Fast CFD Based Optimization of Coal Moving Bed Gasifier

NATIONAL ENERGY TECHNOLOGY LABORATORY

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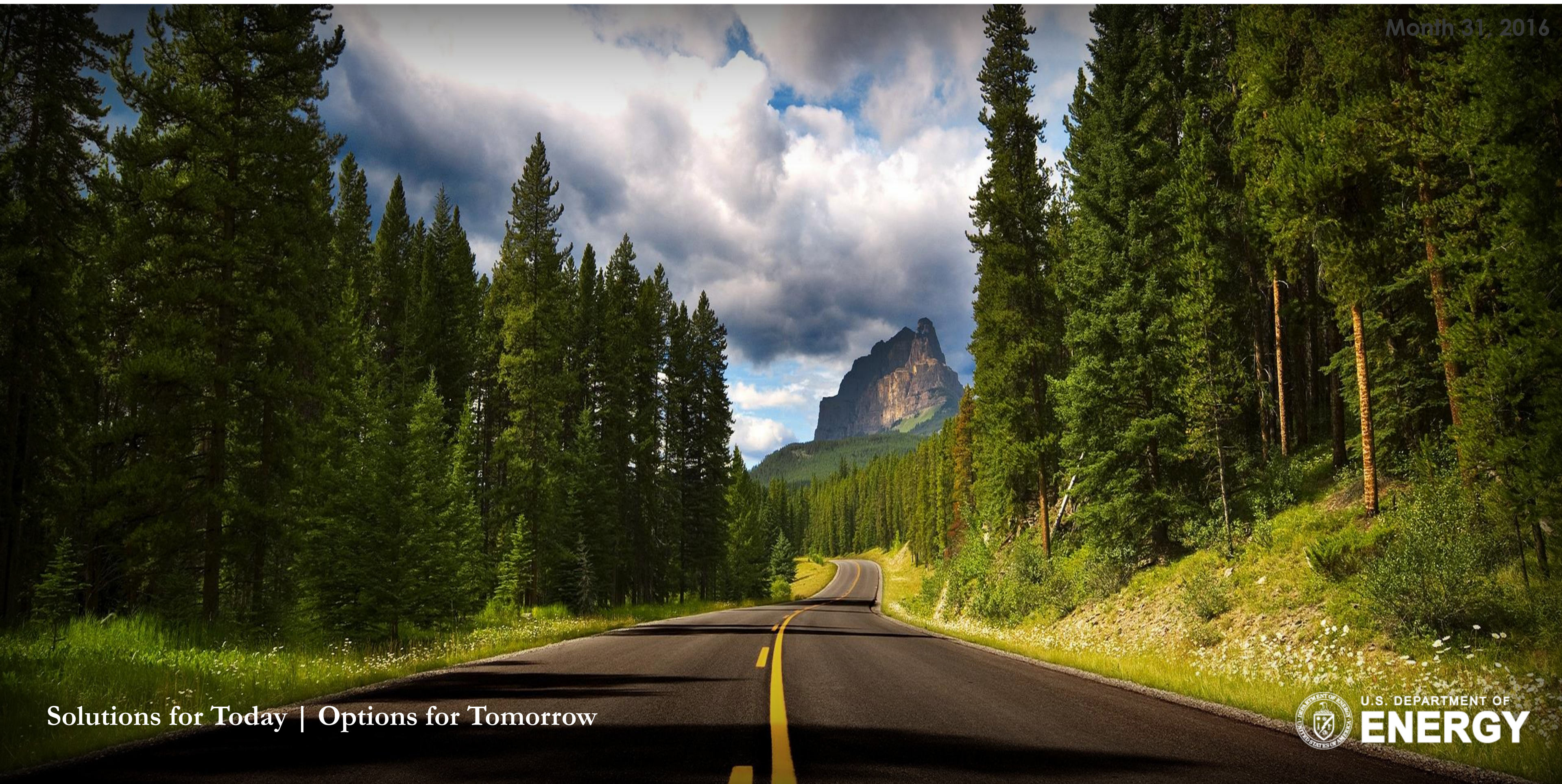


Coal/biomass gasifier simulation

Pilot scale gasifier at Sotacarbo, Italy

Challenges

- Experiment takes several hours to reach steady state
- 3D CFD simulation can only simulate about several seconds to several minutes

Strategies

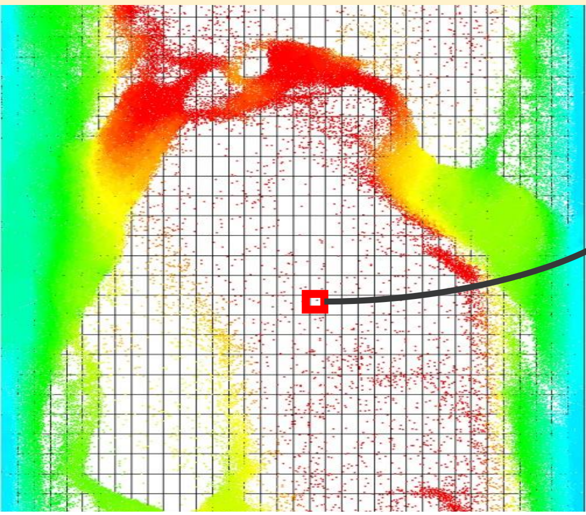
- Long time (several hours) 1D simulation to provide initial condition for 3D simulation
- Coarse grained DEM simulate to speed up 3d simulation and optimization

1-D: DEM

3-D: coarse-grained DEM

Coarse Grained DEM

To capture particle-scale chemical reactions Euler-Lagrangian method

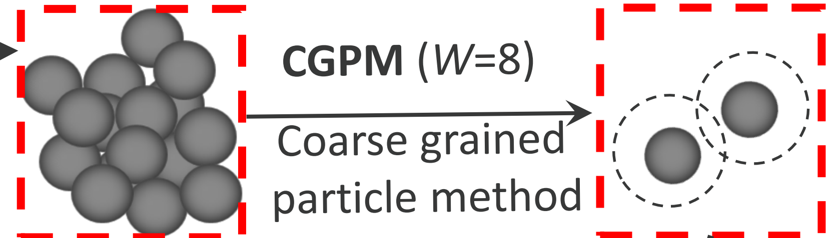


Solid flow = 18.4kg/h
Residence Time=80s
Simulate 400 s, using 100 cores

Particle Number = 6.4 x10^6
Time steps = 1.0x10^{-6}s
Time needed ~ 3.65 YEARs!

Solved by lumping several real particles into a parcel

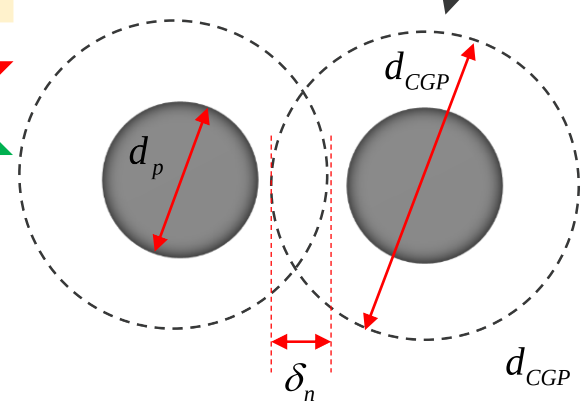
16 particles



Improved Speed

Particle number ↓

Time steps ↑

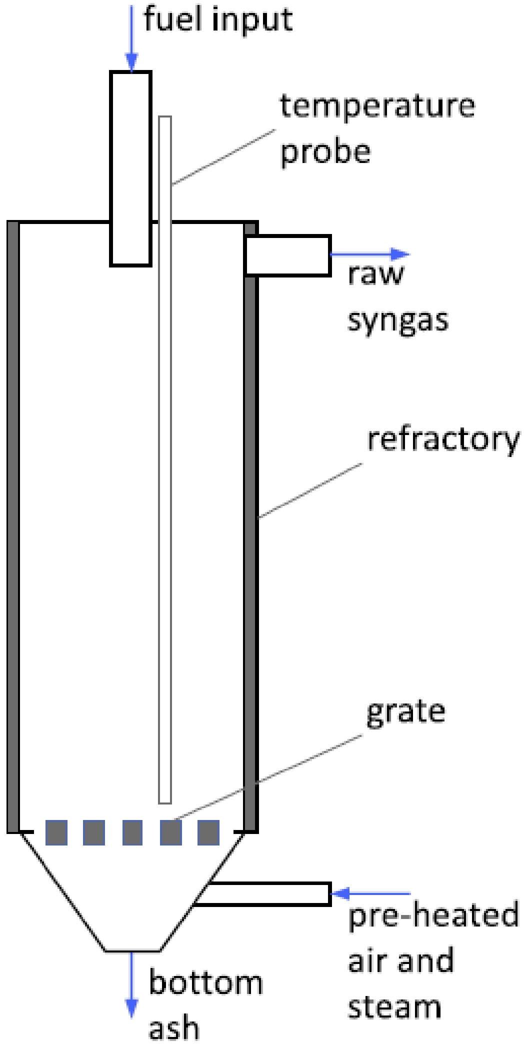


$$d_{CGP} = d_p W^{1/3}$$

Moving Bed Gasifier Experiment[1]

- Coal: 24kg/h, Usibelli, 1300kg/m^3
- Air+H_2O=57.6+3.7 at 250 Celcius
- 140Kpa, coal diameter 5mm-15mm, isolated wall, thermocouple close to center.
- Data for model validation:

a. Syngas compositions (mole fraction, dry basis)
b. Bed temperature profile

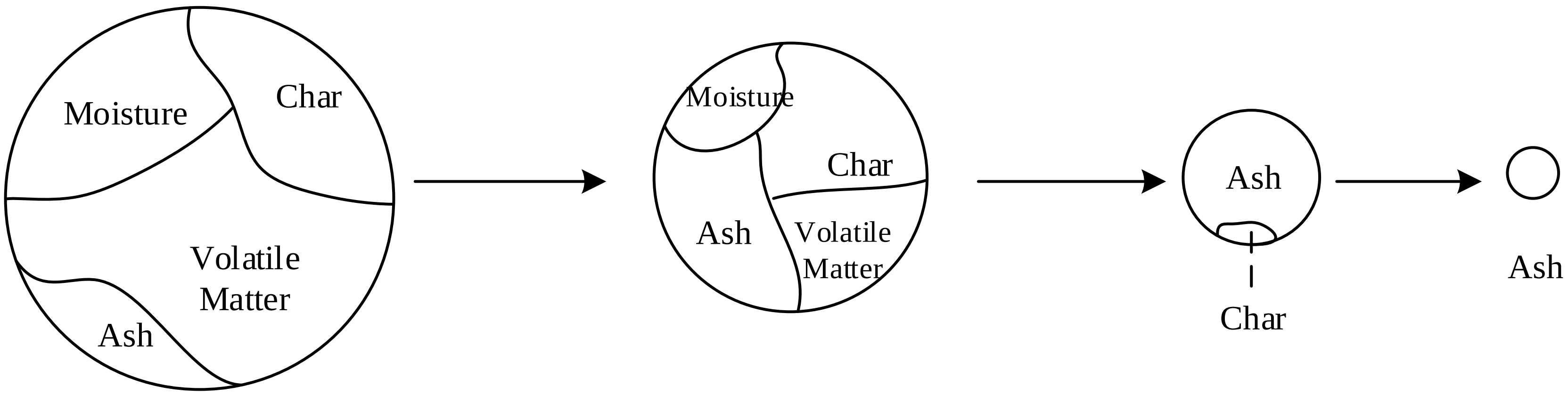


Proximate Analysis		Ultimate Analysis (by weight)	
Fixed Carbon	31.34	**C**	48.56
Moisture	17.64	**H**	5.96
Volatiles	41	**N**	0.50
Ash	10.02	**S**	0.18
		O	17.14
Bulk Density (kg/m^3)	800	**Moisture+Ash**	17.64+10.02

[1] C Frau, F Ferrara, A Orsini, A Perrinau. Characterization of several kinds of coal and biomass for pyrolysis and gasification. Fuel, 2014

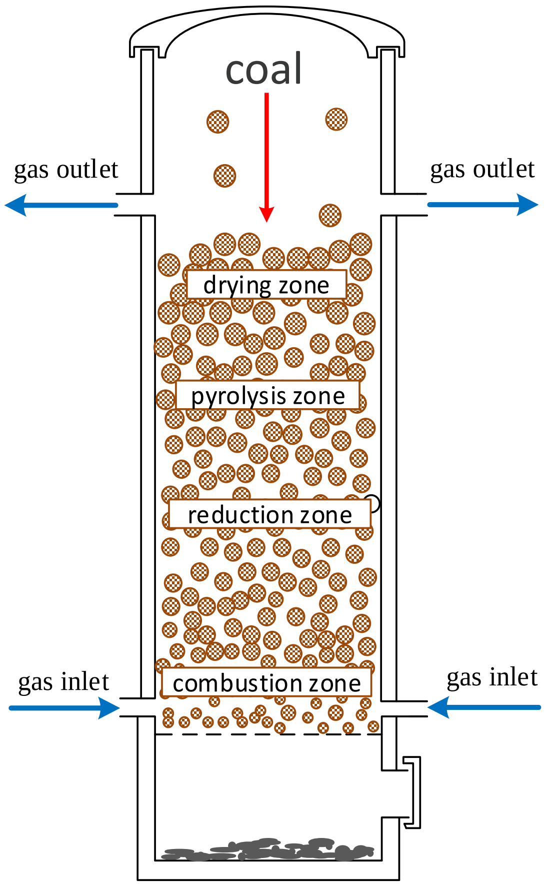
Particle diameter shrinkage model

Constant density for fuel particles:



The diameter of the biomass particles is: $d_p = (\frac{6m_p}{\pi\rho})^{1/3}$

Kinetics



Categories	Reactions: Forward reaction	Reactions: Backward reaction
Drying	$\text{Moisture(coal)} \rightarrow H_2O\text{(gas)}$	
Pyrolysis	$\text{Volatiles} \rightarrow 0.6088CO + 0.3962CH_4 + 2.2469H_2 + 0.4665H_2O + 0.093\text{tar} + 0.1932CO_2$	
Gasification	$\text{Char}+H_2O \rightarrow CO+H_2$	$CO + H_2 \rightarrow \text{Char} + H_2O$
	$\text{Char}+CO_2 \rightarrow 2CO$	$2CO \rightarrow \text{Char} + CO_2$
	$\text{Char} + 2H_2 \rightarrow CH_4$	$CH_4 \rightarrow \text{Char} + 2H_2$
	$\text{Char} + O_2 \rightarrow CO_2$	
Gas phase reactions	$CO+\frac{1}{2}O_2 \rightarrow CO_2$	
	$H_2+\frac{1}{2}O_2 \rightarrow H_2O$	
	$CH_4+2O_2 \rightarrow CO_2+2H_2O$	
	$CO+H_2O \rightarrow CO_2+H_2$	
	$CO_2 + H_2 \rightarrow CO + H_2O$	

Simulation Strategy

01

1

1-D Startup

This simulates the ignition and startup phase of the gasifier.

02

2

1-D steady state

4 hour simulation at steady state feeding conditions

03

3

Map 1-D to 3-D

“Copy” 1-D solid phase details to 3-D case as I.C.

04

4

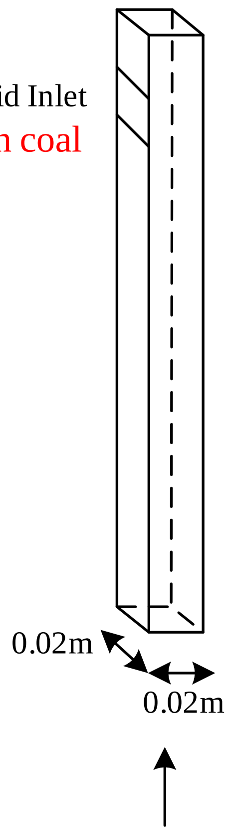
3-D steady state

Run 3-D simulations for at least 600s to steady state.

1D-4 hour simulation to steady state

1D: 2dp*2dp*2m, DEM

Syngas Outlet

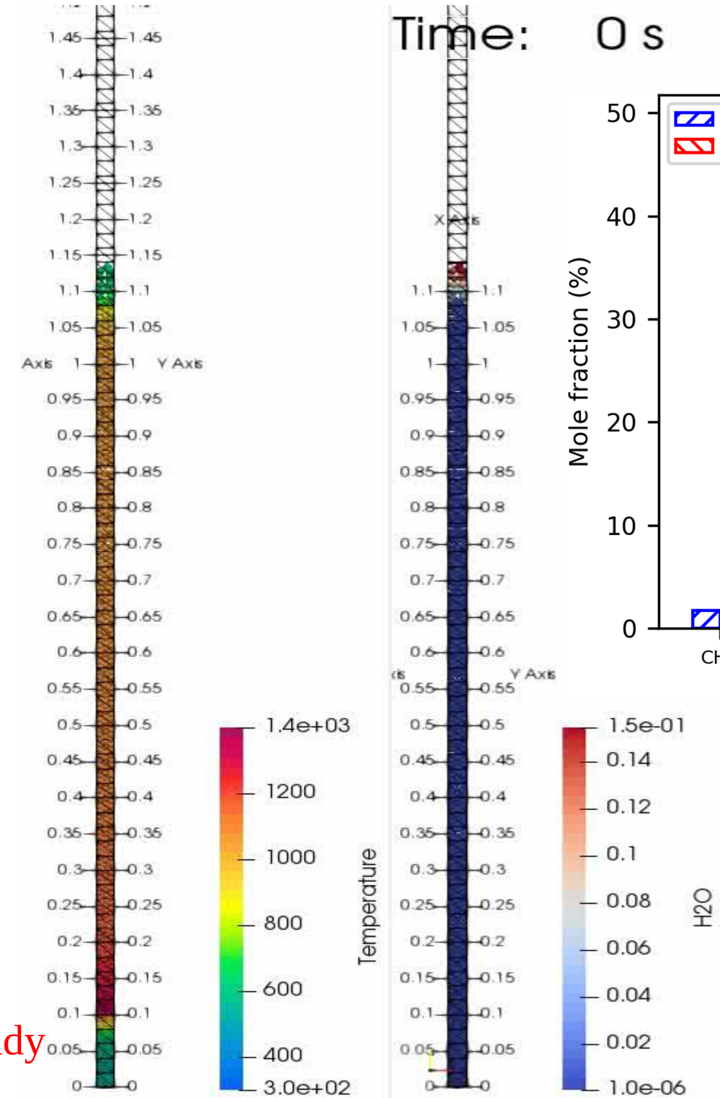


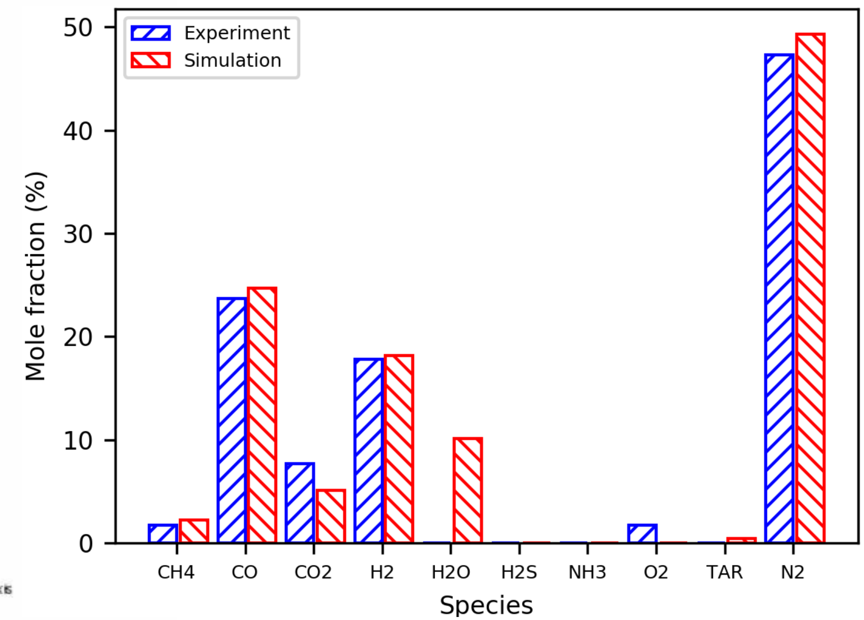
24kg/h coal

Gas Inlet

20kg/h air for startup

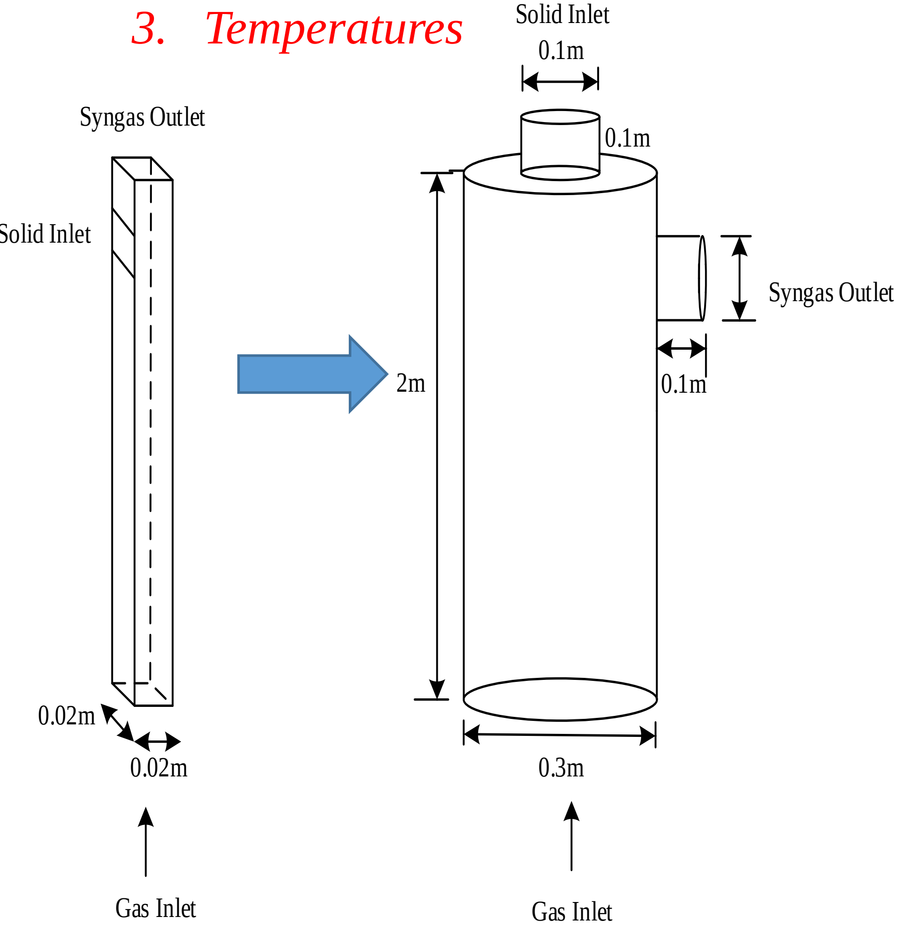
Air+H_2O=57.6+3.7 for steady state

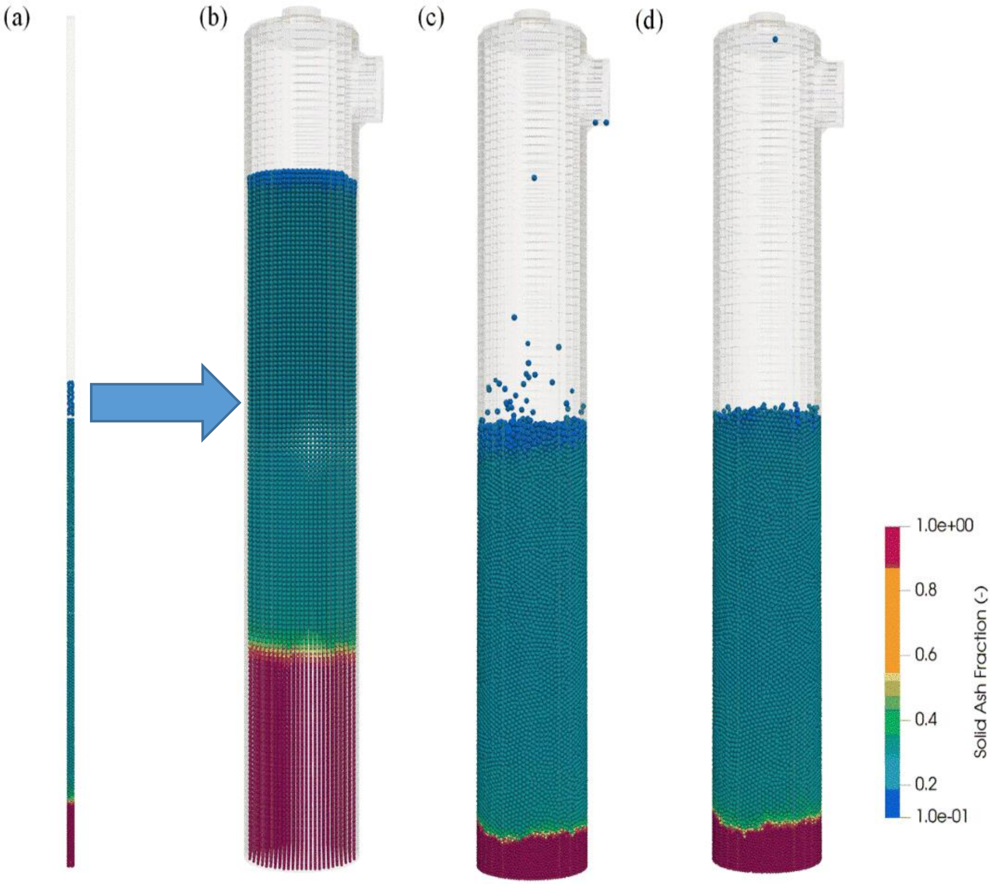




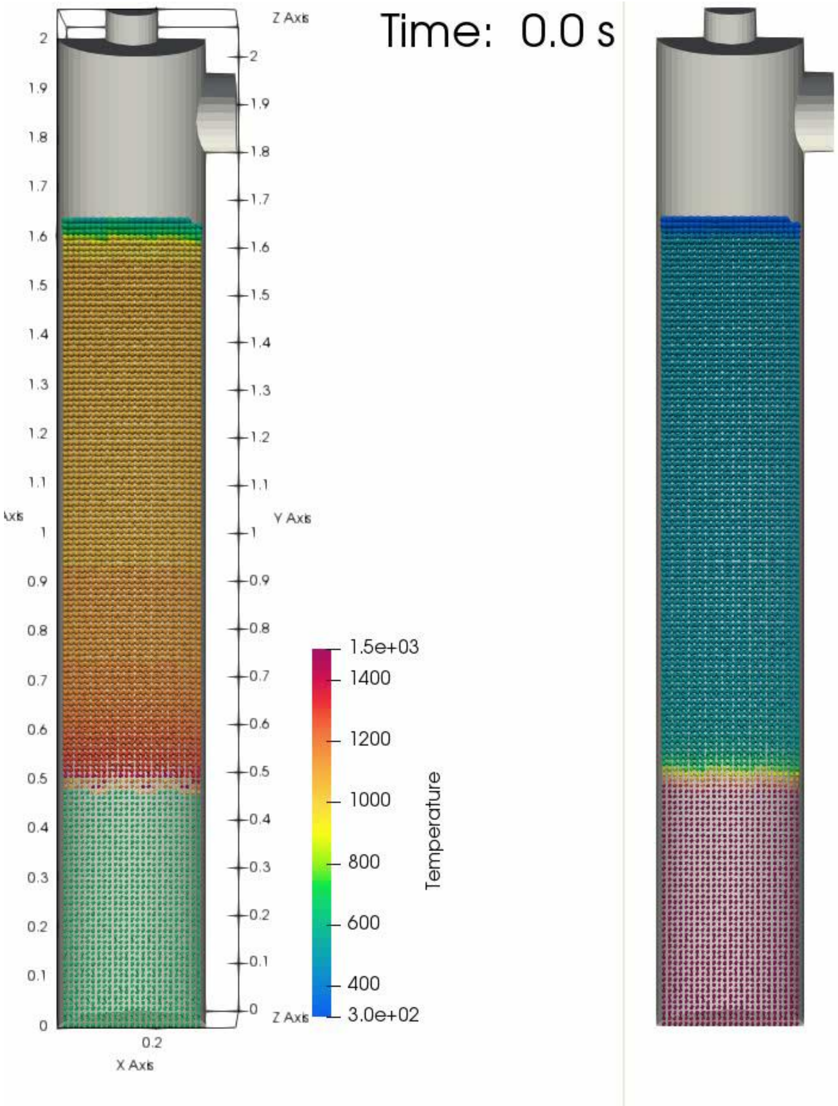
1-D to 3-D mapping

Solid phase mapping:
1. *Solid compositions*
2. *Diameters*
3. *Temperatures*

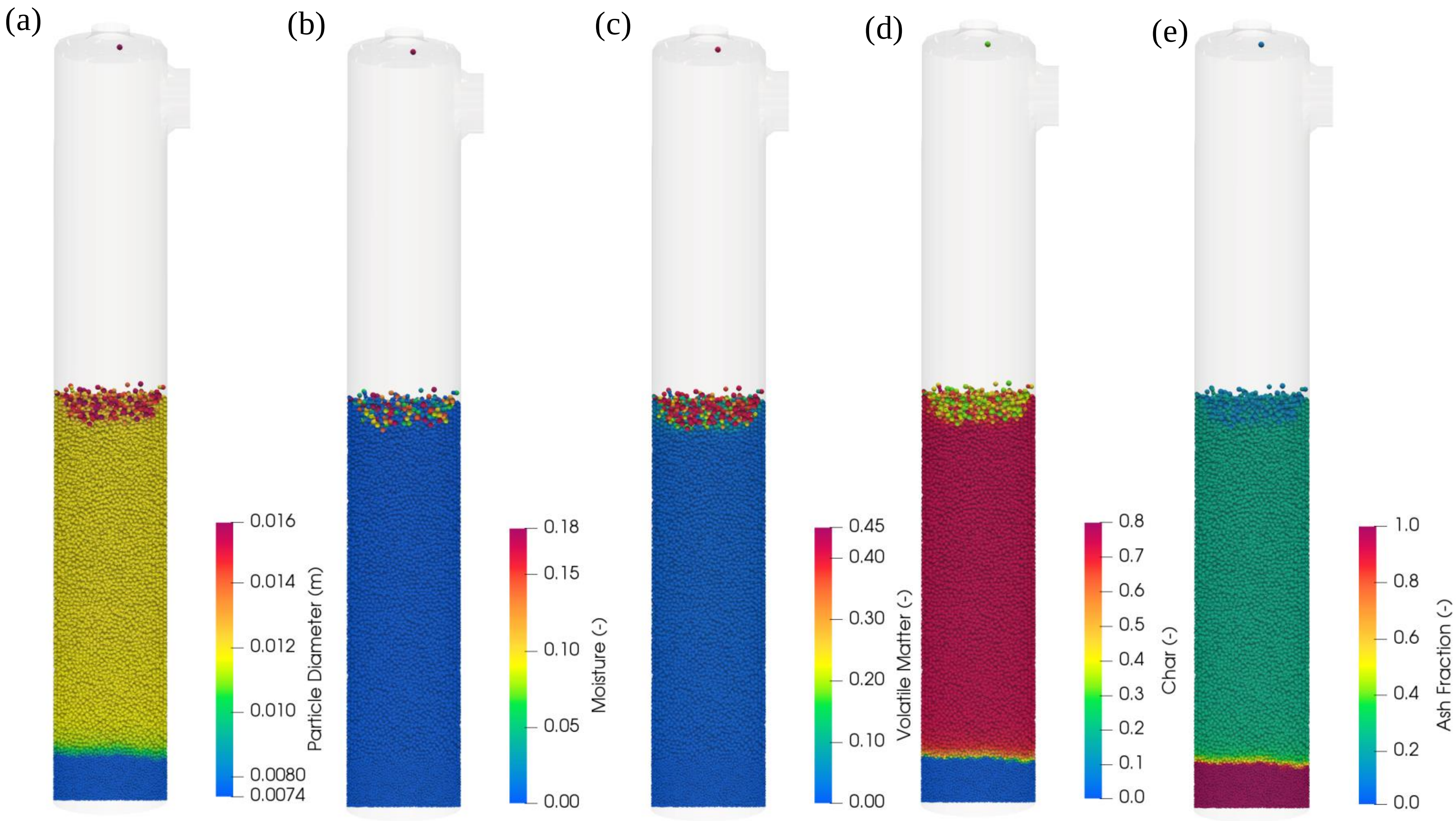




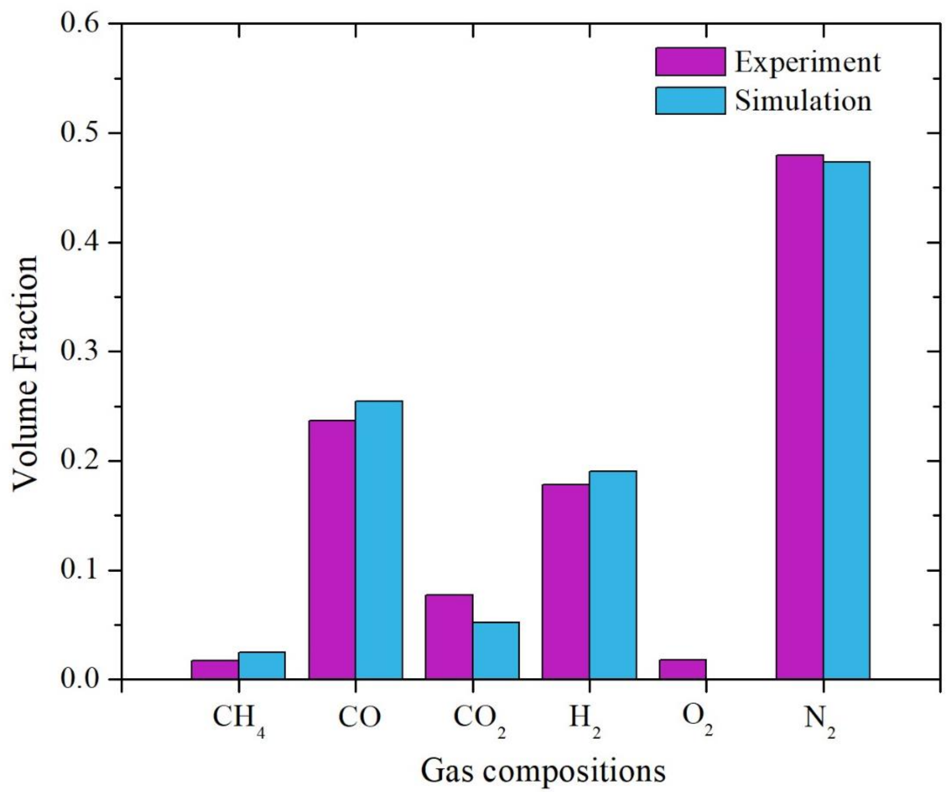
3-D CGDEM 10min simulation

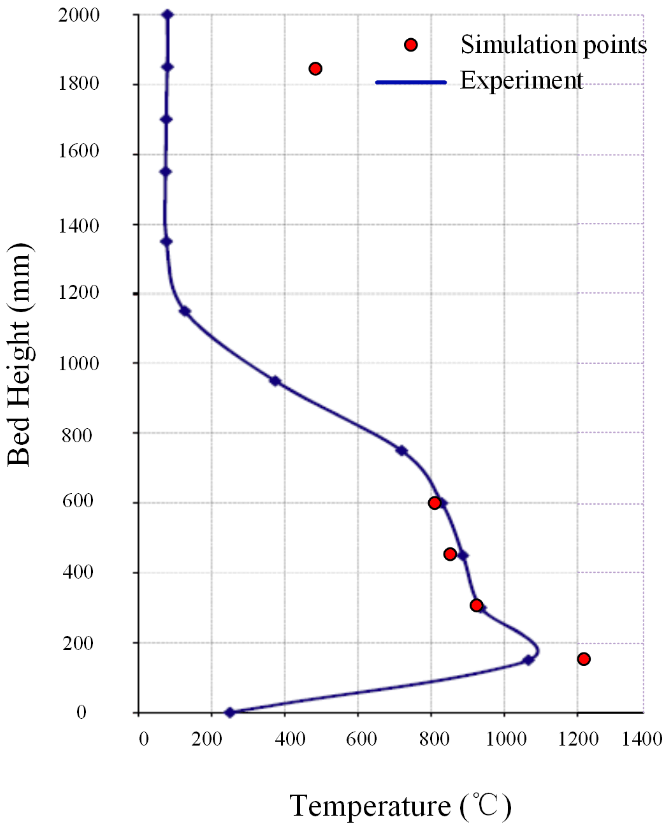


3D-CGDEM simulation results at steady state



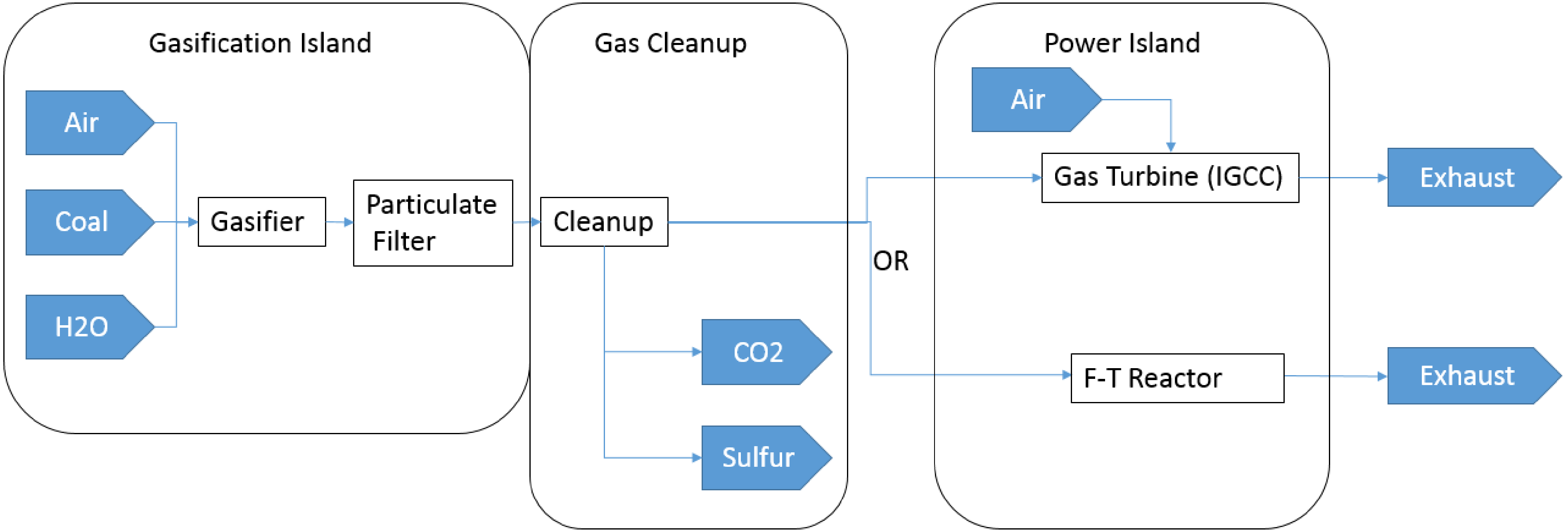
3-D CGDEM simulation VS. Experiment





Optimization Gas Products: IGCC or F-T

Integrated gasification combined cycle or the Fischer–Tropsch process



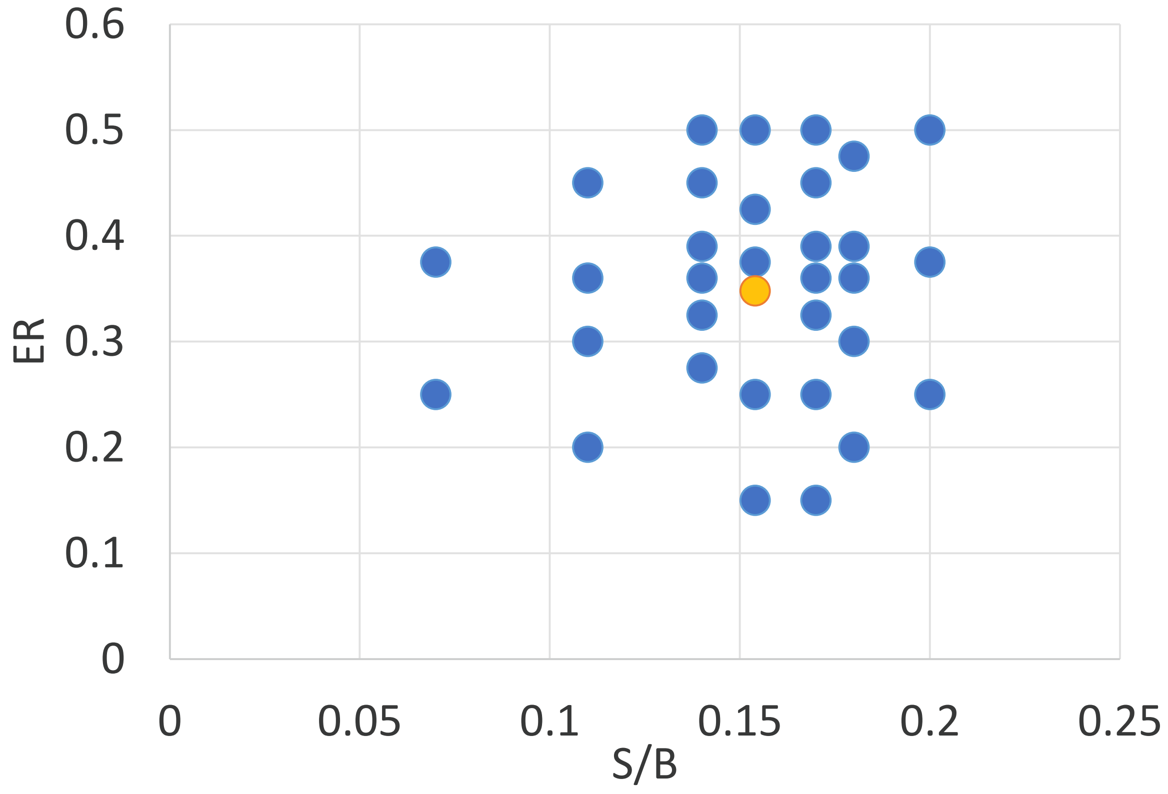
Ref: H Ghezel-Ayagh, Stephen Jolly, Dilip Patel, and David Stauffer. Solid Oxide Fuel Cell System Utilizing Syngas from Coal Gasifiers. Process Engineering of Energy Systems. dx.doi.org/10.1021/ie300841m | Ind. Eng. Chem. Res. 2013, 52, 3112−3120

Optimization Cases

Major parameters:

$$ER = \frac{\text{actual air/fuel ratio}}{\frac{\text{air}}{\text{fuel}}\text{ ratio for stoichiometric combustion}}$$

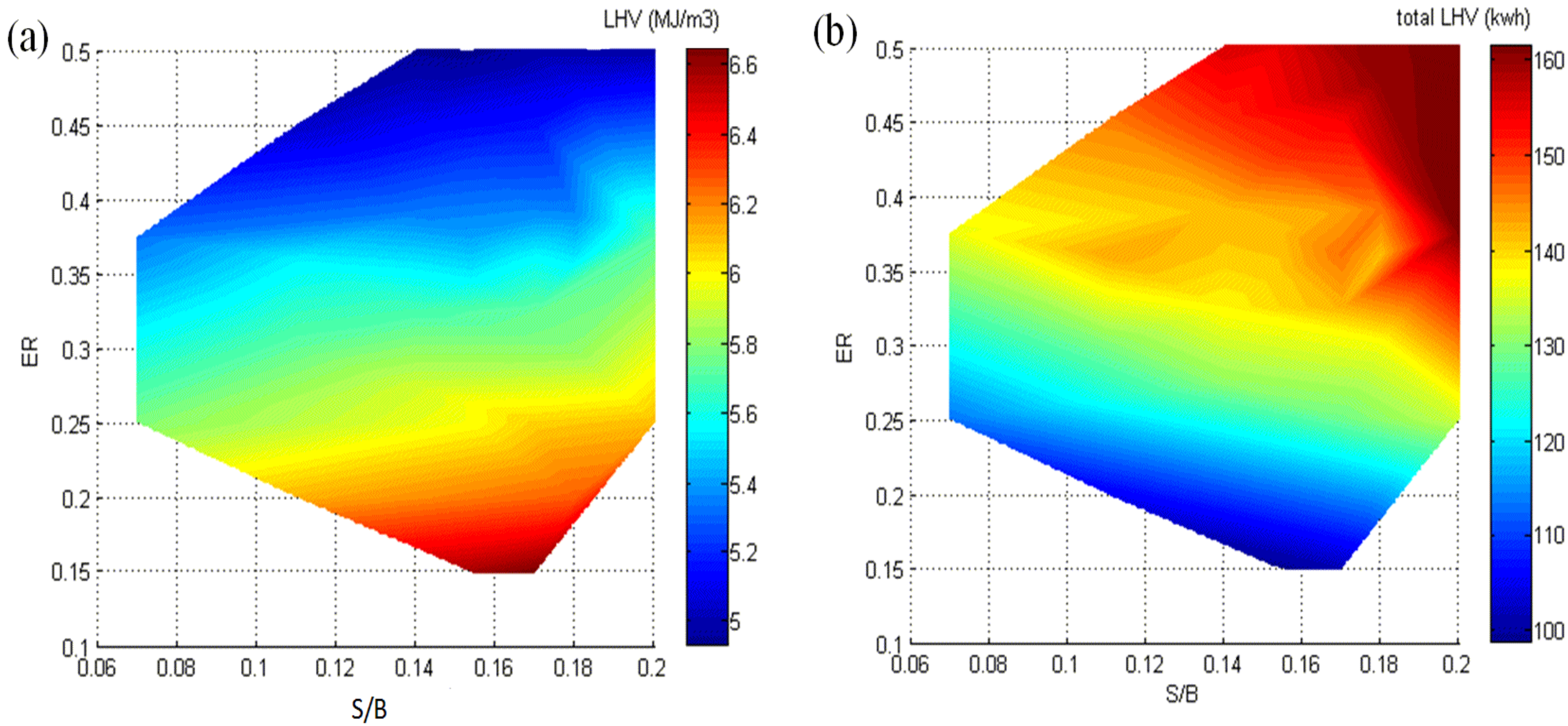
S/B=Water/Biomass mass ratio



Optimization For IGCC

For IGCC: the goal is to use the conserved energy, we search for the maximum heating value

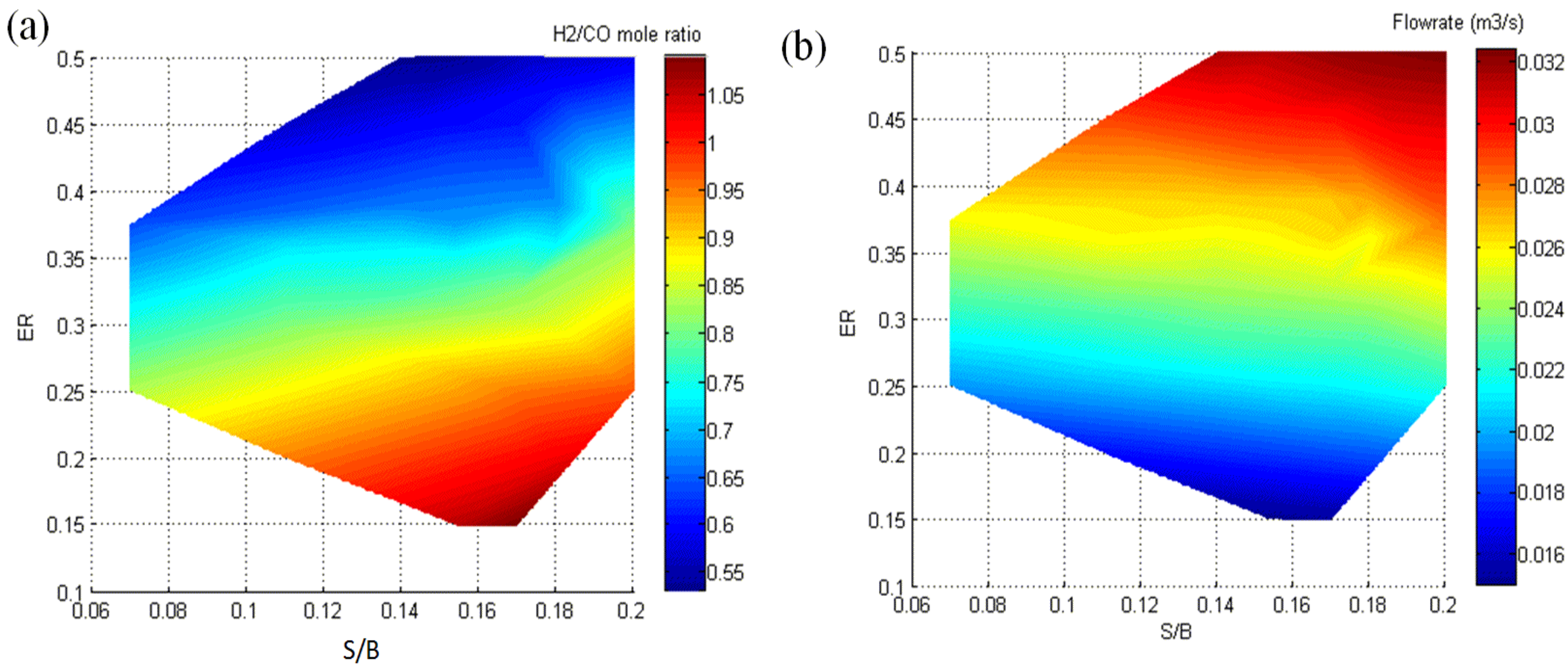
LHV(MJ/m^3)=CO×12.636+H2×10.798+CH4×35.818+C2H4×59.036+C2H6×63.772
Total LHV(kwh)=LHV(MJ/m^3) ×Flowrate (m^3/s)*1000(MJ/kJ)



Optimization for F-T

Fischer-Tropsch process: $(2n+1)\ H_2\ +\ n\ CO \rightarrow C_n H_{(2n+2)}\ +\ n\ H_2O$

We search for H_2/CO at 2.0



Scaleup to 1MW - Demonstration

Acknowledgement-MFS Group

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MFiX Multiphase Flow with Interphase eXchanges

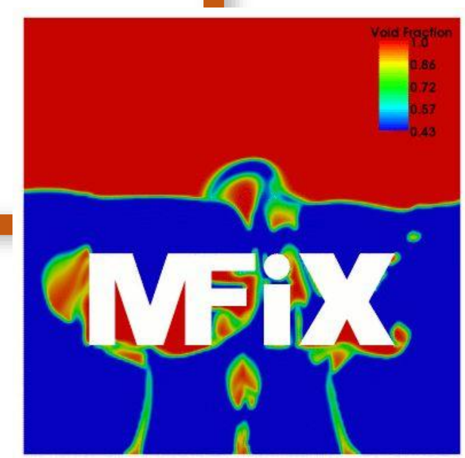
C3M Carbonaceous Chemistry for Computational Modeling

Nodeworks

Tracker

Acknowledgement

THANKS!



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