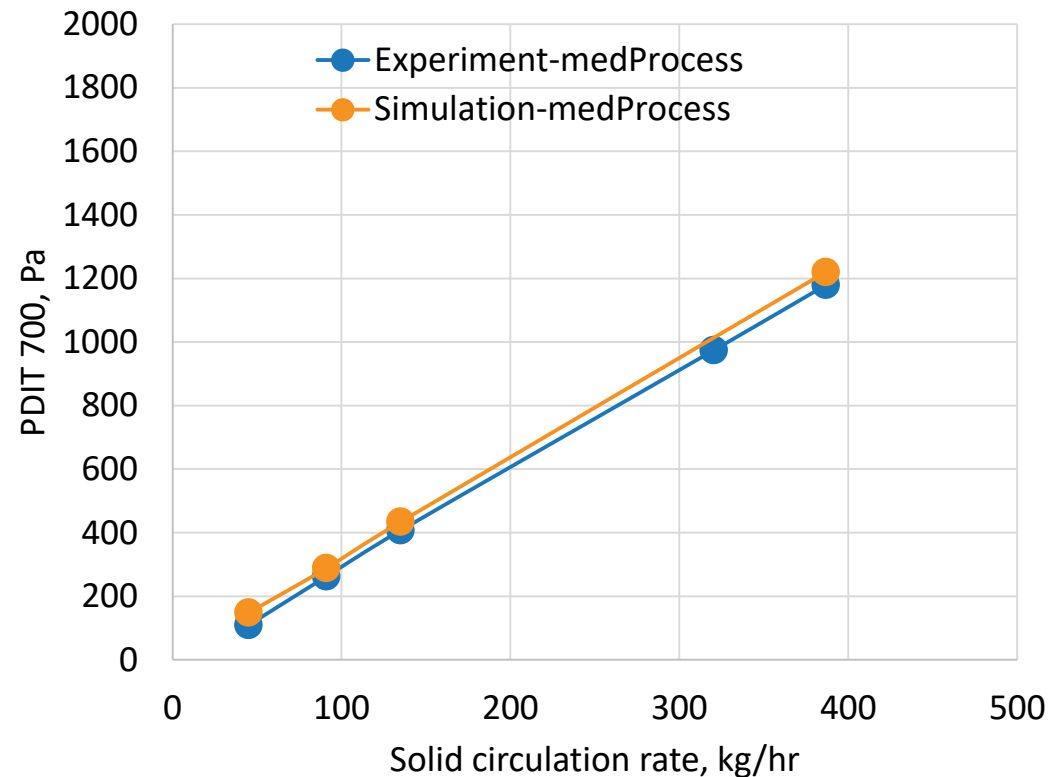
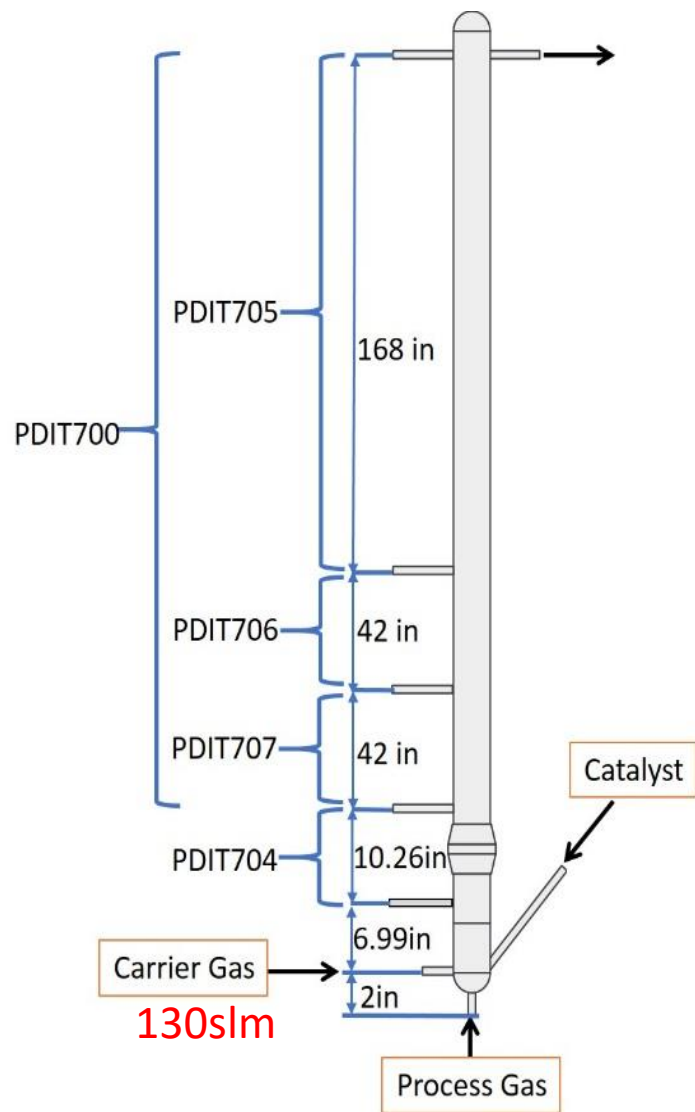


computational cost



- 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

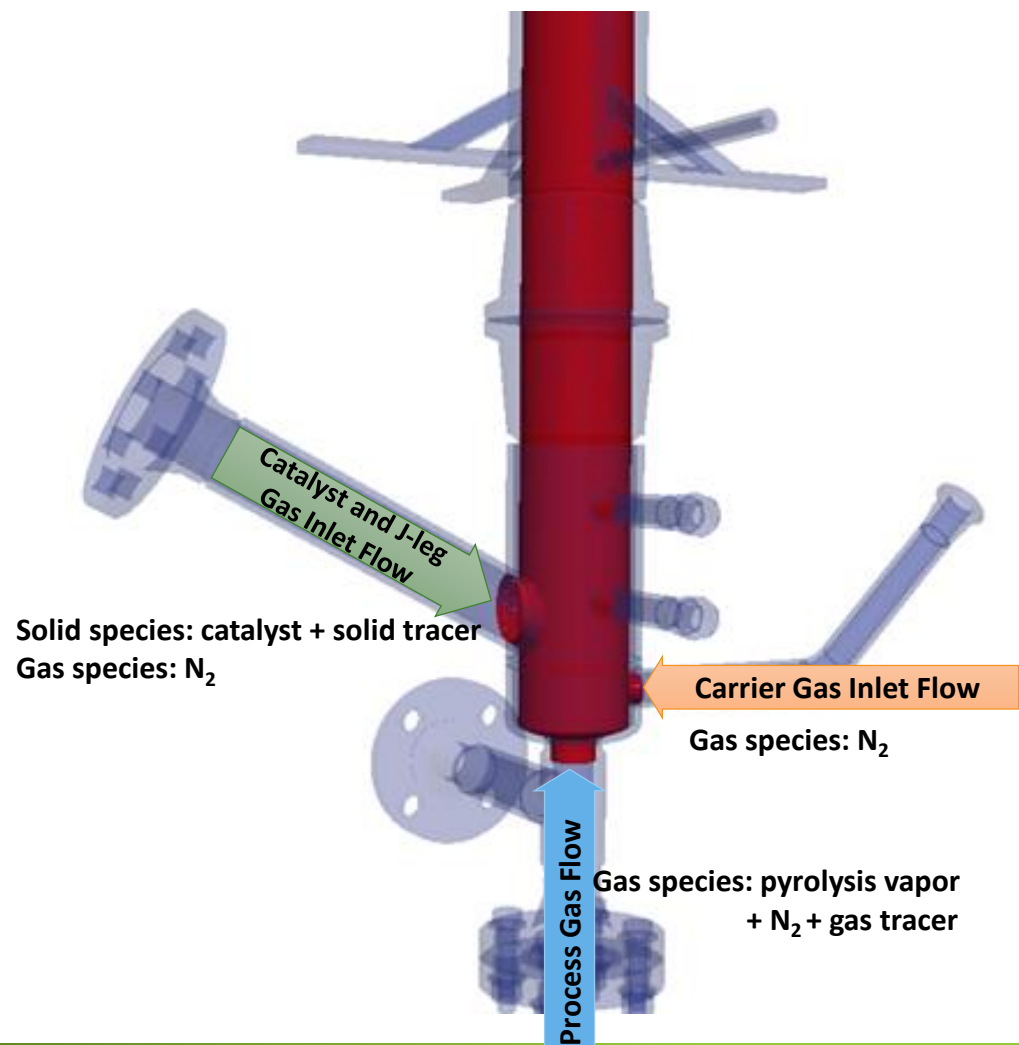
Multiphase Hydrodynamics Simulation in the R-cubed Riser



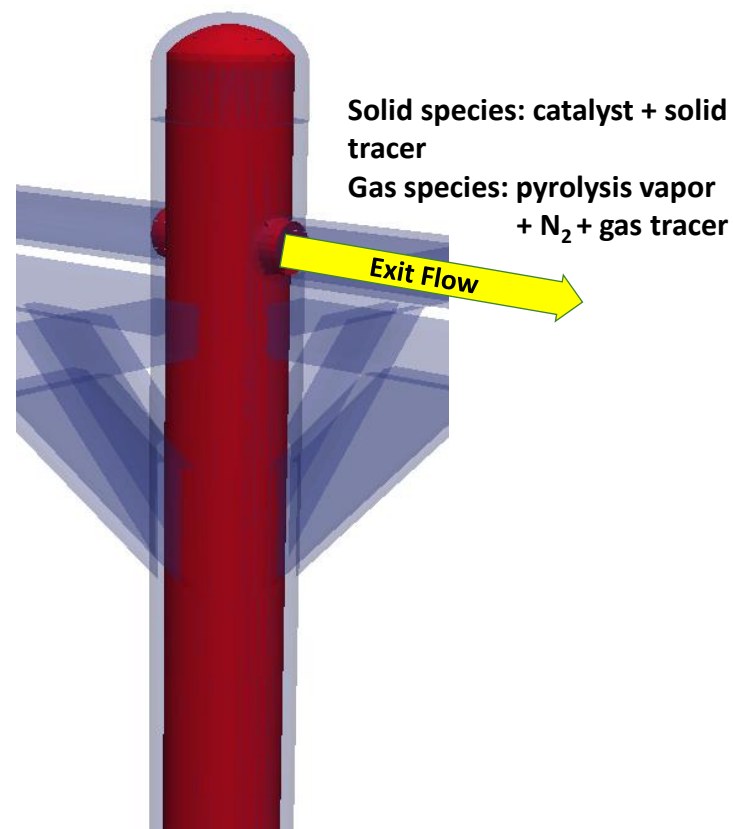
- Pressure drop PDIT 700 almost linearly increase with the solid circulation rate.
- Simulation agree well with experiment data

Residence Time Distribution Simulation in the R-cubed Riser

Inlet configuration



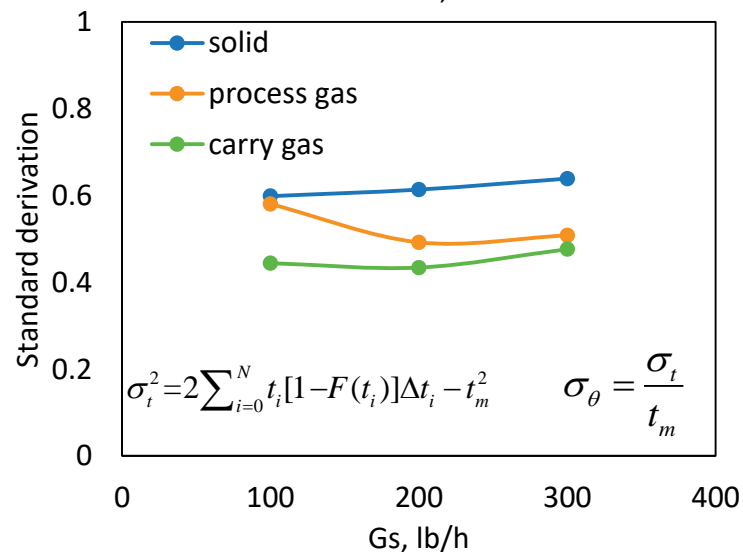
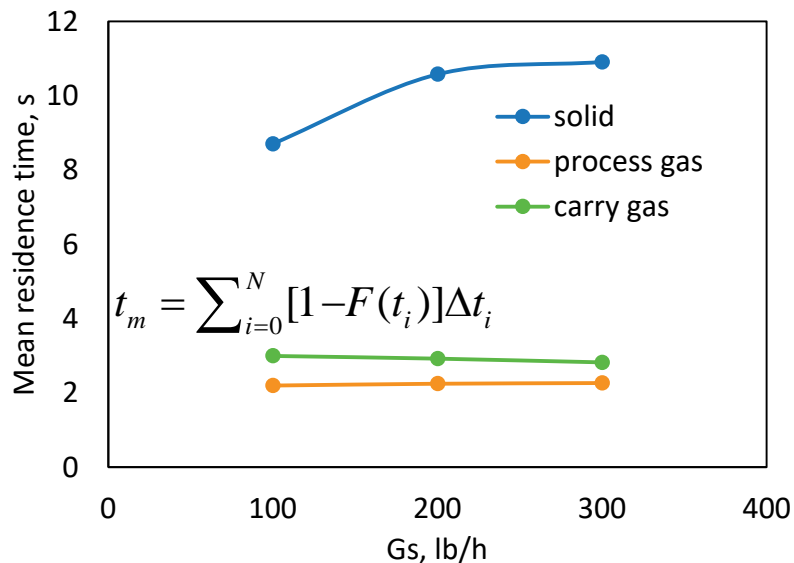
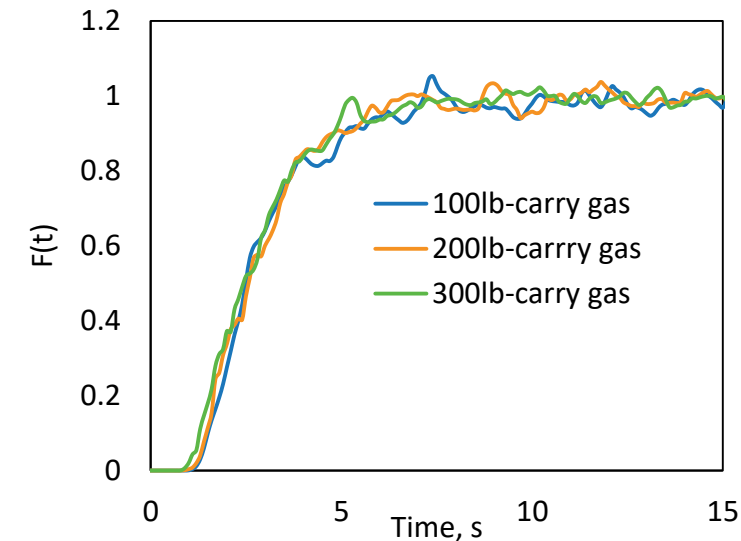
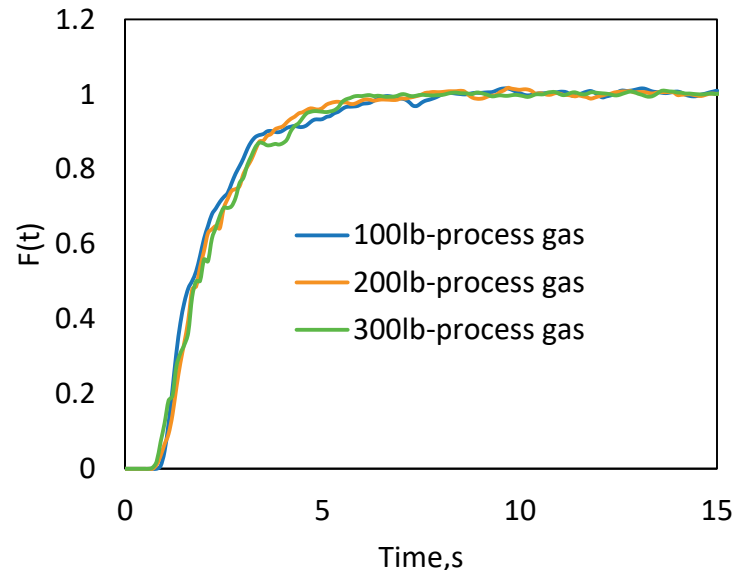
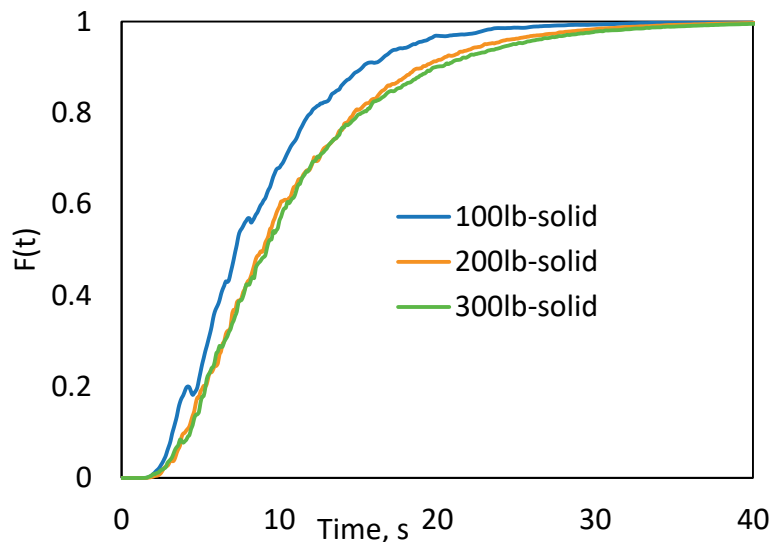
Outlet configuration



Tracer injection for non-reacting flow RTD

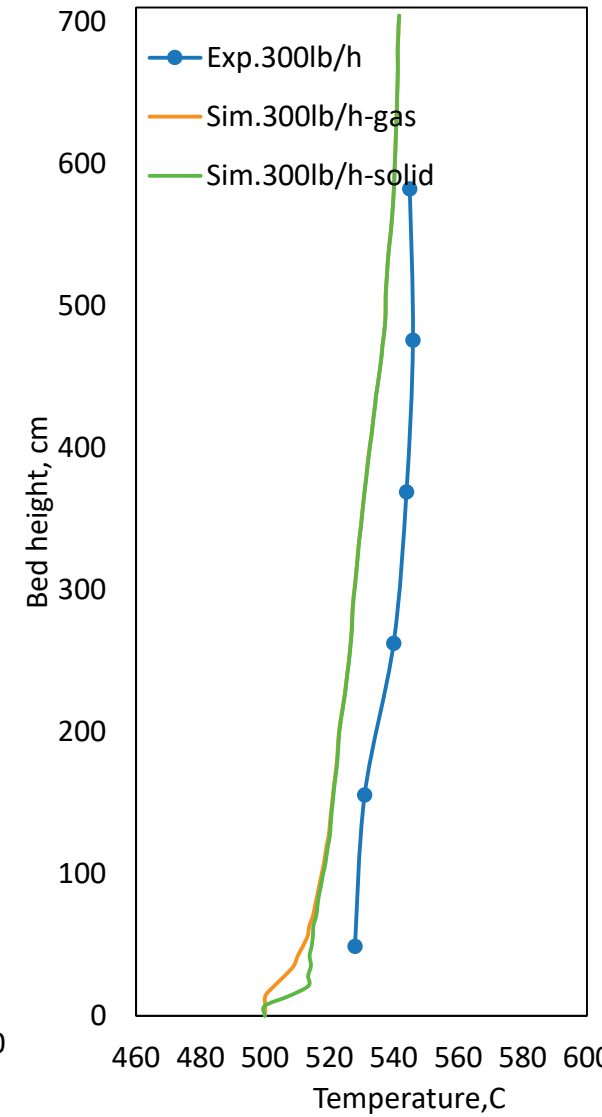
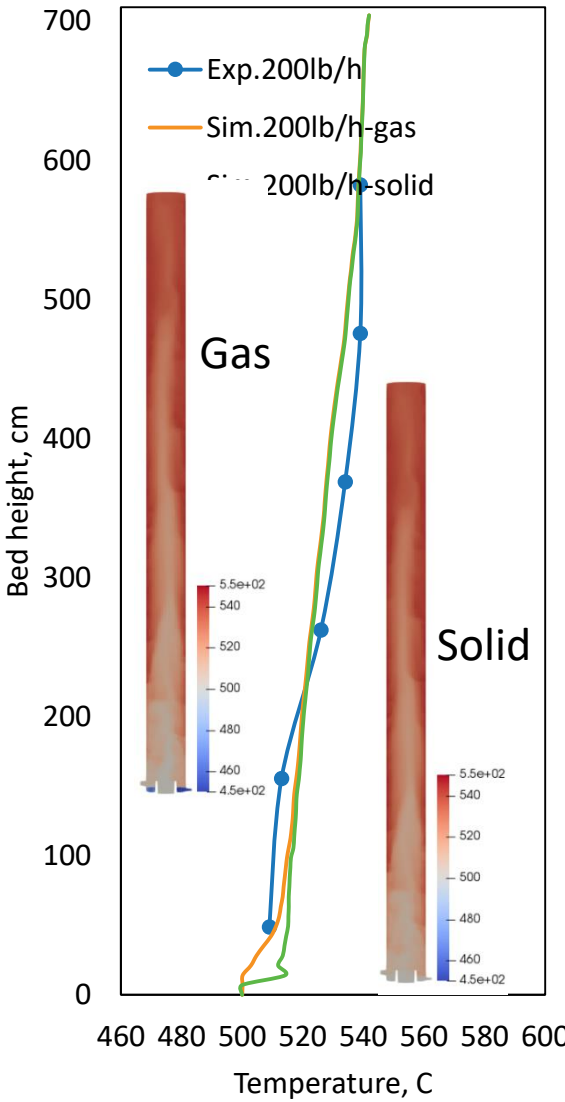
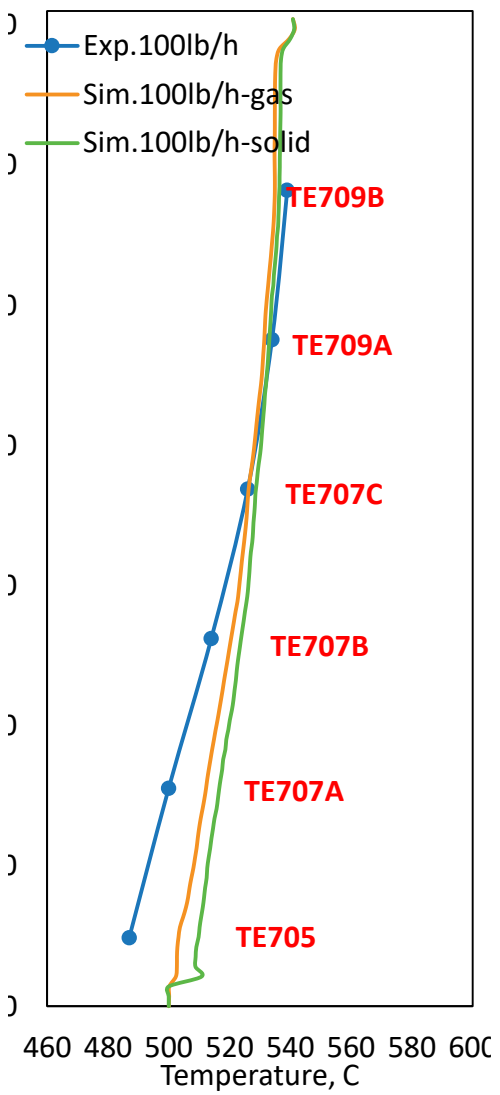
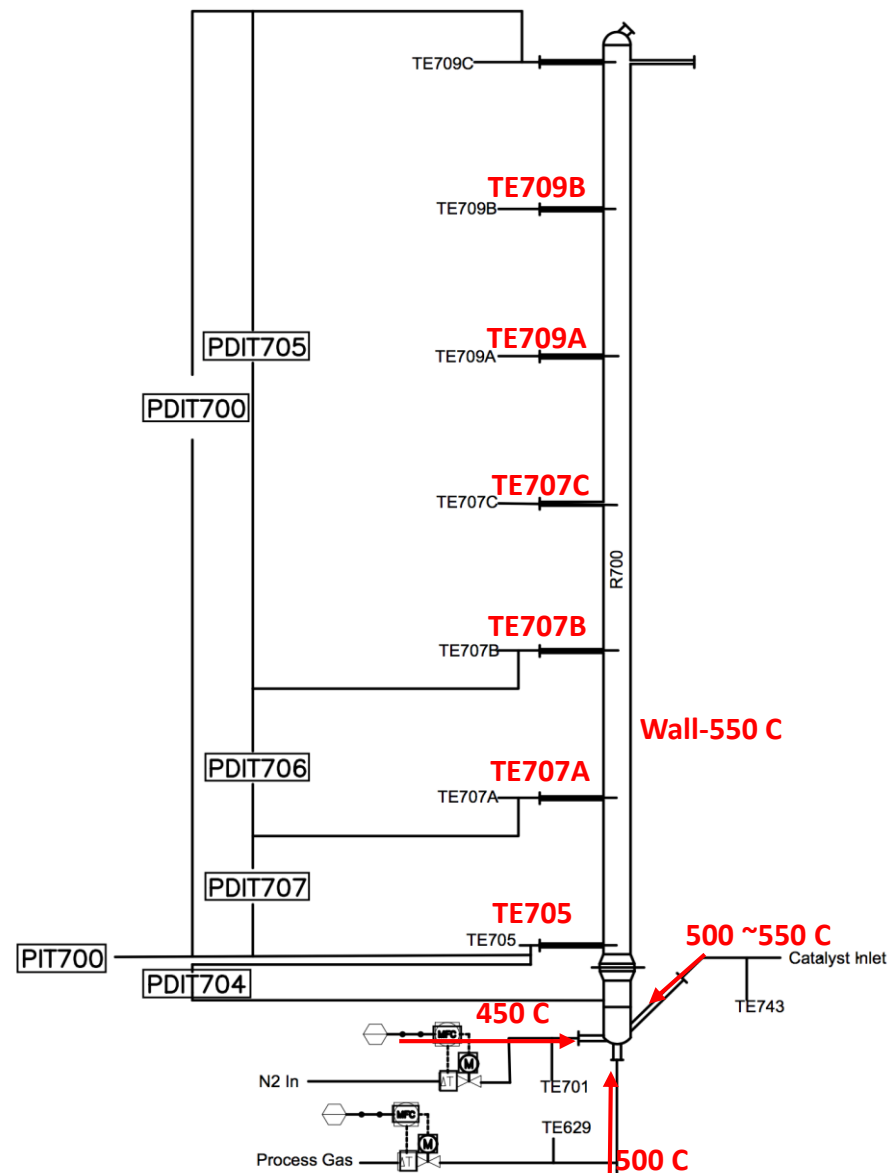
- Continuous tracer injections start at 65s of elapsed time into the simulation
- Gas tracers are given the same properties as process gas and carrier gas
- The solid tracer is given the same properties as the catalyst
- A volume fraction of 5% was used for each tracer
- The tracer outlet concentration is monitored at the top exit

Residence Time Distribution Simulation in the R-cubed Riser



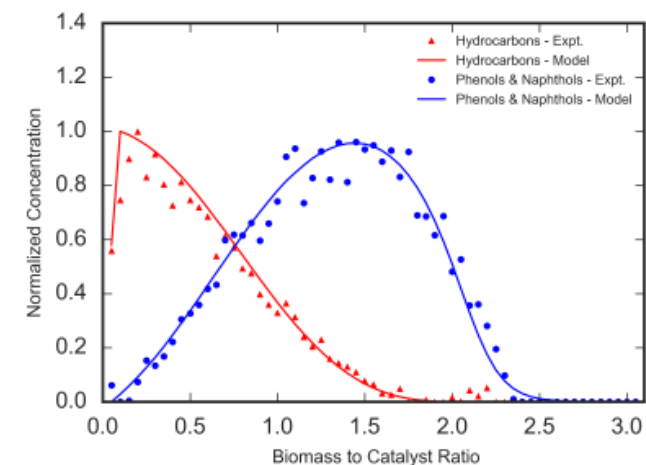
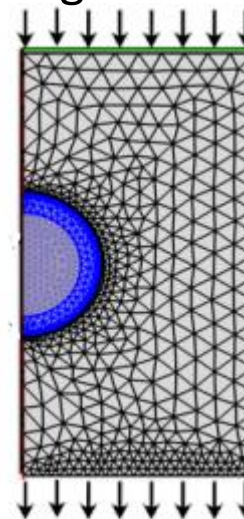
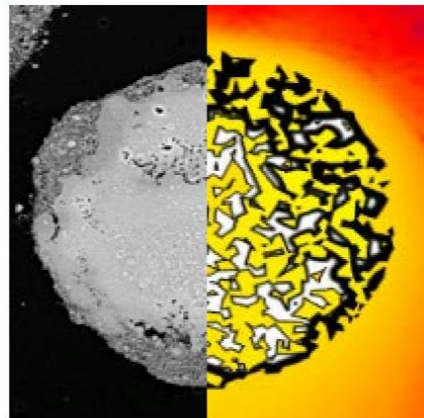
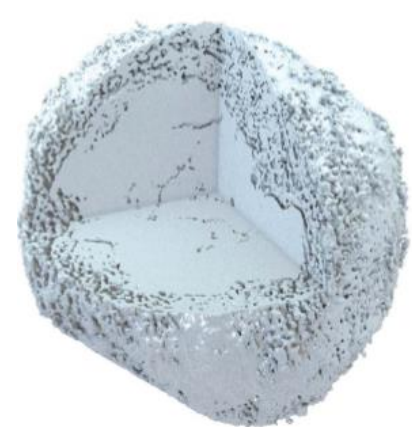
- Mean residence time of solid slightly increase with the solid circulation rate.
- Mean residence time of gas keep almost unchanged.
- Normalized variance of solid slightly increase with the solid circulation rate.

Heat Transfer Simulation in the R-cubed Riser

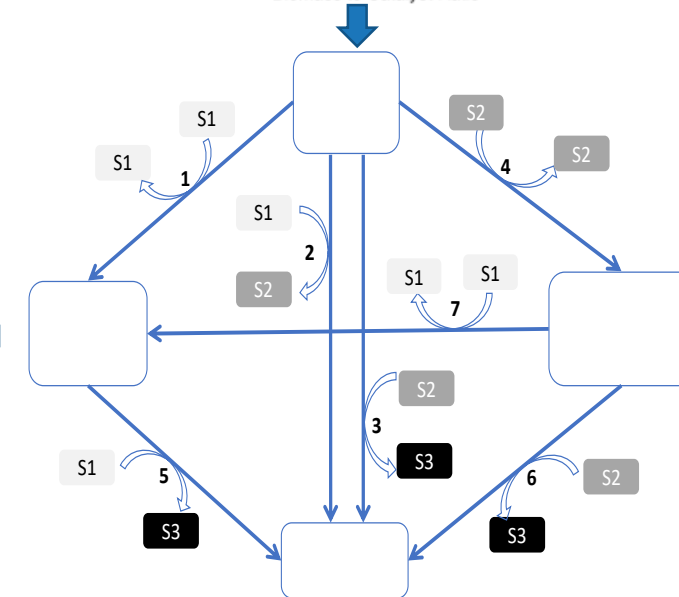
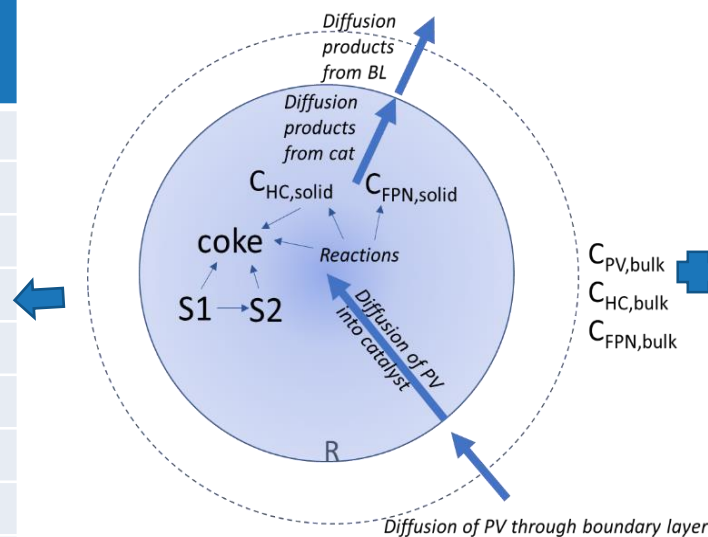


NREL VPU Kinetic Model

- Kinetics from NREL experiments and mesoscale modeling*



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



S1- Fresh Active Sites S2- Intermediate Sites S3- Deactivated Sites

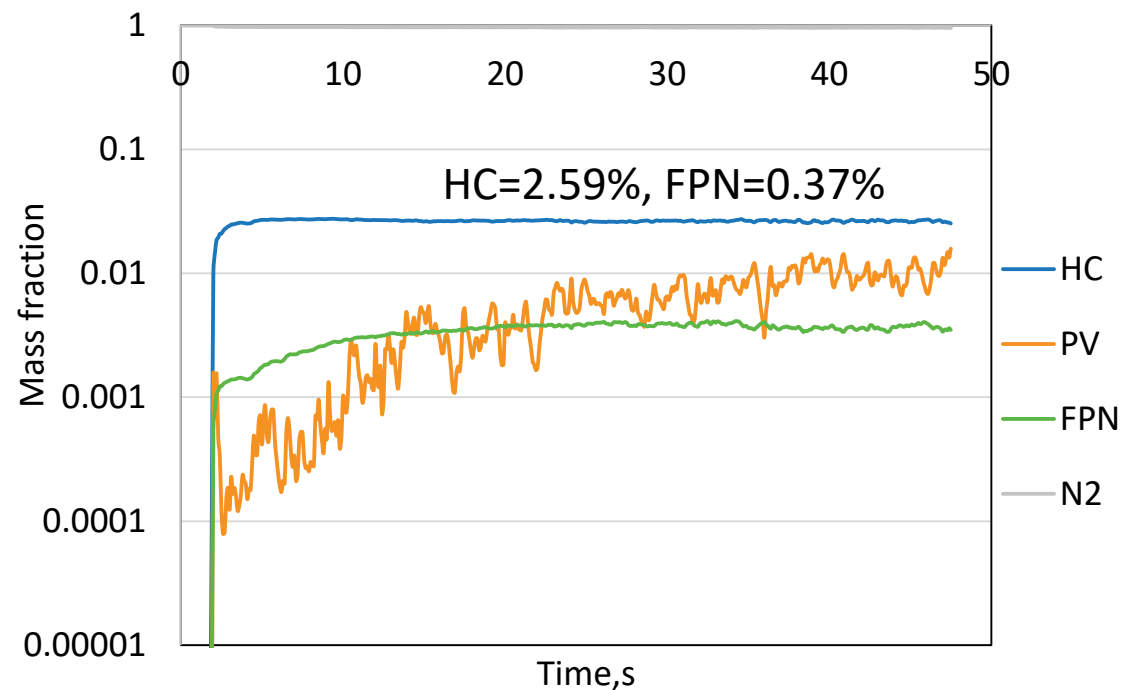
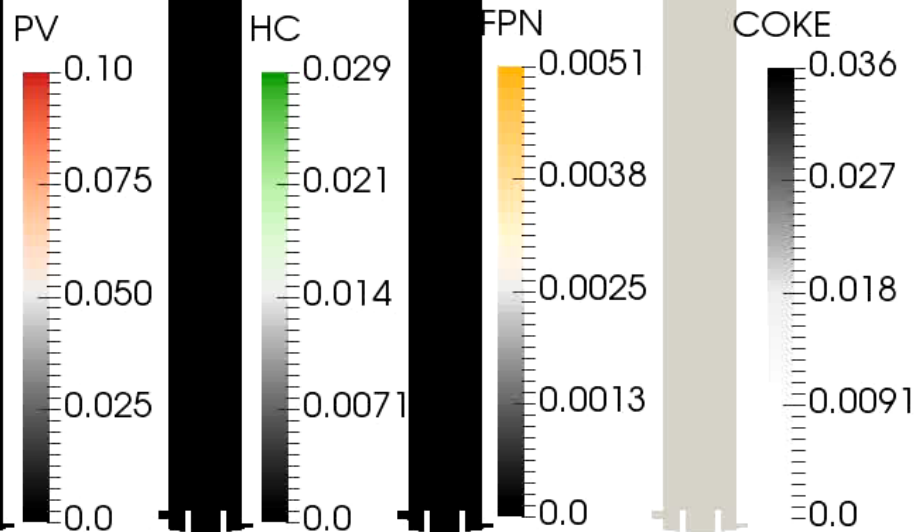
Intra and outer particle diffusion

*NREL 2017 Q4 report.

Reaction Simulation in the R-cubed Riser

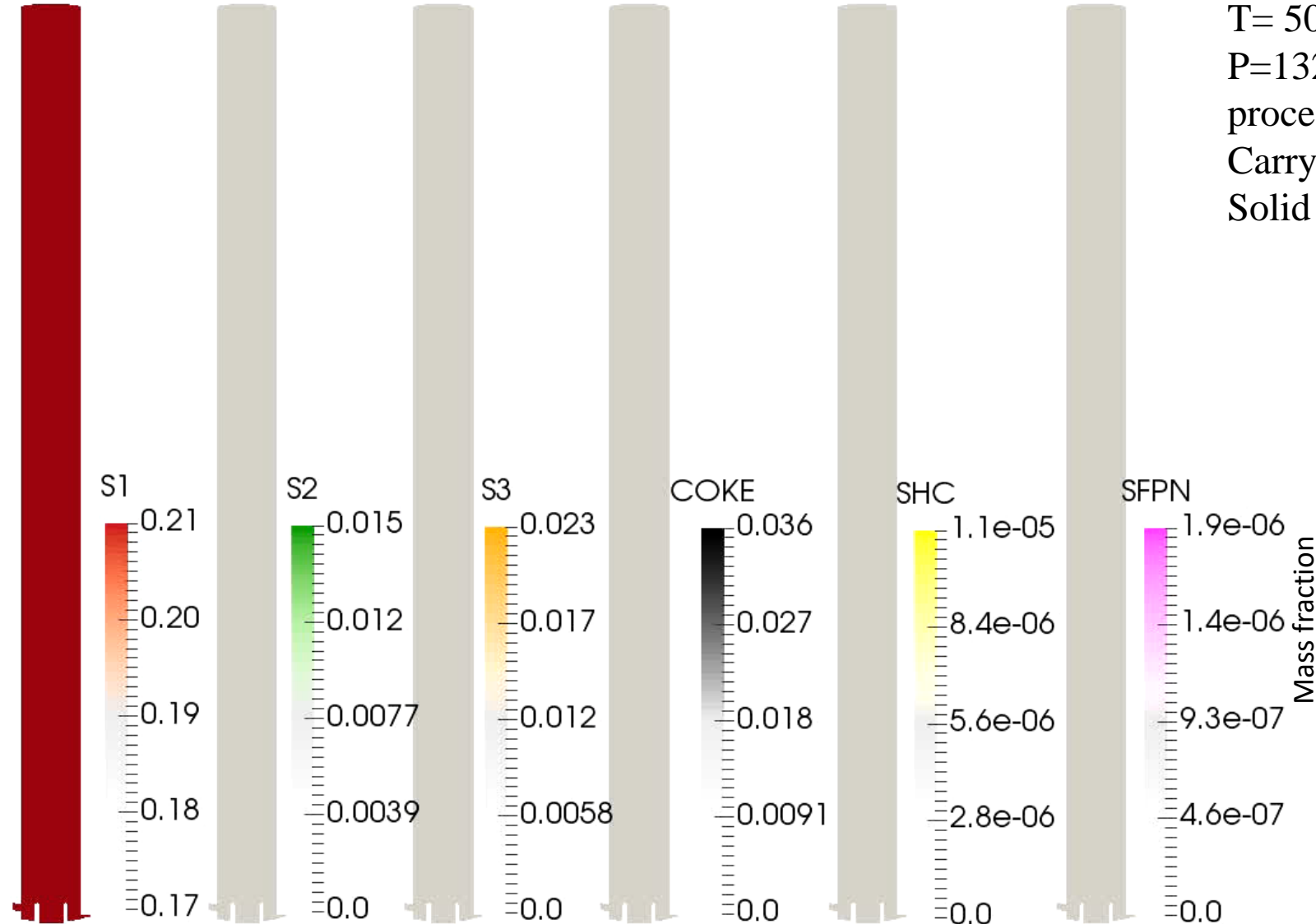
Time: 0.0 s

- 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

Time: 0.0 s



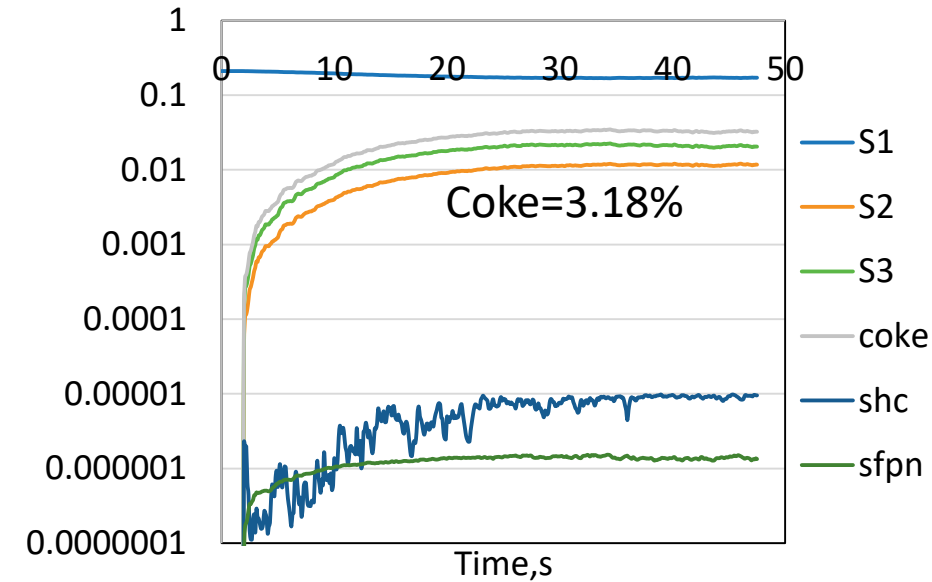
T= 500 degree C

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

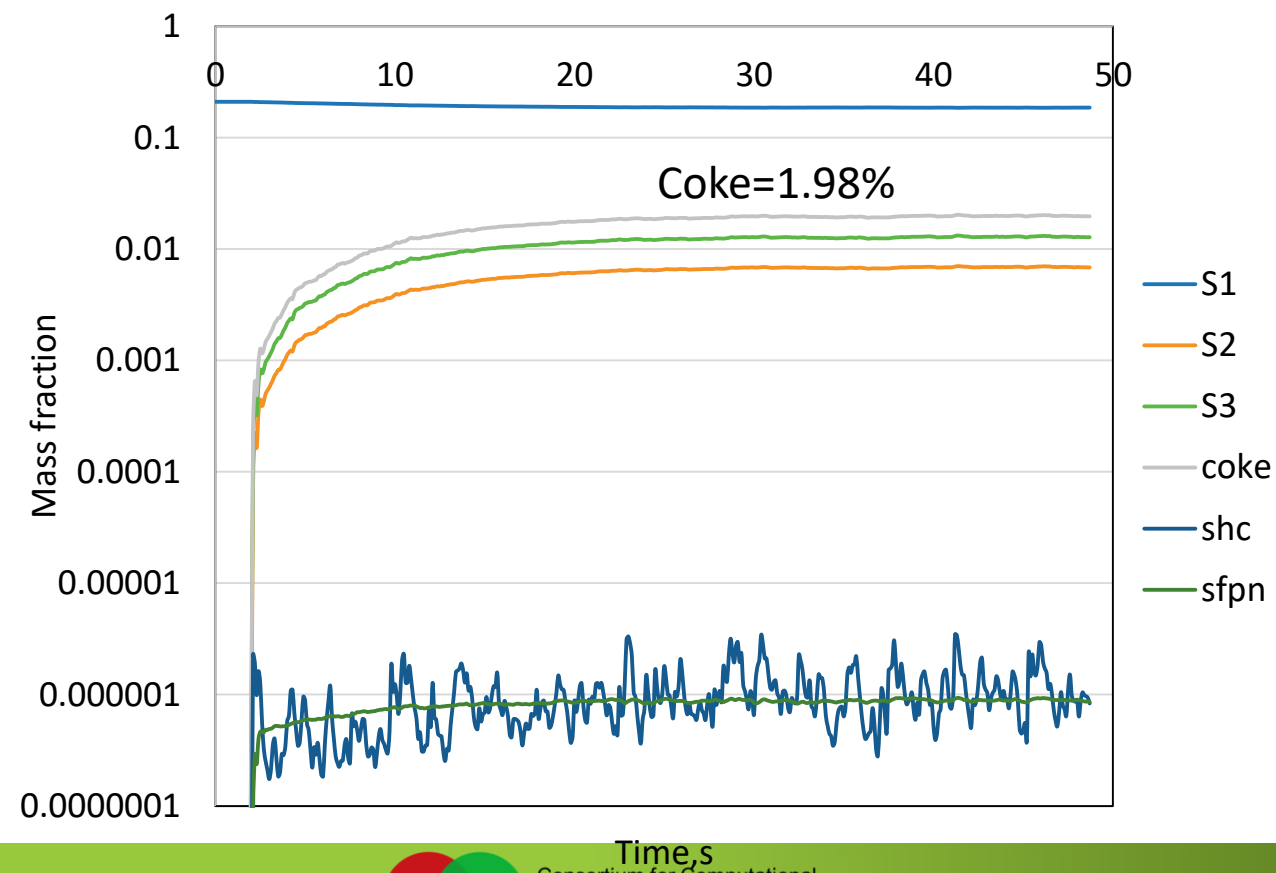
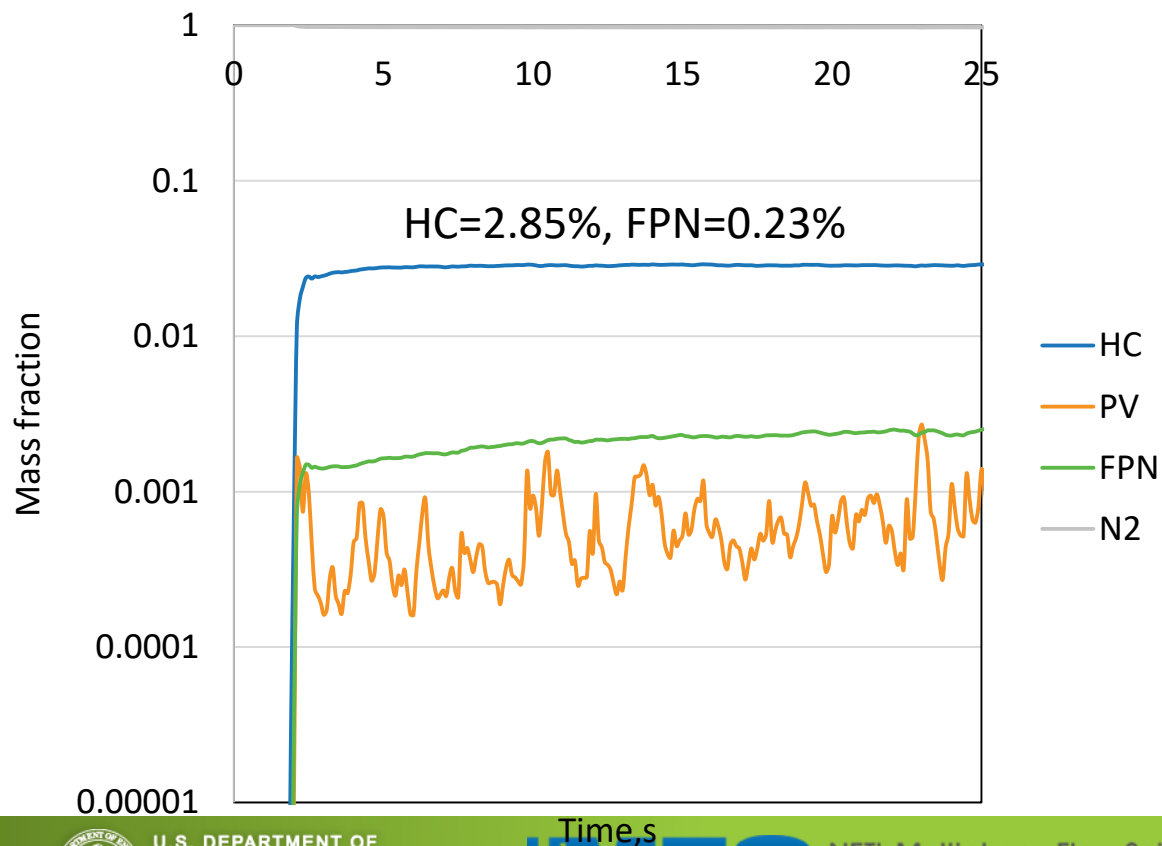
T= 500 degree C

P=132 kPa

process gas: 400SLM, 10% biomass vapor, 90% N2

Carry gas: 130 SLM, N2

Solid circulation rate=200lb/hr



Reaction Simulation in the R-cubed Riser

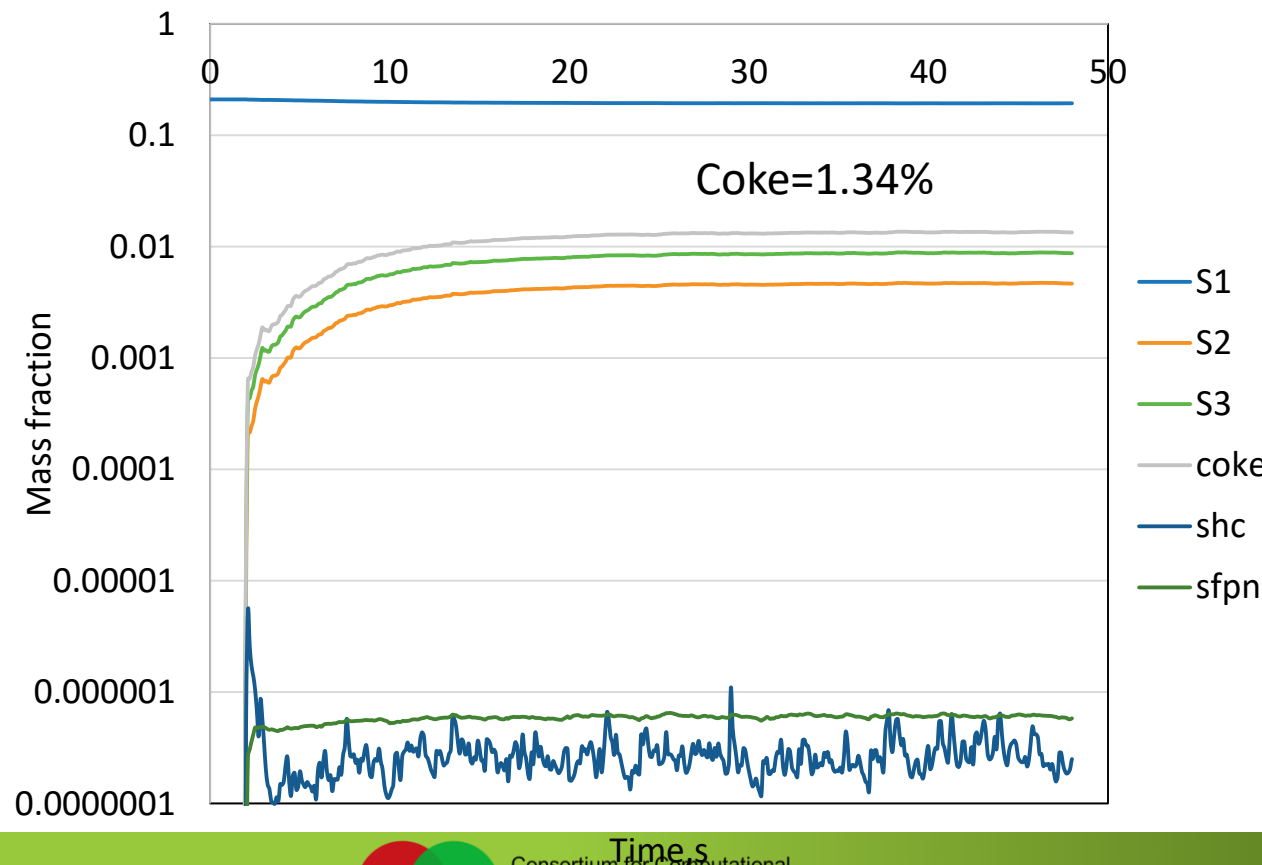
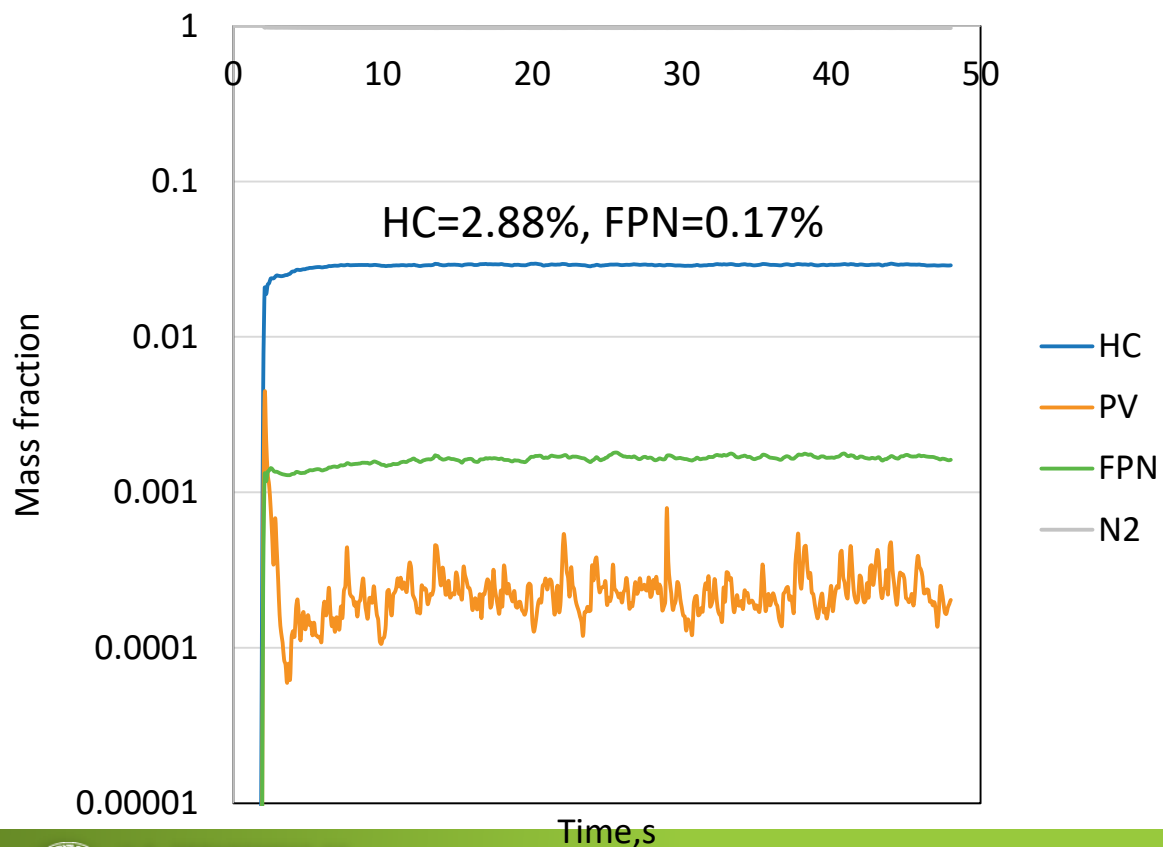
T= 500 degree C

P=132 kPa

process gas: 400SLM, 10% biomass vapor, 90% N2

Carry gas: 130 SLM, N2

Solid circulation rate=300lb/hr



- MFiX simulations were performed to study flow hydrodynamics in the VPU riser and results were compared with the NREL non-reacting flow experimental data.
- Validated hydrodynamics model was applied to study the gas/solid RTDs under different operating conditions.
- MFiX simulations were performed for study heat transfer in the VPU riser and results were compared with the NREL non-reacting flow experimental data.
- 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



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.



Jim Parks
Gavin Wiggins
Stuart Daw
Emilio Ramirez
Charles Finney



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



Roger Rousseau
Vanda Glezakou
Sneha Akhade
Simuck Yuk
Asanga Padmaperuma



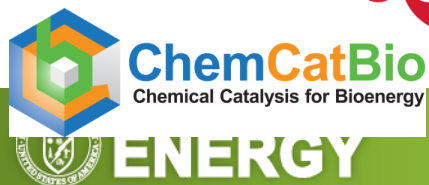
Xi Gao
Tingwen Li
William Rogers
Madhava Syamlal
Rupen Panday
Cheng Li
Huda Ashfaq
Bryan Hughes



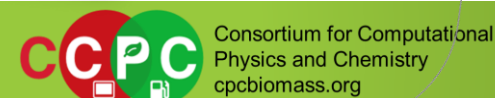
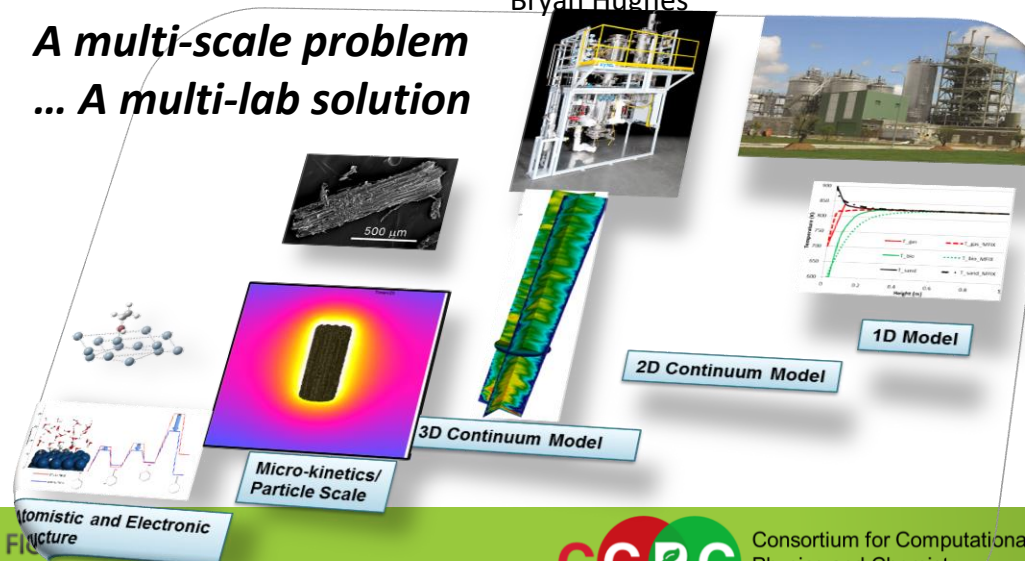
Larry Curtiss
Rajeev Assary
Lei Cheng
Cong Liu
Dale Pahlis

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)



**A multi-scale problem
... A multi-lab solution**



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.