Application of an Efficient Discrete Particle Model to Simulate an Industrial FCC Regenerator

Liqiang Lu & Sofiane Benyahia
NETL

2017 NETL Workshop on Multiphase Flow Science

Aug 8, 2017, Morgantown, W.V.

Solutions for Today | Options for Tomorrow

Outline

1. General Introduction of Discrete Particle Models
2. Coarse Grained Hard Sphere (CGHS)
3. Verification and Validation of CGHS
4. Simulation of an industrial FCC regenerator using CGHS
5. Concluding remarks

Discrete Particle Models: From Atoms to Planets

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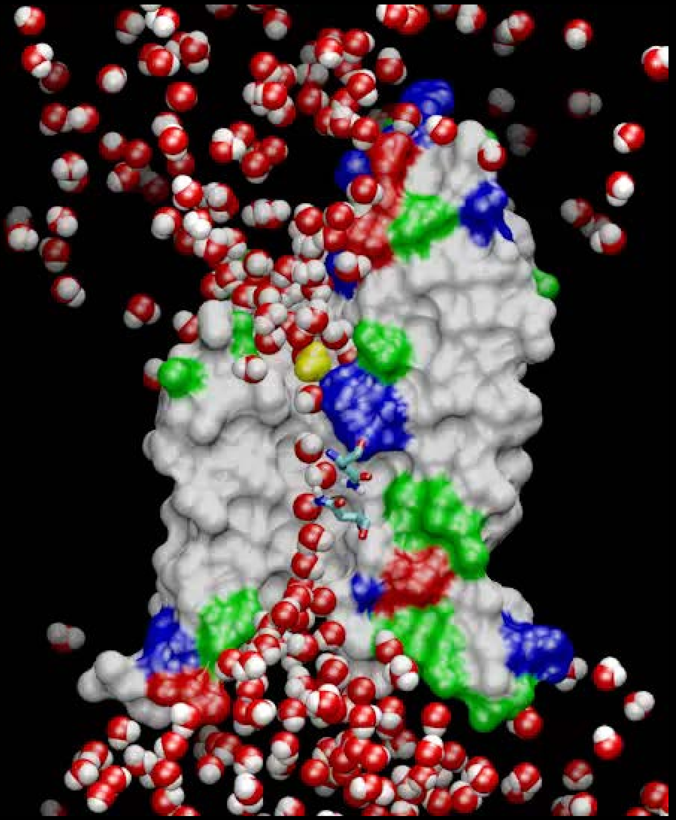
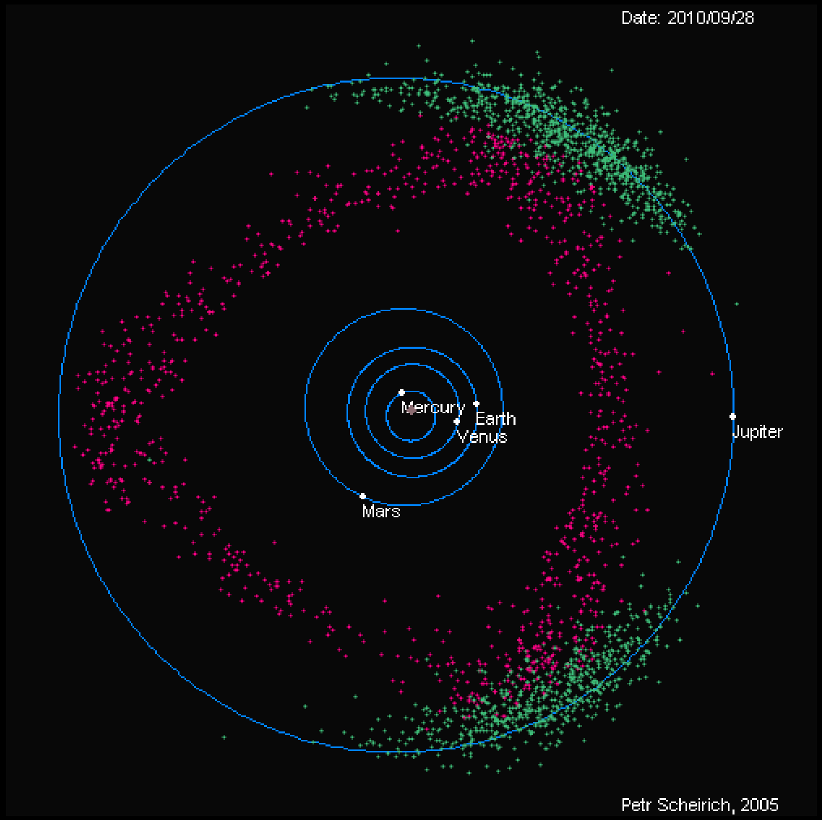
Water Molecular in Cell Membrane



http://www.ks.uiuc.edu/Gallery/Movies/ChannelProteins/

Asteroids in Solar System



http://sajri.astronomy.cz/asteroidgroups/groups.htm

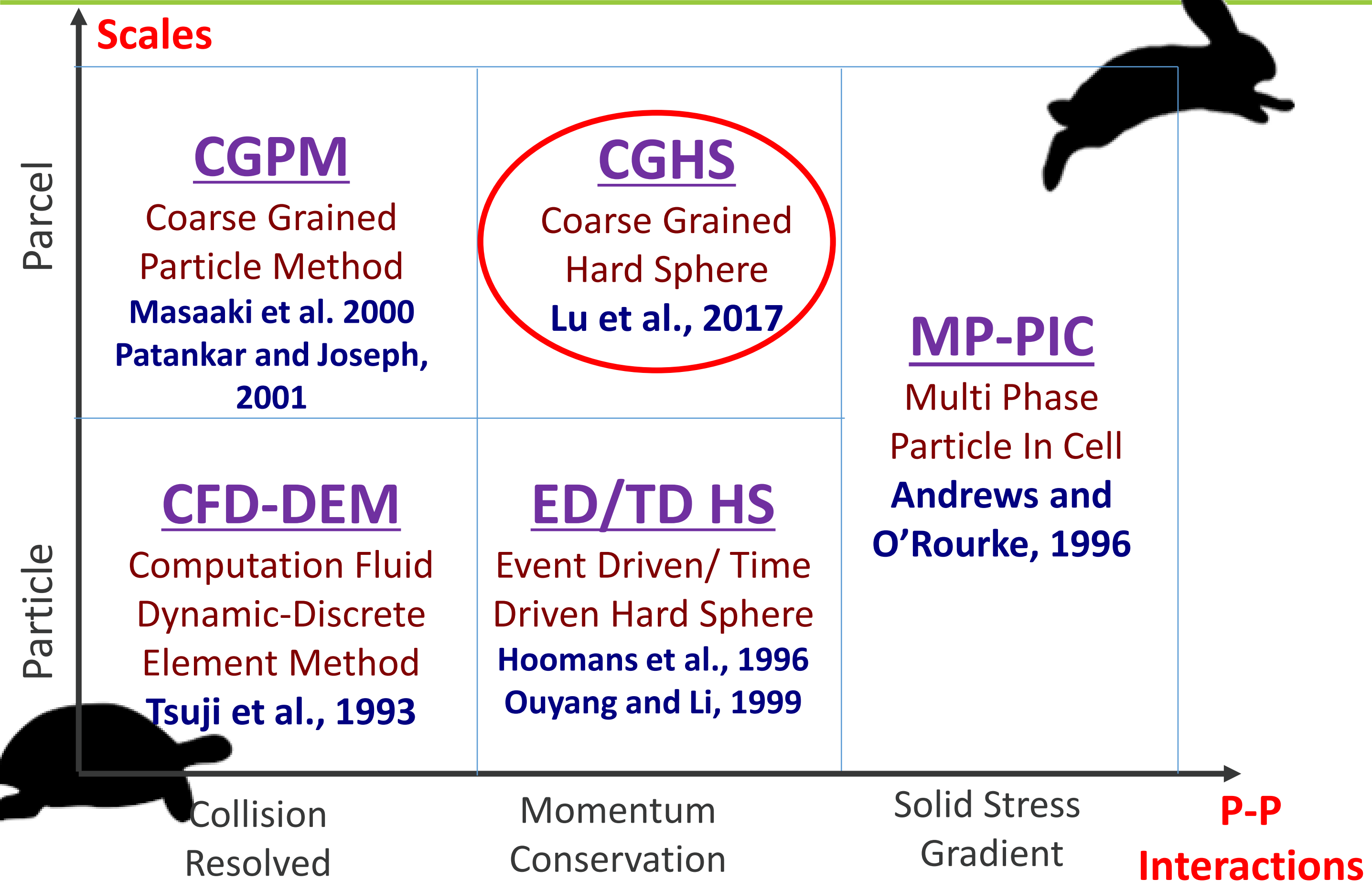
$d\mathbf{x}/dt = \mathbf{v}$; $d\mathbf{v}/dt = \mathbf{F}/m$

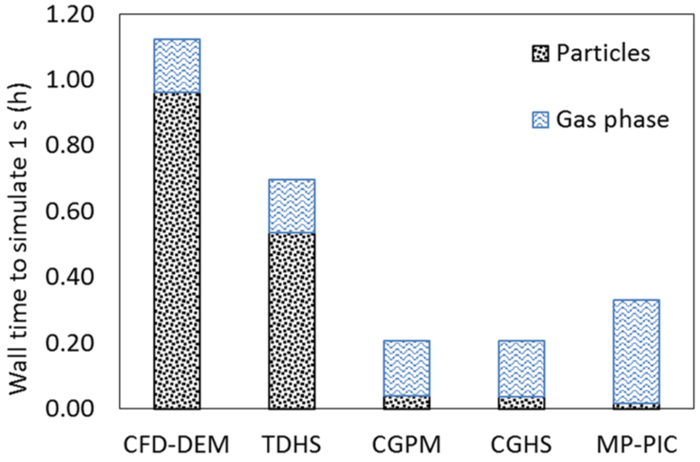
Based on the SCALES of PARTICLES and their INTERACTIONS

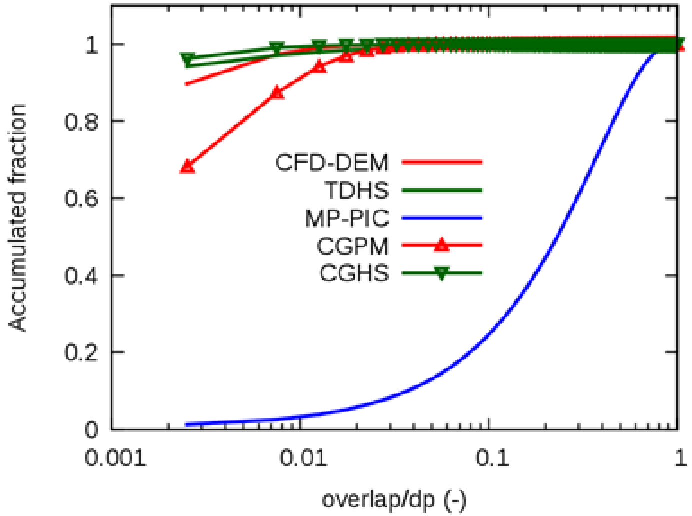
- Molecular Dynamic
- Dissipative Particle Dynamic
- Pseudo-Particle Method
- Hard-Sphere Method
- Discrete Element Method
- Coarse Grained Hard Sphere
- Coarse Grained DEM
- Particle In Cell
- Smooth Particle Hydrodynamics

There is nothing cannot be simulated with DPM. If there is one, just make the particle smaller or larger.

Discrete Particle Models: widely used DPMs in gas-solids flow







Lu, L.; Gopalan, B.; Benyahia, S., 2017. Assessment of different discrete particle methods ability to predict gas-particle flow in a small-scale fluidized bed. Industrial & Engineering Chemistry Research, *56*, 7865–7876

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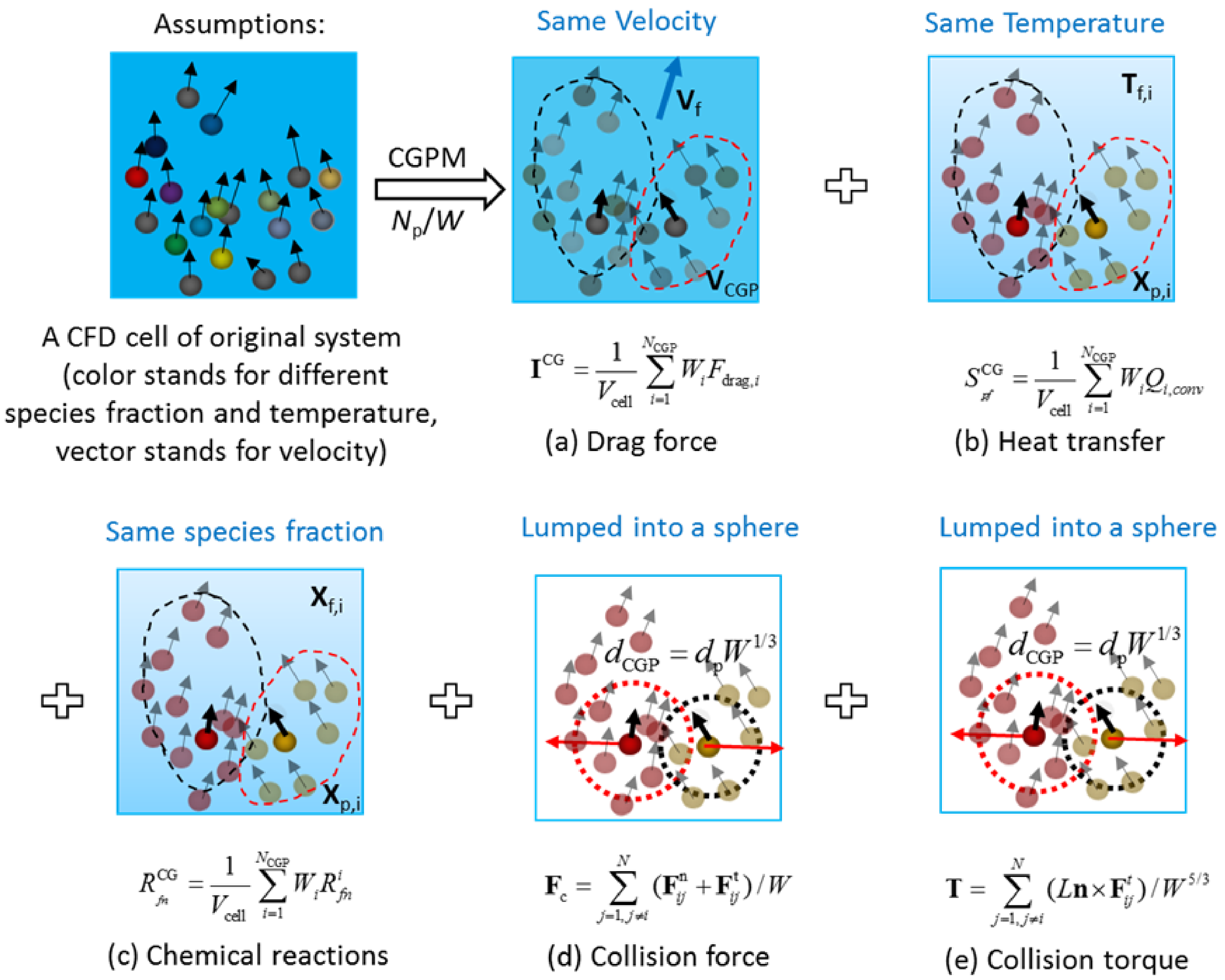
CGHS: Basic Assumptions and different models in CG



	Spring	Dashpot	Friction
M1	$k_{CGP} = k_p$	$e_{CGP} = e_p$	$\mu_{CGP} = \mu_p$
M2	$k_{CGP} = Wk_p$	$e_{CGP} = e_p$	$\mu_{CGP} = \mu_p$
M3	$k_{CGP} = Wk_p$	$\ln e_{CGP} = W^{1/2} \ln e_p$	$\mu_{CGP} = \mu_p$
M4	$k_{CGP} = W^{1/3} k_p$	$e_{CGP} = e_p$	$\mu_{CGP} = \mu_p$
M5	$k_{CGP} = k_p$	$e_{CGP} = (1-(e_p^2-1) W^{1/3})^{1/2}$	$\mu_{CGP} = \mu_p$

M1	Sakano et al.,2000, Jan.J.Multi.Fow.; Patankar and Joseph, 2001, Int. J. Multi. Flow
M2	Sakai et al. 2009, CES
M3	Benyahia and Galvin, 2010, I&ECR
M4	Radl et al. 2011, 8th Conf. CFD in Oil &Gas; Thakur et al., 2016 Pow.Tec.
M5	Lu et al. 2014, CES

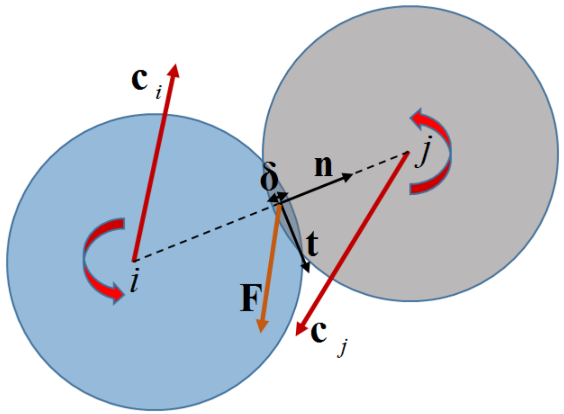
CGHS: From DEM to HS

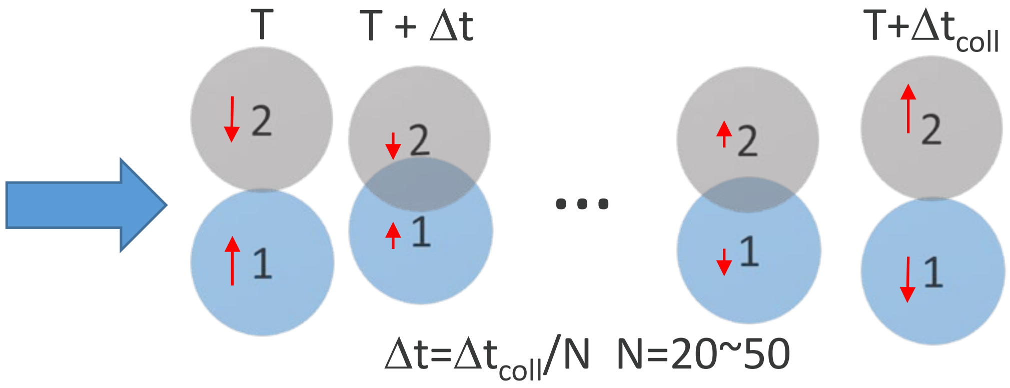
- Soft-sphere

$$m\frac{d\mathbf{c}_i}{dt}=\mathbf{F}$$

$$I\frac{d\boldsymbol{\omega}_i}{dt}=\frac{d}{2}(\mathbf{n}\times\mathbf{F})$$

F: *contact force*



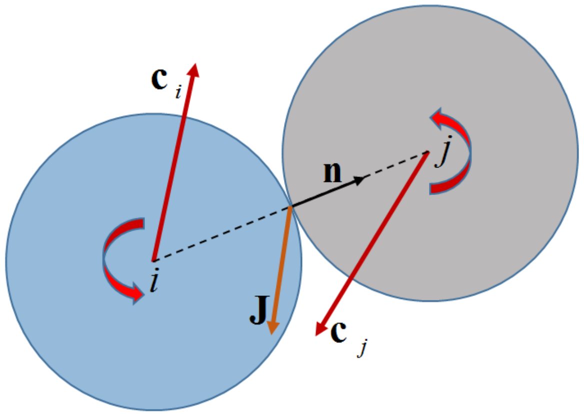


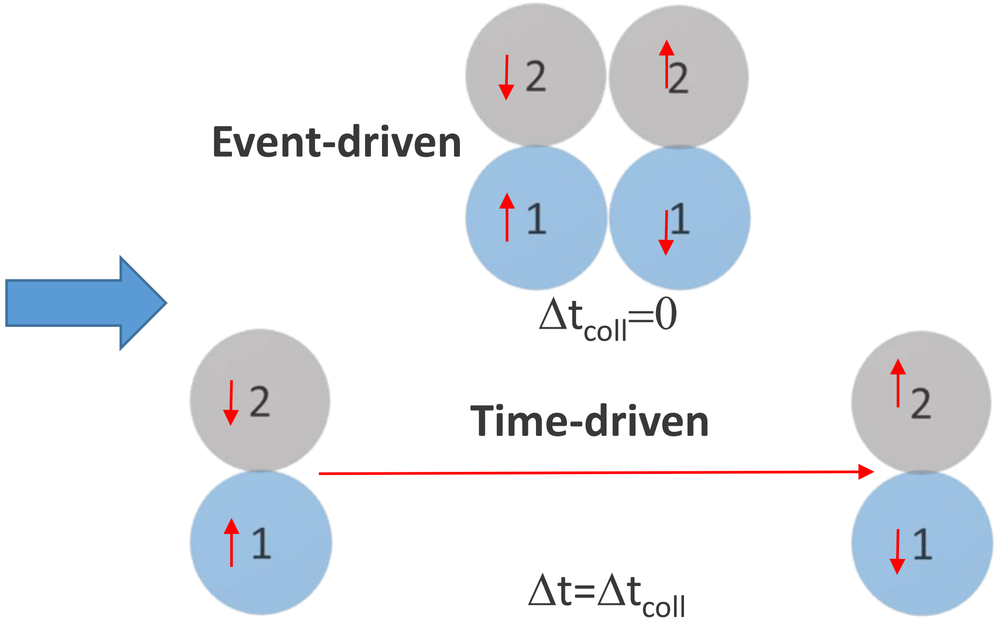
- Hard-sphere

$$m(\mathbf{c}_i'-\mathbf{c}_i)=\mathbf{J}$$

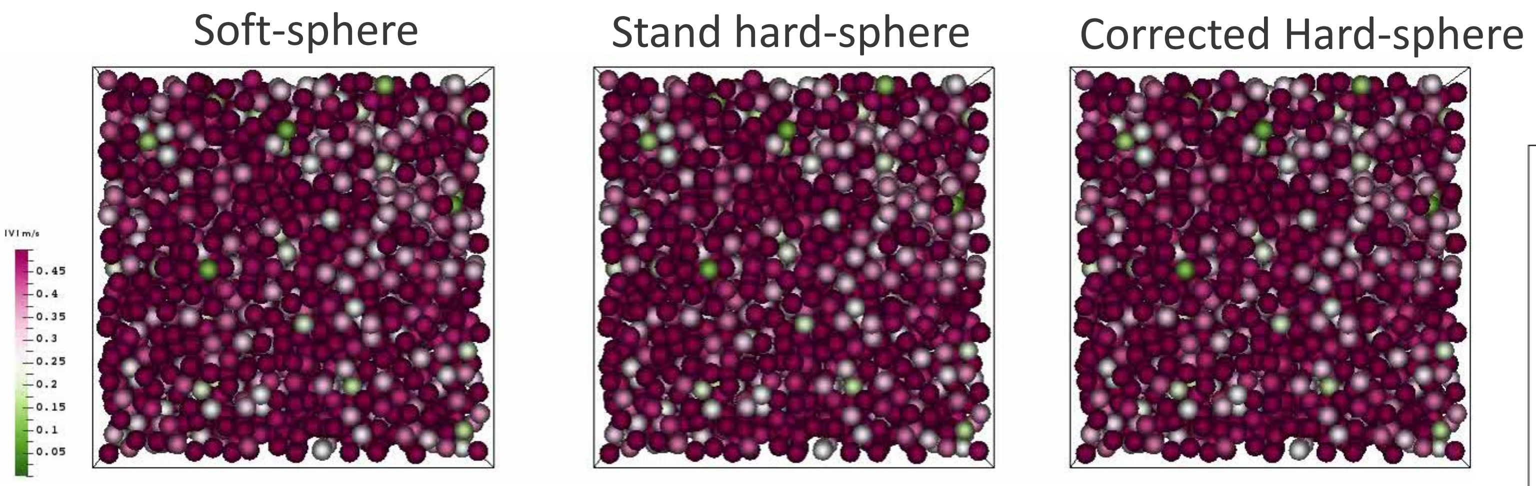
$$I(\boldsymbol{\omega}_i'-\boldsymbol{\omega}_i)=\frac{d}{2}(\mathbf{n}\times\mathbf{J})$$

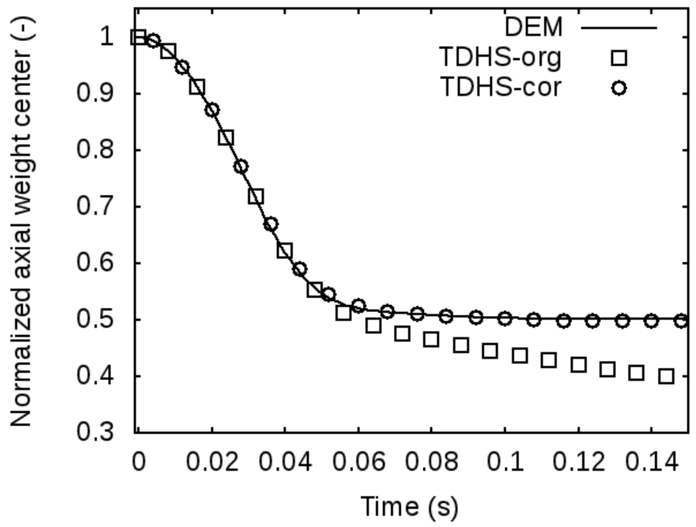
J: *impulse*

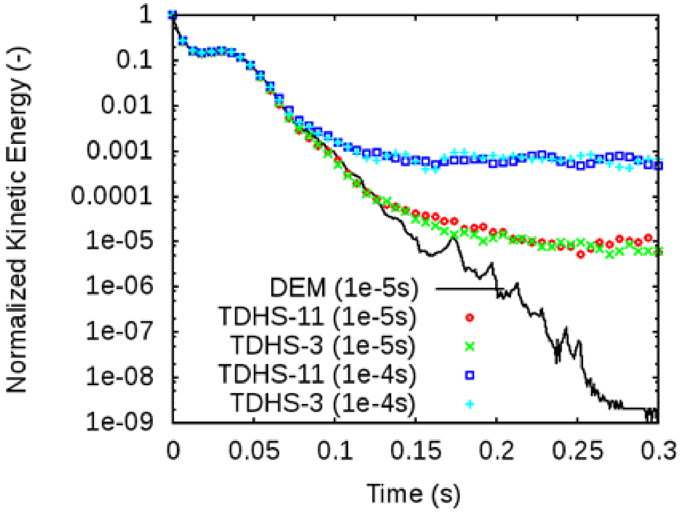


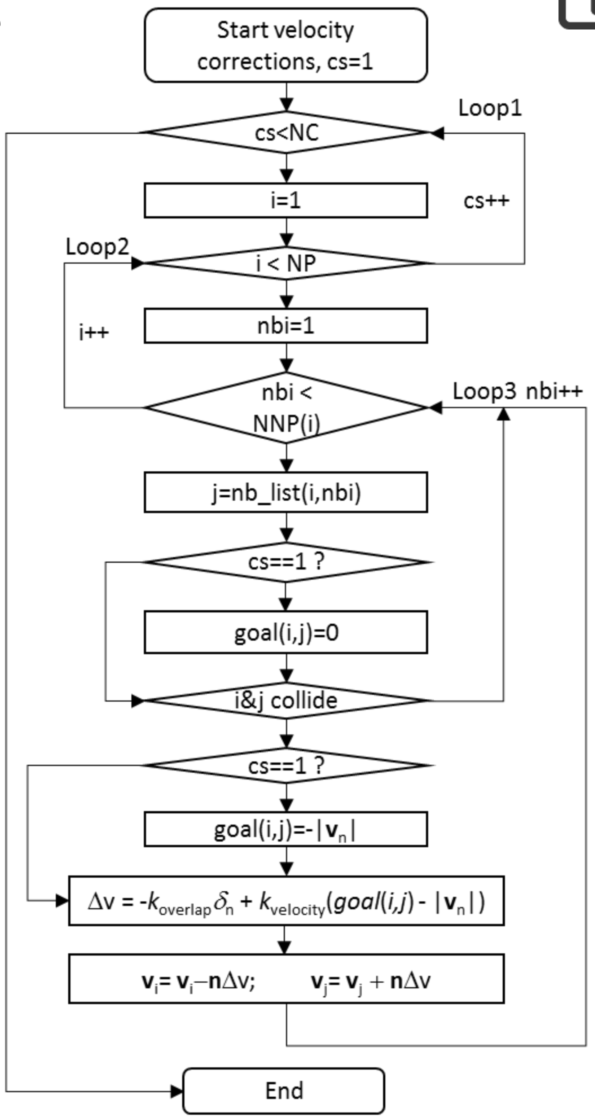


CGHS: Eliminating unphysical overlaps in HS









Lu, L.; Li, T.; Benyahia, S., 2017. An efficient and reliable predictive method for fluidized bed simulation. AIChE Journal, DOI: 10.1002/aic.15832

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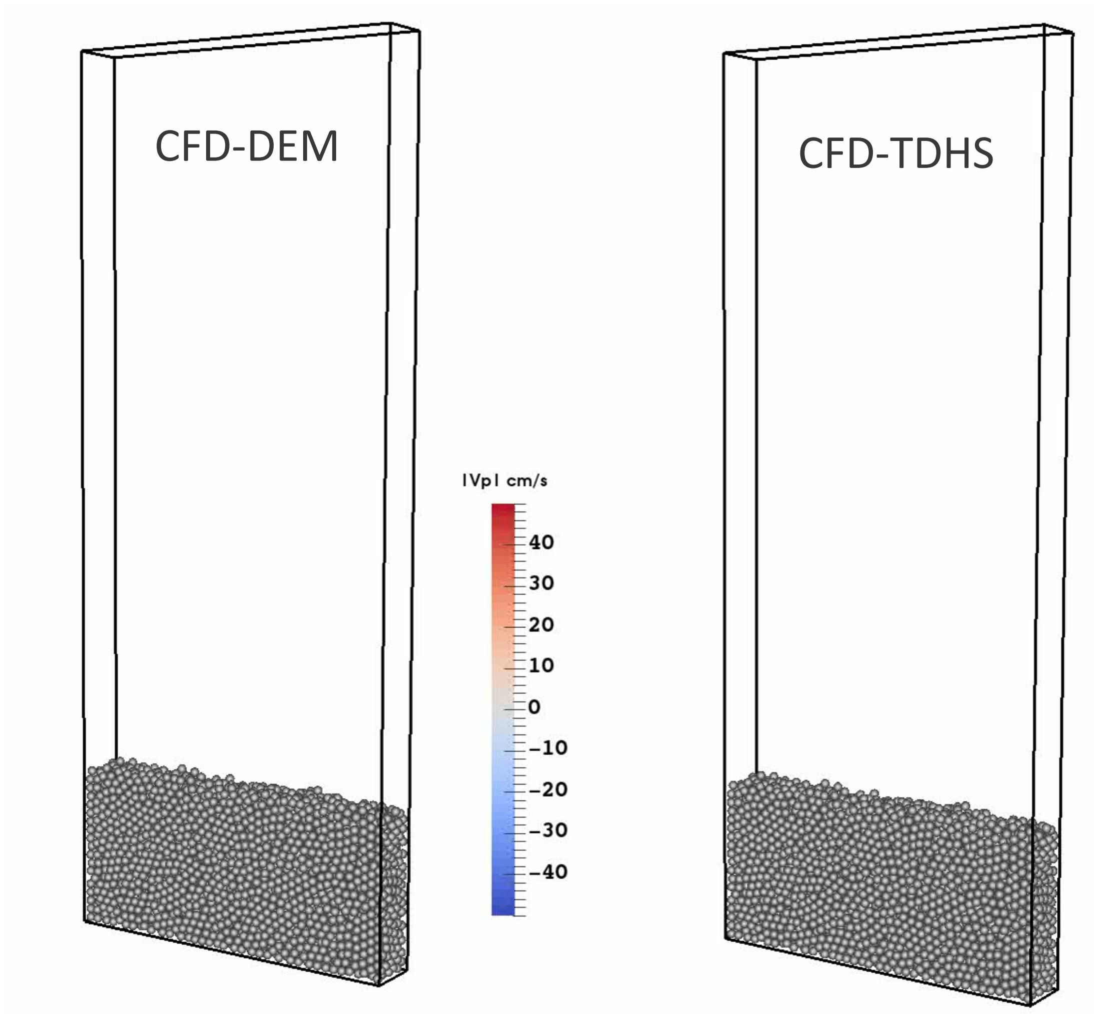
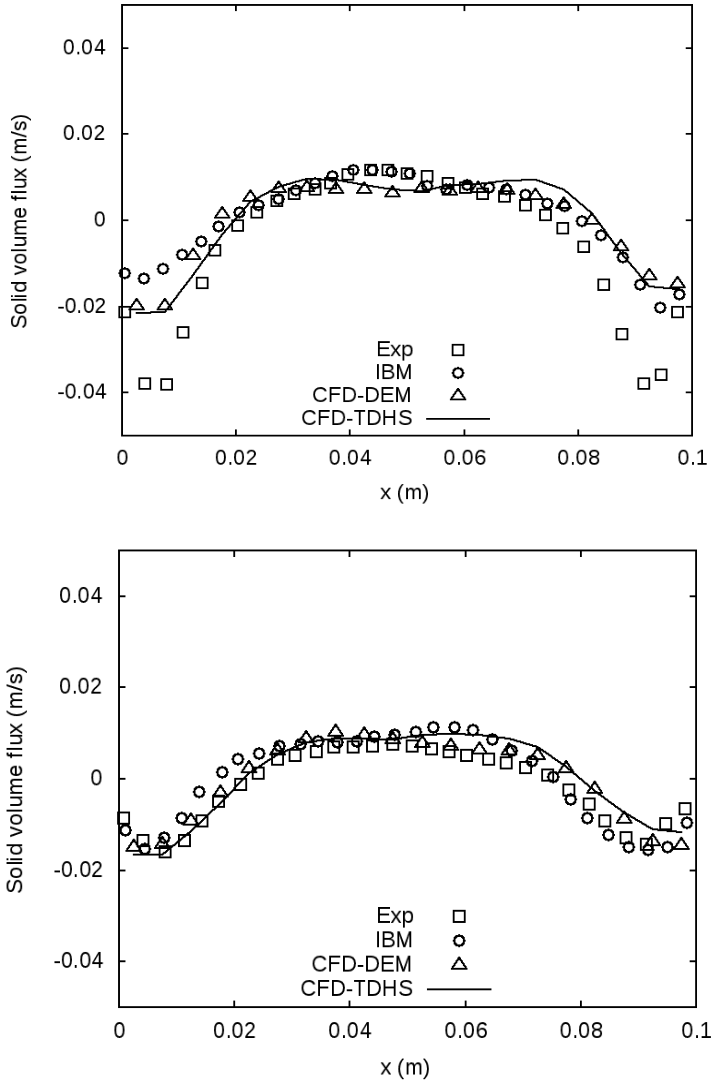
V&V: TDHS in small bubbling fluidized bed





[Lu, L.; Li, T.; Benyahia, S., 2017. An efficient and reliable predictive method for fluidized bed simulation. AIChE Journal, DOI: 10.1002/aic.15832]

V&V: Verification of CGHS in a virtual bubbling fluidized bed

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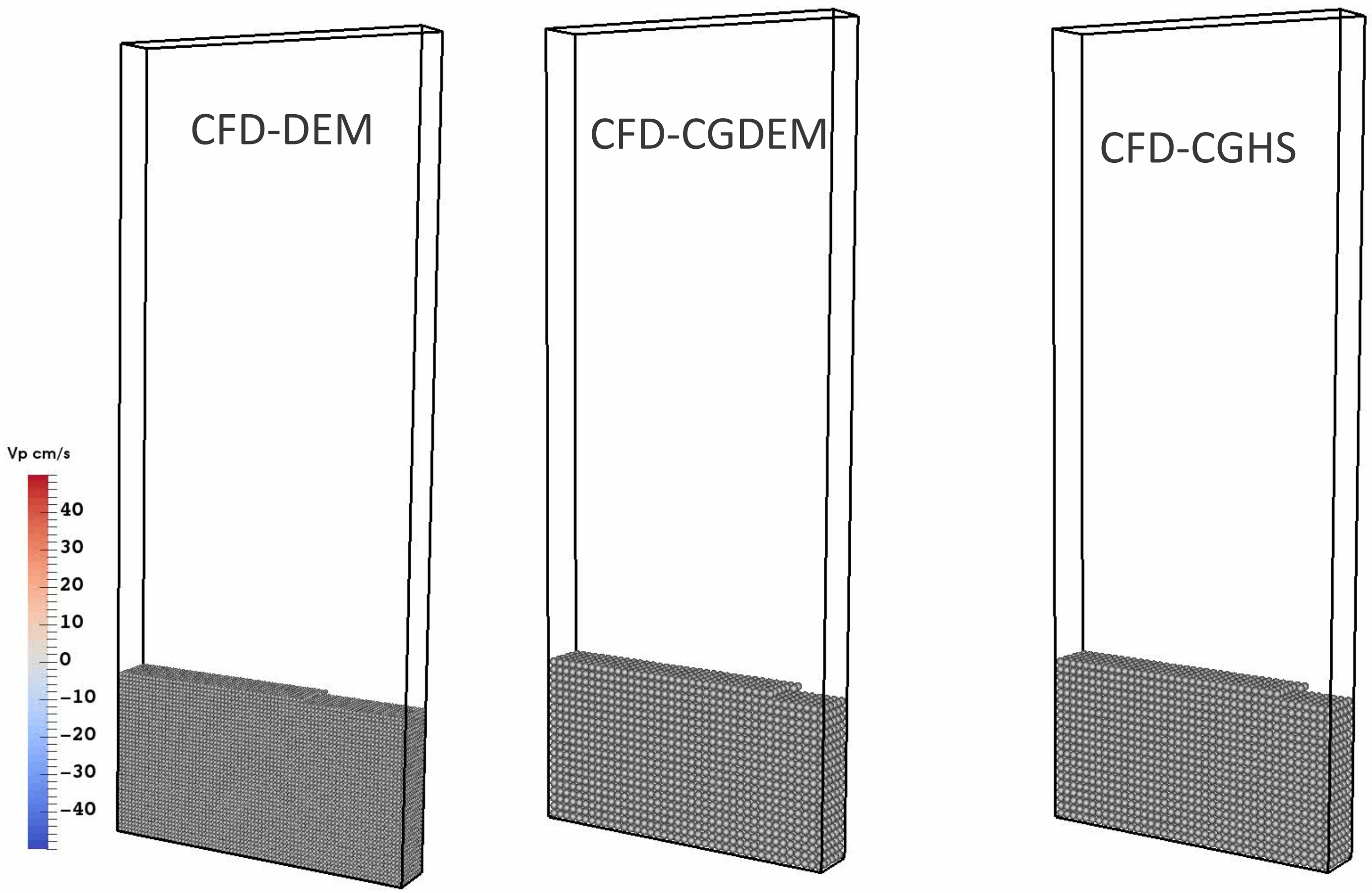
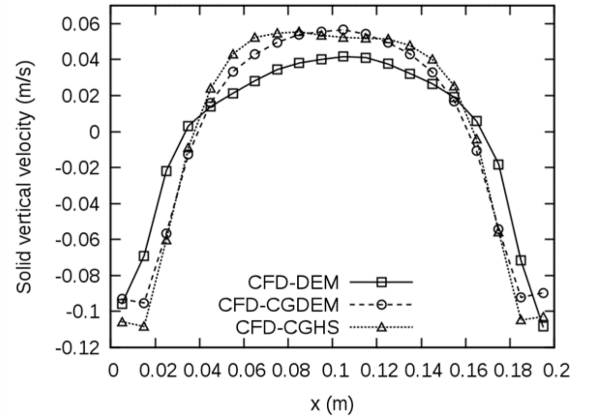
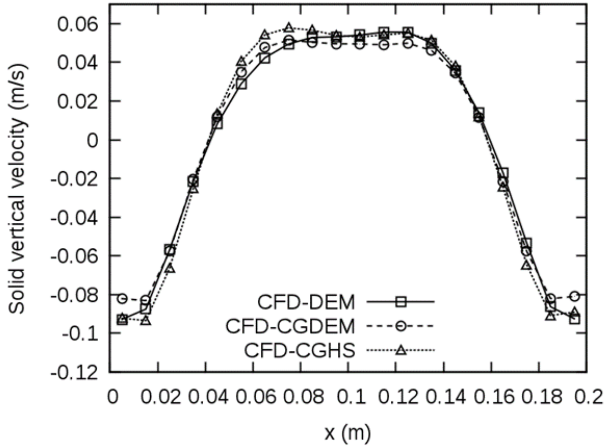


9.56 hour | 0.31 hour | 0.08 hour

CPU time for solids phase



(b) Height = 0.11 m

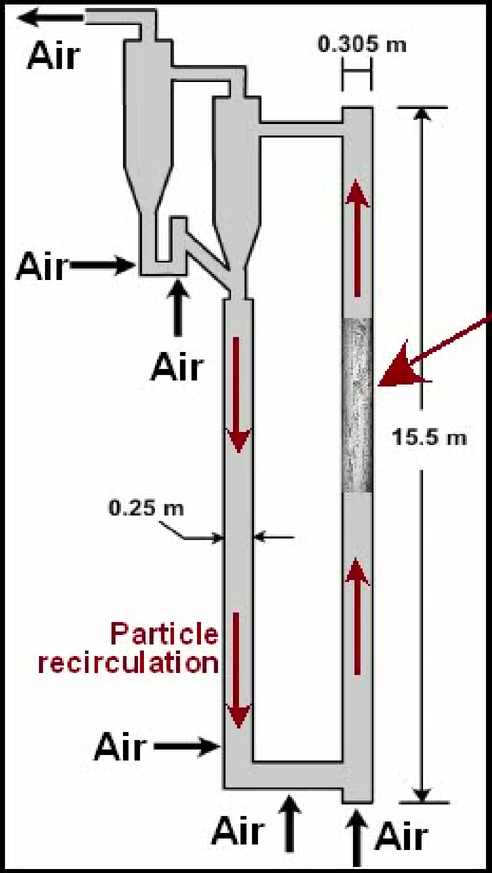


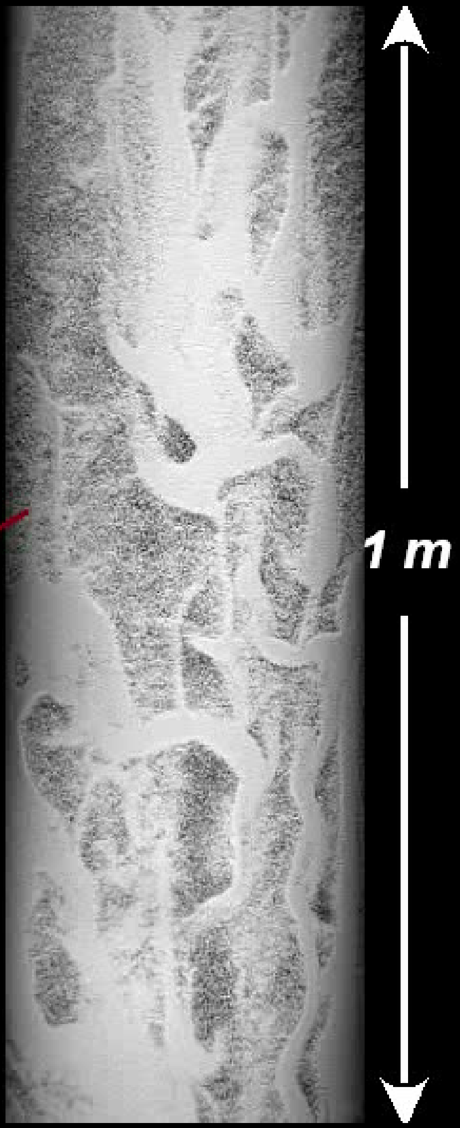
(a) Height = 0.05 m

Thousand-Fold Speedup of Discrete-Particle-Based Computer-Aided Reactor Design and Scale-up. 2017
Liqiang Lu and Sofiane Benyahia. TechConnect 2017, Washington D.C. U.S.

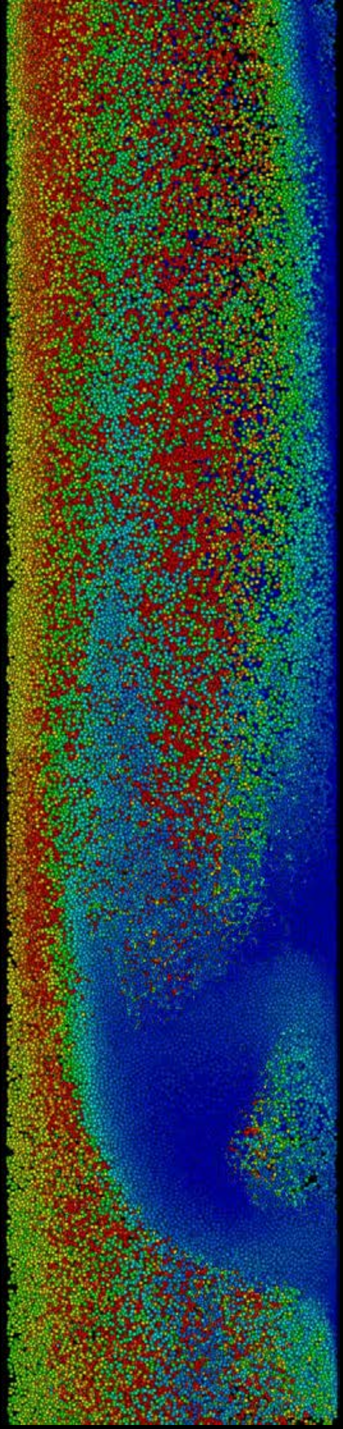
V&V of CGHS: Validation in large circulating fluidized bed

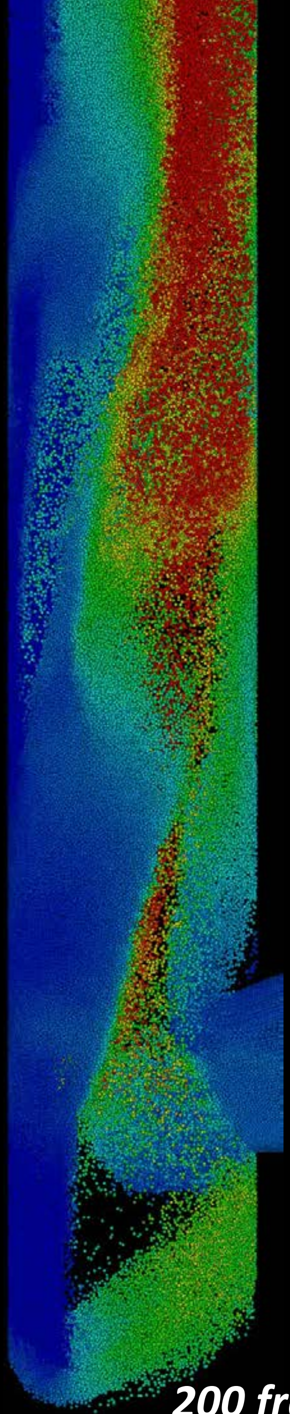
Particle flow field in NETL's Circulating Fluidized Bed (CFB) system.





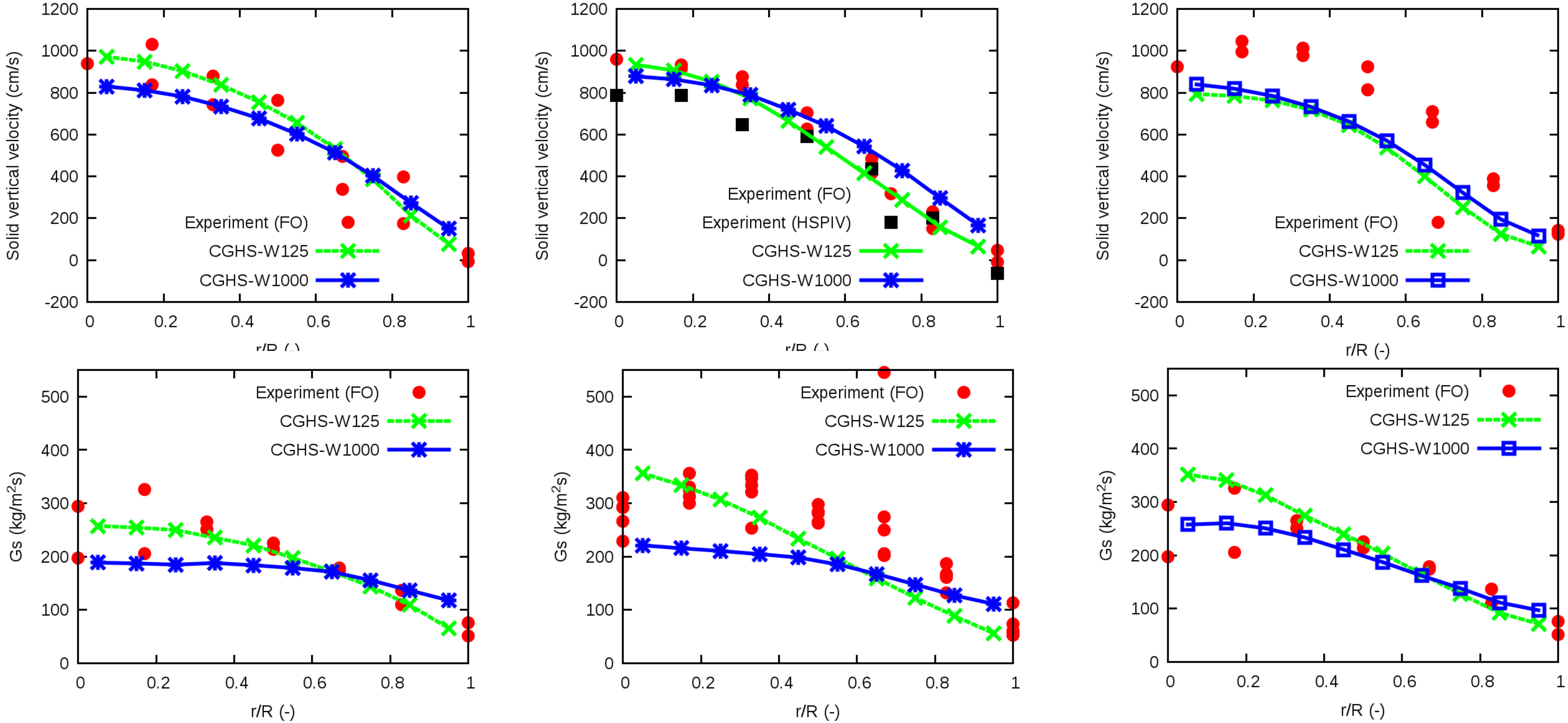
Shaffer & Gopalan, PIV





200 frames/sec

V&V of CGHS: Validation in large circulating fluidized bed



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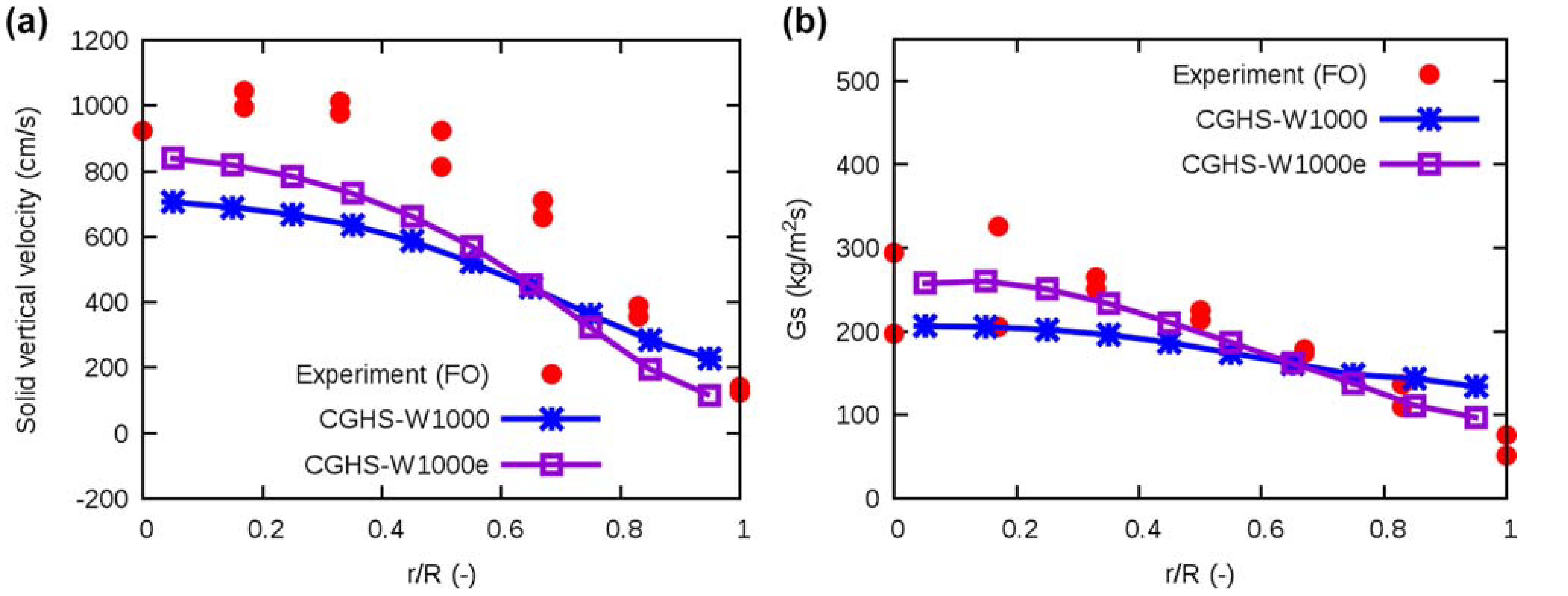
V&V of CGHS: Validation in large circulating fluidized bed



Improvements in radial profiles of solids vertical velocity and flux at height 13.33 m from case W1000 (e = 0.5) to case W1000e (e = 0.14).

Lu, L.; Li, T.; Benyahia, S., 2017. An efficient and reliable predictive method for fluidized bed simulation. AIChE Journal, DOI: 10.1002/aic.15832

V&V of CGHS: other validations of Coarse Graining

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- **Collision parameters**
  - **Benyahia** S, Galvin JE. **2010**, Estimation of Numerical Errors Related to Some Basic Assumptions in Discrete Particle Methods. ***Ind. Eng. Chem. Res.*** 49(21):10588-10605.
  - **Lu, L.,** Xu, J., Ge, W., Yue, Y., Liu, X., Li, J., **2014**. EMMS-based discrete particle method (EMMS–DPM) for simulation of gas–solid flows. **Chemical Engineering Science** 120, 67-87.

- **Chemical reactions**
  - **Lu, L.,** Yoo, K., Benyahia, S., **2016**. Coarse-Grained-Particle Method for Simulation of Liquid–Solids Reacting Flows. **Industrial & Engineering Chemistry Research** 55, 10477-10491.

- **Heat transfer**
  - **Lu, L.**; Morris, A.; Li, T.; **Benyahia**, S., **2017.** Extension of a coarse grained particle method to simulate heat transfer in fluidized beds. ***Int. J. Heat Mass Transfer,*** *111*, 723-735.

- **Drag corrections/CFD grid/parcel size**
  - **Lu, L.**; Konan, A.; **Benyahia**, S., **2017.** Influence of grid resolution, parcel size and drag models on bubbling fluidized bed simulation. **Chemical Engineering Journal**, *326*, 627-639.

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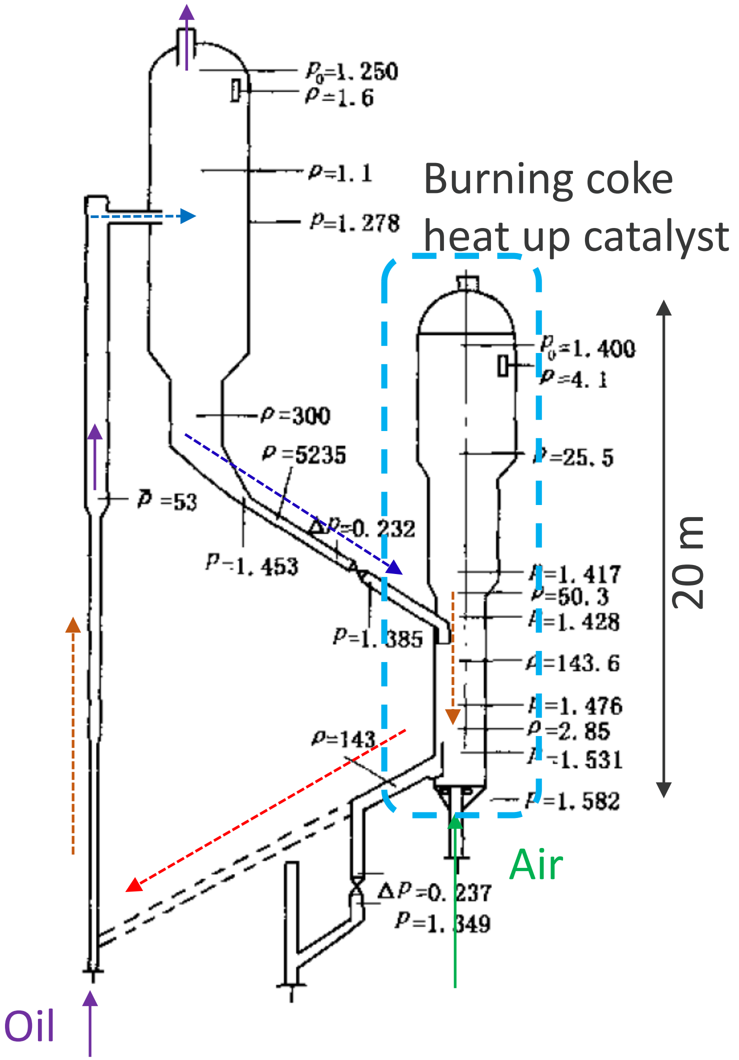
FCC Regenerator: Geometry and boundary conditions



Boundary conditions

Term	Simulation Value	Industrial data
Bottom inlet air velocity, m/s	0.495	NA (not available)
Bottom inlet air pressure, kPa	160	160
Bottom inlet air temperature, K	573	573
Bottom inlet air oxygen mass fraction	0.2320	0.2320
Bottom inlet air carbon dioxide mass fraction	0.0005	0.0005
Bottom inlet air carbon monoxide mass fraction	0.0000	0.0000
Bottom inlet air water vapor mass fraction	0.0000	0.0000
Bottom inlet air nitrogen mass fraction	0.7675	0.7675
Top outlet pressure, kPa	140	140
Spent catalyst inlet air velocity, m/s	0.5	NA (not available)
Spent catalyst inlet air pressure, kPa	140	NA
Spent catalyst inlet air temperature, K	735	NA
Spent catalyst inlet air oxygen mass fraction	0.0212	NA
Spent catalyst inlet air carbon dioxide mass fraction	0.2617	NA
Spent catalyst inlet air carbon monoxide mass fraction	0.0093	NA
Spent catalyst inlet air water vapor mass fraction	0.0416	NA
Spent catalyst inlet air nitrogen mass fraction	0.6662	NA
Spent catalyst mass flow rate, kg/s	22.7	22.7
Spent catalyst carbon mass fraction	0.00900	0.00900
Spent catalyst hydrogen mass fraction	0.00072	0.00072
Spent catalyst Temperature, K	753	753
Spent catalyst inlet voidage	0.9	NA
Regenerated catalyst outlet pressure, kPa	140	NA
Regenerated catalyst outlet solid mass flow rate, kg/s	22.7	22.7
Walls Momentum transfer	Non slip	NA
Walls Heat transfer	Adiabatic	NA
Walls Species transfer	Zero flux	NA

Lu, C., Wang, Z., 2002. Fluid Catalytic Cracking Technology. China Petrochemical Press, Beijing.

FCC Regenerator: Numerical parameters

Numerical parameters

Term	Simulation Value
Cartesian grid in x direction	15
Cartesian grid in y direction	90
Cartesian grid in z direction	15
Convection term discrete scheme	Superbee
Linear equation solver	BICGS
Hydrodynamic residual	1.0×10^{-3}
Temperature residual	1.0×10^{-3}
Species residual	1.0×10^{-3}
Gas phase time step, s	Adaptive and no larger than 1.0×10^{-3}
Solid phase time step, s	1.0×10^{-3}
Coarse grained particle diameter, m	0.048
Particle-particle restitution coefficient	0.1
Particle-particle spring constant, kg/s^2	1000
Particle-particle friction coefficient	0.1
Particle-wall restitution coefficient	0.1
Particle-wall spring constant, kg/s^2	1000
Particle-wall friction coefficient	0.1

Computation Speed: 1000 s for 5 days using only 64 cores

Catalyst Space time: 200 s

Correlations for the gas mixture properties

Property	Corrections
Density	$\rho_g = P/RT\sum \frac{Y_{gi}}{M_{gi}}$
Viscosity	$\mu_g = 1.672\times10^{-6}\sqrt{T} - 1.058\times10^{-5}$
Thermal conductivity	$\lambda_g = 5.526\times10^{-5}\sqrt{T} + 0.01155$
Heat capacity	$C_g = \sum Y_{gi} C_{gi}$
Molecular weight	$M_g = 1/\sum \frac{Y_{gi}}{M_{gi}}$

FCC Regenerator: Drag correction, Species. & Heat transfer

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Drag corrections

$$\beta_{Gao}=\begin{cases}150\dfrac{(1-\varepsilon_f)^2\mu_f}{\varepsilon_f d_{p*}^2}+1.75\dfrac{(1-\varepsilon_f)\rho_f\left|\mathbf{v}_f-\mathbf{v}_p\right|}{d_{p*}}, & \varepsilon_f\le 0.800\\ \dfrac{5}{72}\dfrac{\varepsilon_f(1-\varepsilon_f)\rho_f\left|\mathbf{v}_f-\mathbf{v}_p\right|}{d_{p*}(1-\varepsilon_f)^{0.293}}C_{D*}, & 0.800<\varepsilon_f\le 0.933\\ \dfrac{3}{4}\dfrac{\varepsilon_f(1-\varepsilon_f)\rho_f\left|\mathbf{v}_f-\mathbf{v}_p\right|}{d_p}C_{D0}\varepsilon_f^{-2.65}, & 0.933<\varepsilon_f\le 0.990\\ \dfrac{3}{4}\dfrac{\varepsilon_f(1-\varepsilon_f)\rho_f\left|\mathbf{v}_f-\mathbf{v}_p\right|}{d_p}C_{D0}, & 0.990<\varepsilon_f\le 1.000\end{cases}$$

Gao, J., Lan, X., Fan, Y., Chang, J., Wang, G., Lu, C., Xu, C., 2009. CFD modeling and validation of the turbulent fluidized bed of FCC particles. AIChE Journal 55, 1680-1694.

Chemical reactions and Heat transfer

$$\mathrm{CH_{12n}}+\left(\frac{r+0.5}{r+1}+3n\right)\mathrm{O_2}\rightarrow\frac{r}{r+1}\mathrm{CO_2}+\frac{1}{r+1}\mathrm{CO}+6n\mathrm{H_2O}$$

$$\mathrm{C}+\mathrm{O_2}\rightarrow\mathrm{CO_2}, Q=-393.51kJ/mol$$

$$\mathrm{C}+\tfrac{1}{2}\mathrm{O_2}\rightarrow\mathrm{CO}, Q=-110.54kJ/mol$$

$$2\mathrm{H}+\tfrac{1}{2}\mathrm{O_2}\rightarrow\mathrm{H2O}\ , Q=-241.82kJ/mol$$

Chang, J., Wang, G., Lan, X., Gao, J., Zhang, K., 2013. Computational Investigation of a Turbulent Fluidized-bed FCC Regenerator. Industrial & Engineering Chemistry Research 52, 4000-4010.

FCC Regenerator: Hydrodynamics

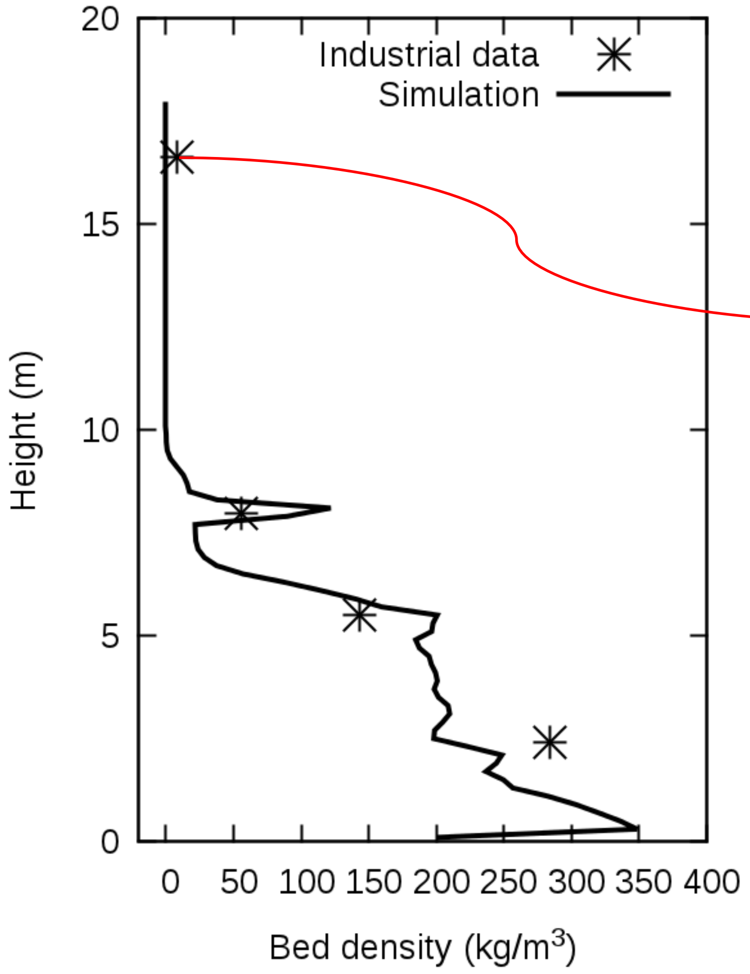
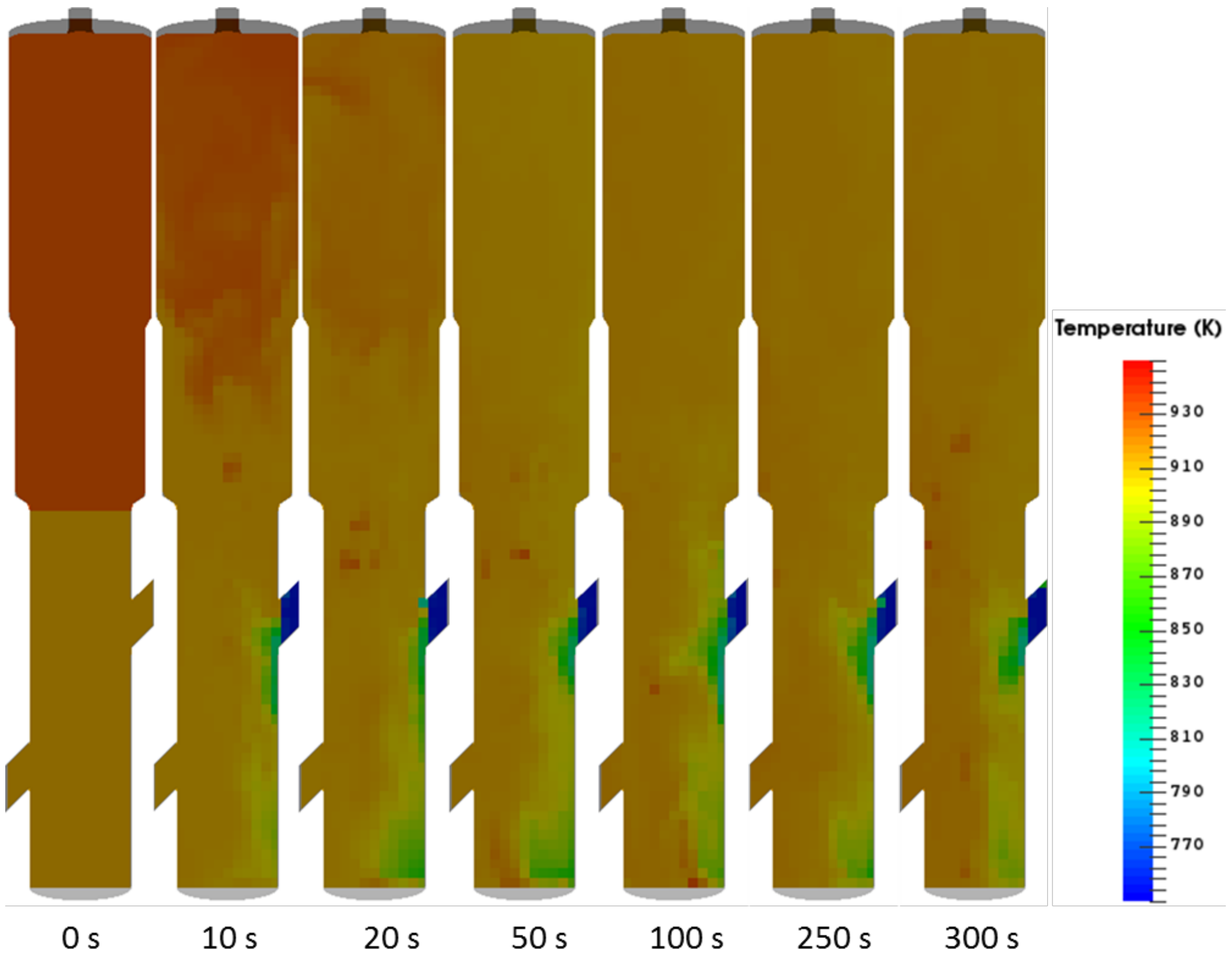


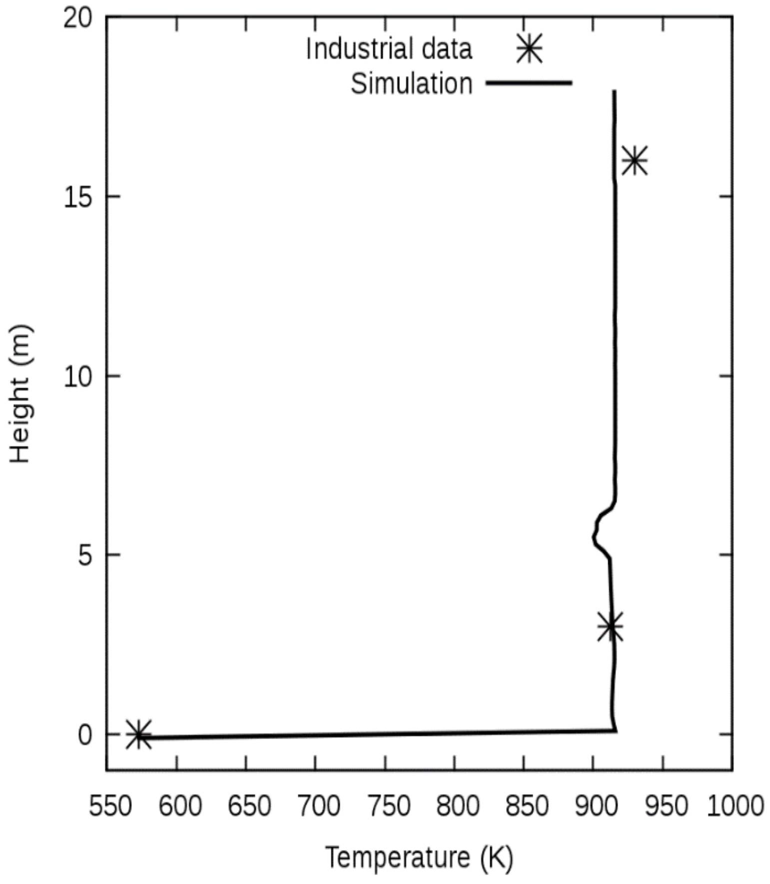
Figure 1. Comparison of predicted (averaged from 500 s to 1000 s) bed densities with industrial data

- Exp: very small but still measurable
- Sim: 0

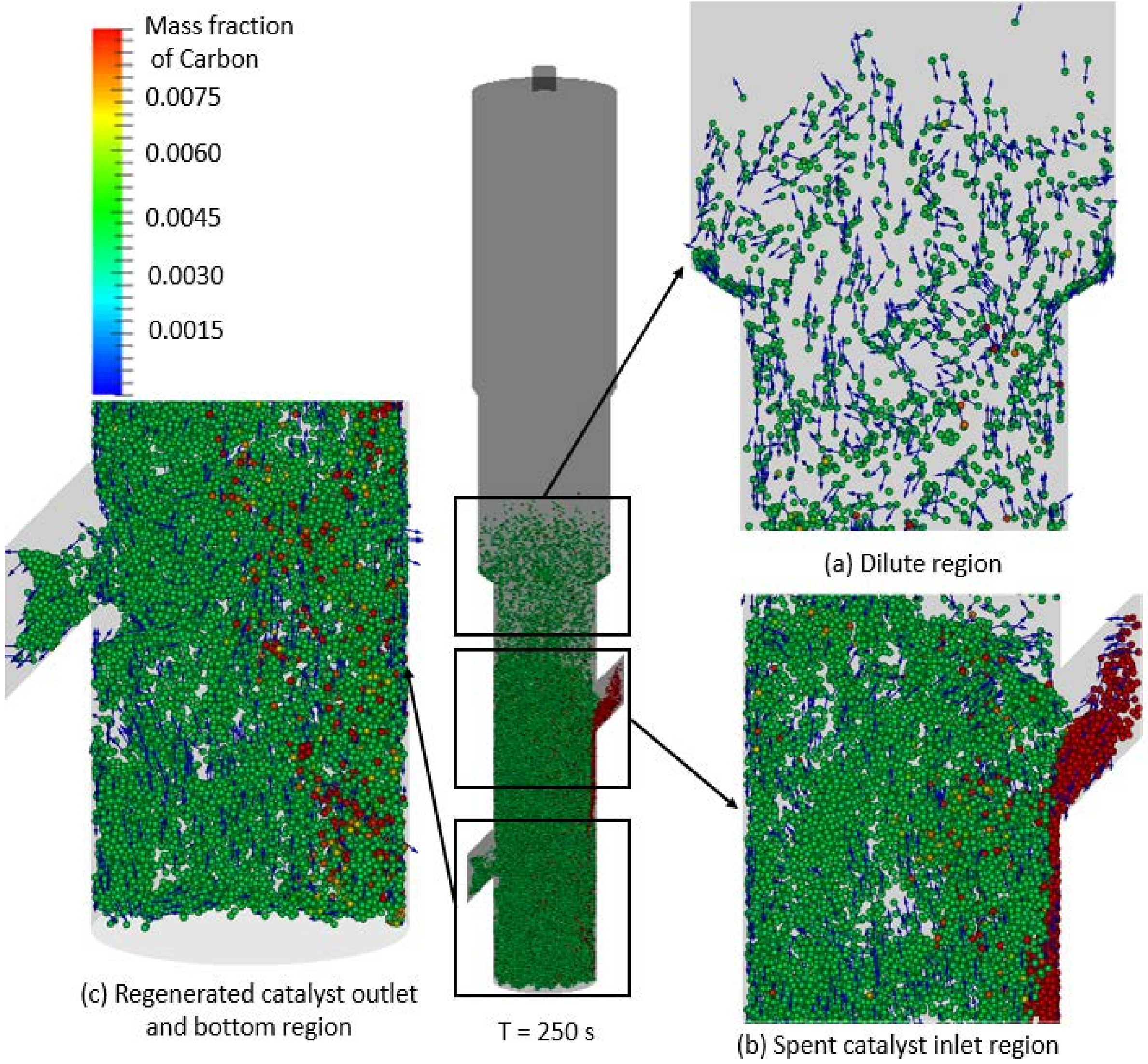
- This PSD was not provided by the industrial data and, so, was not considered in the simulation.
- In reality, small particles, or fines, in a PSD will generally be entrained to the freeboard region. [Grace and Sun, 1991]

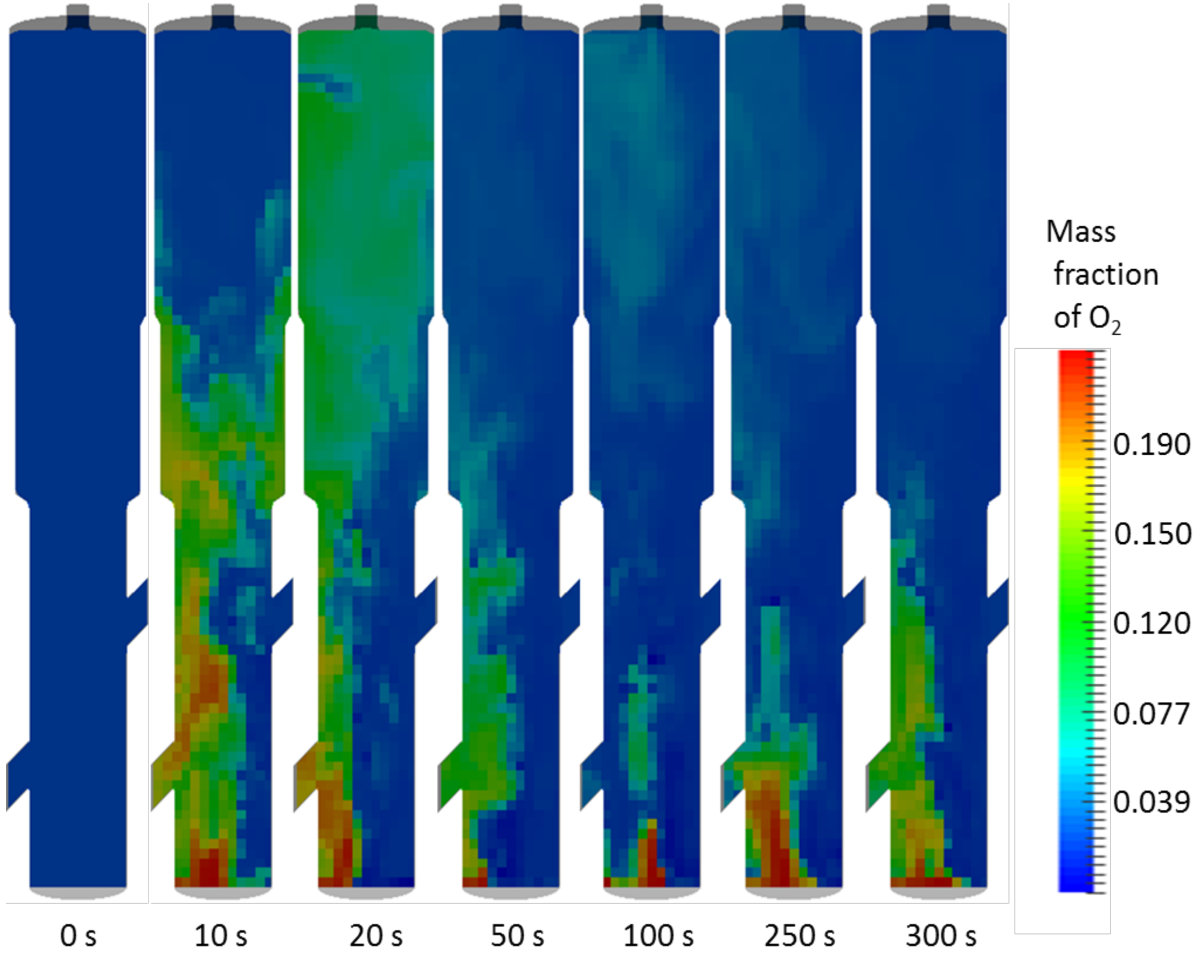
FCC Regenerator: Temperature



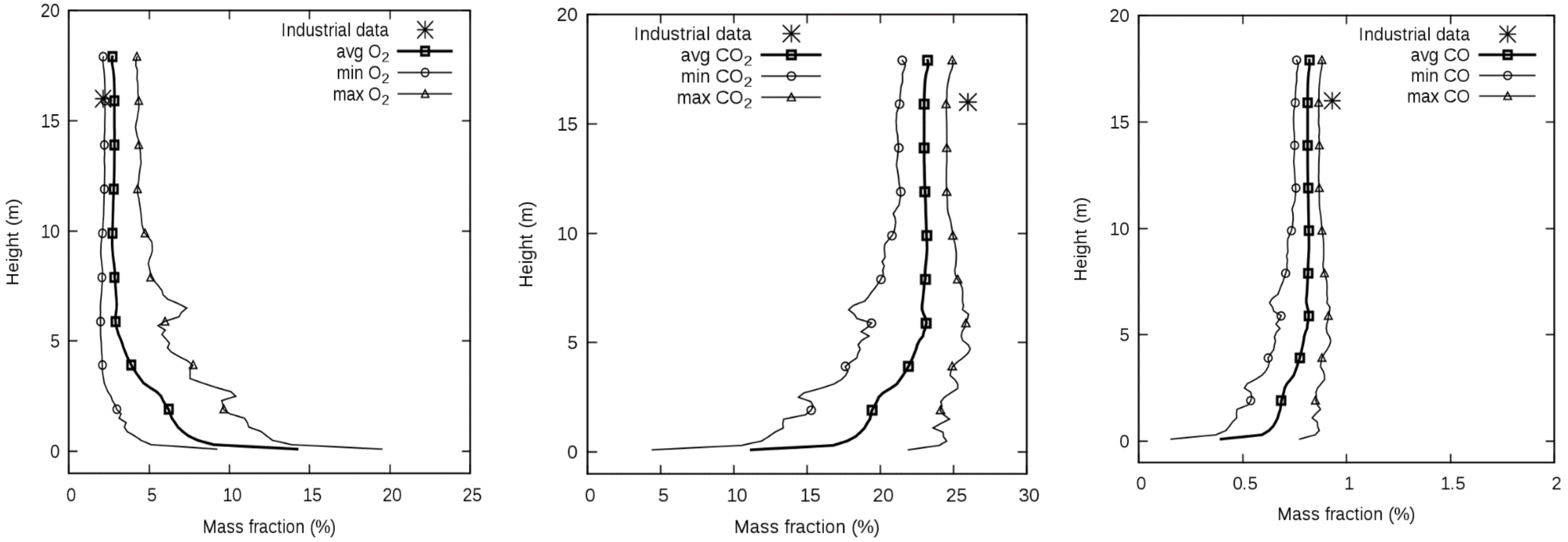


FCC Regenerator: Species





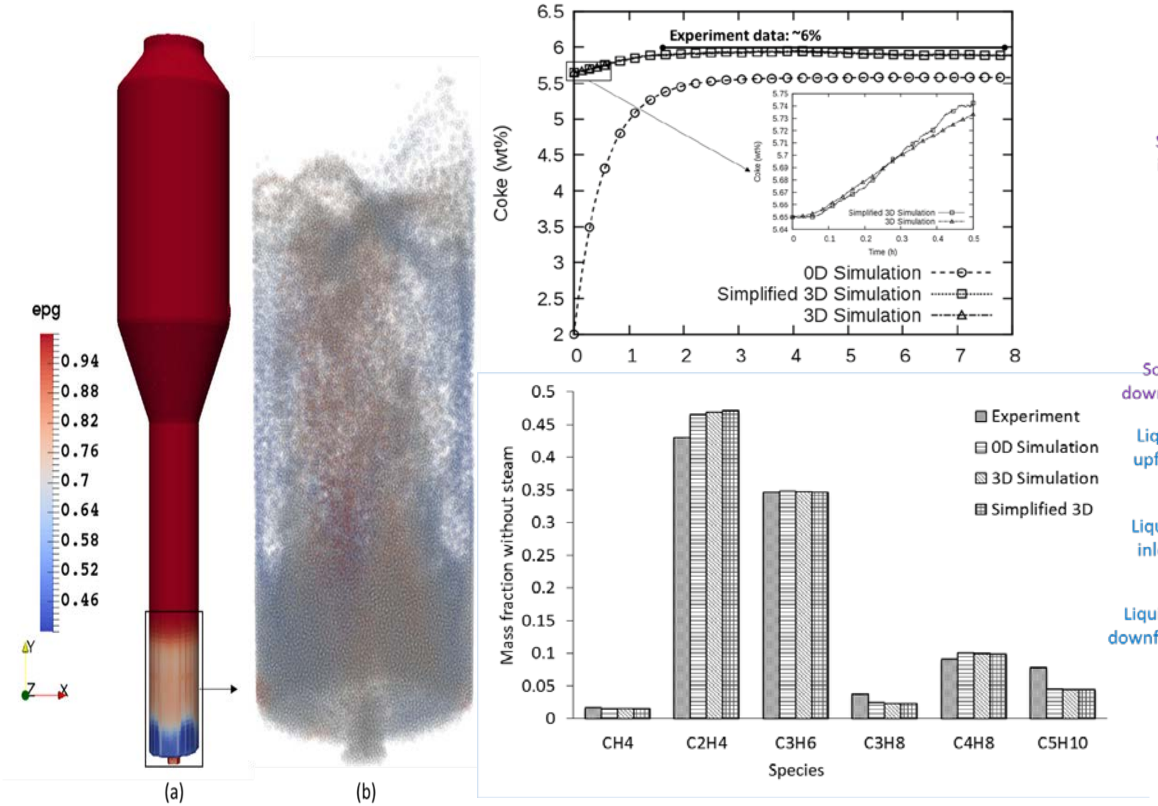
FCC Regenerator: Species



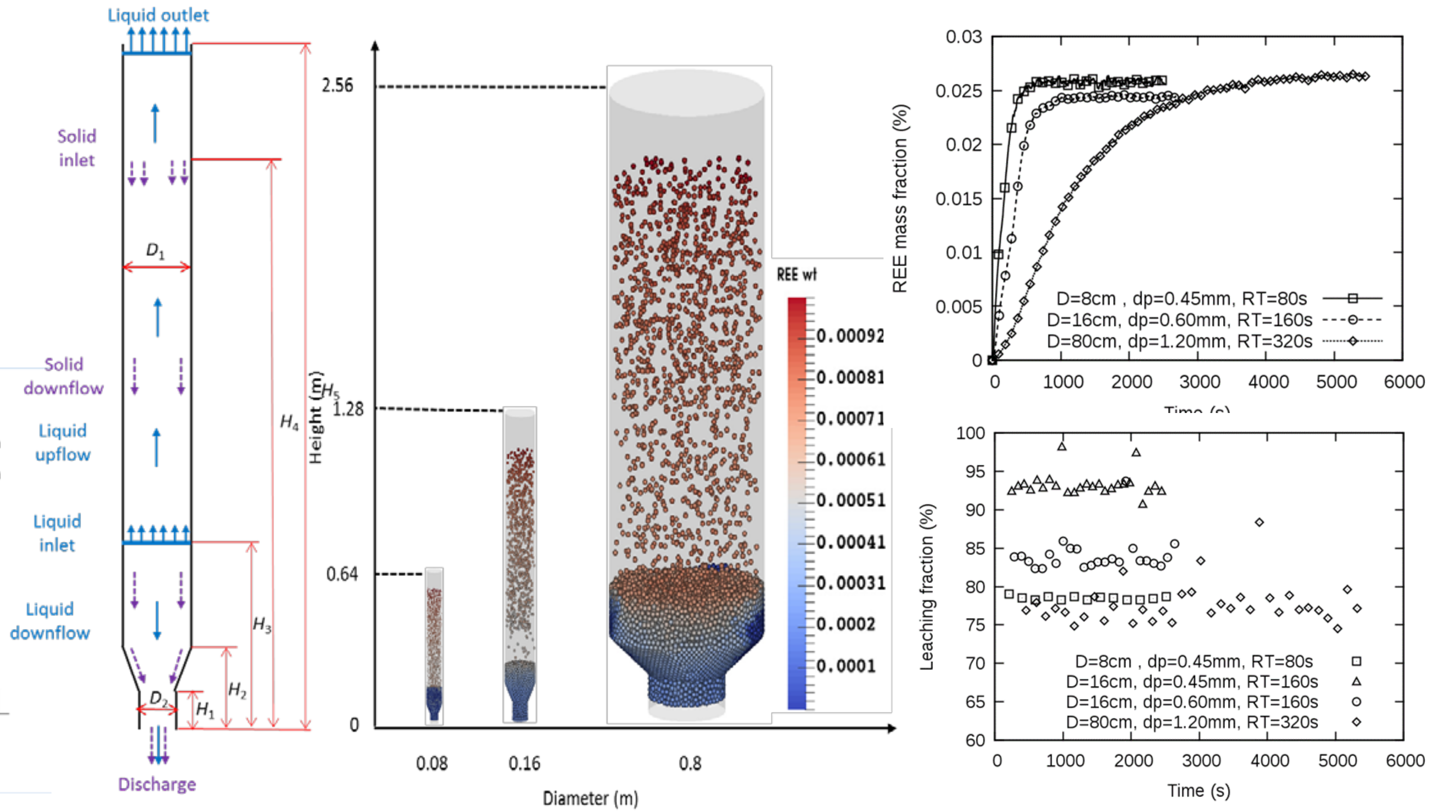
Concluding Remarks

- Simulation of large-scale reactors can be achieved in just few days of wall-clock time using minimal computer resources using CGHS
- The computation accuracy can be improved by reducing time step and parcel size

Methanol-To-Olefins (MTO) Reactor

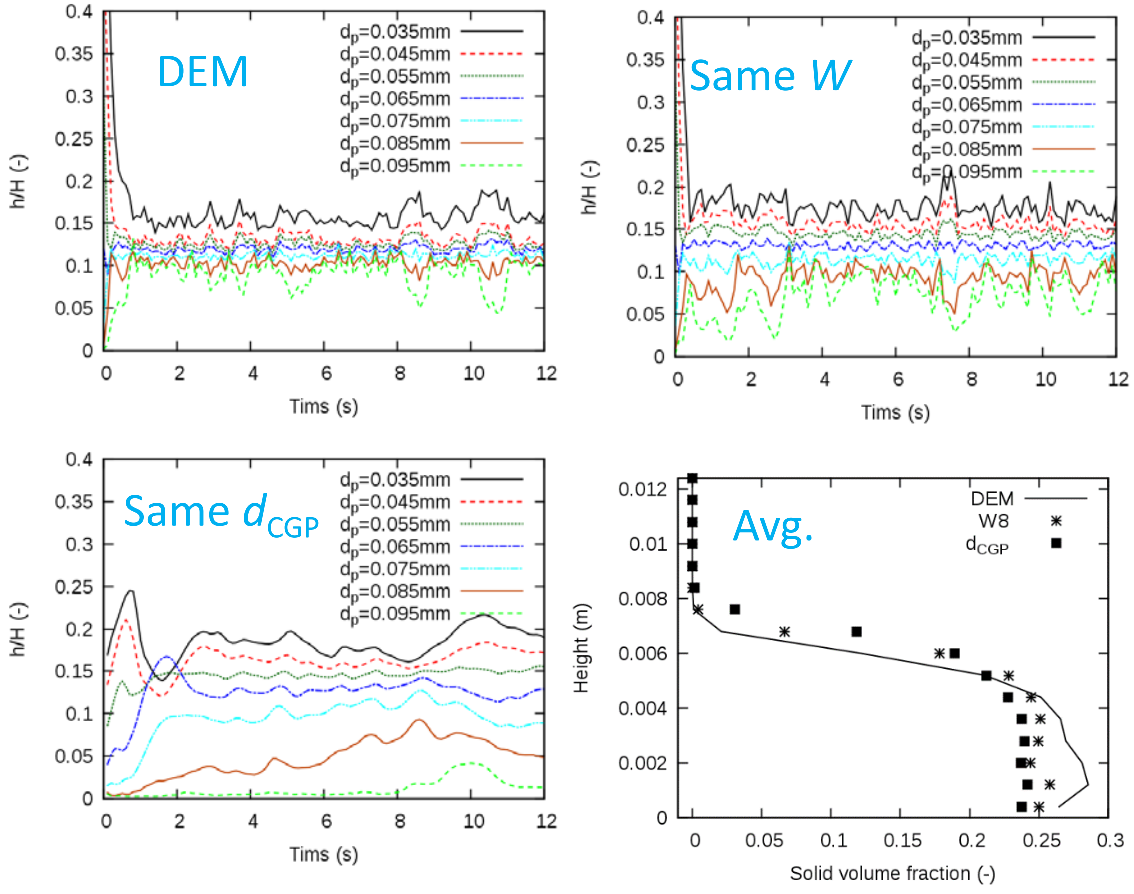


Rare-Earth-Element Leaching Reactor

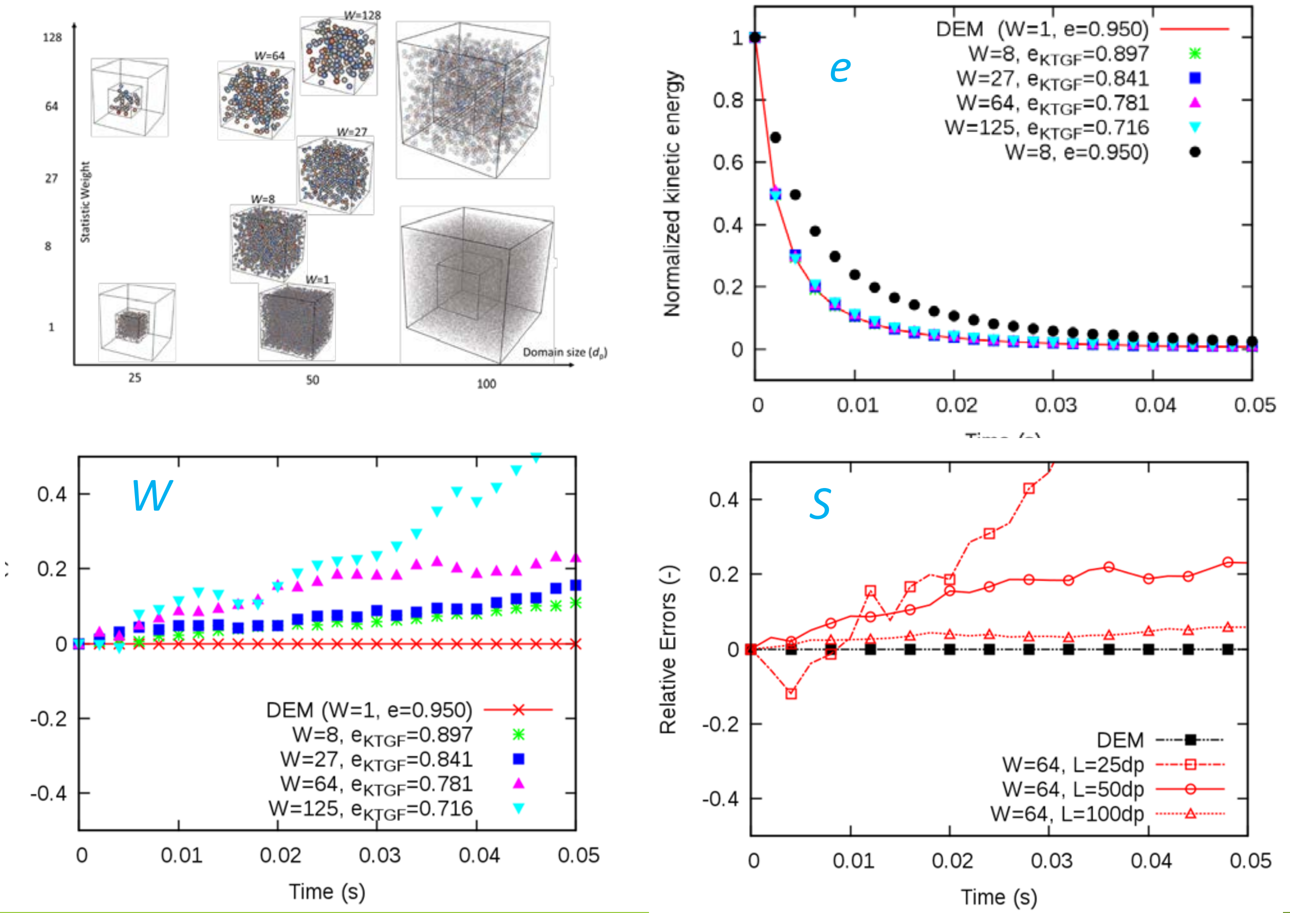


Ongoing Researches

Extension to polydisperse system:
FCC particles as an example



Uncertainty Quantifications:
Homogeneous cooling as an example



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Justin Finn, Ph.D.
Justin Weber
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Liqiang Lu, Ph. D.
Madhava Syamlal, Ph. D.
Mark Meredith
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Pankaj Saha, Ph. D.
Rupen Panday
Sofiane Benyahia, Ph.D.
Subhodeep Banerjee, Ph. D.
Terry Jordan

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