An Euler-Euler CFD Model for Biomass Gasification in Fluidized Bed

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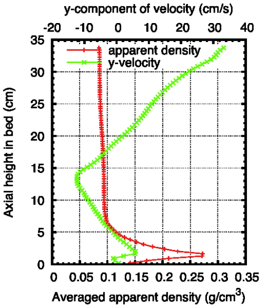
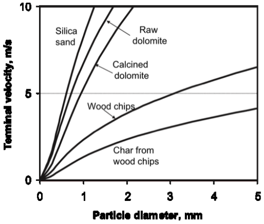
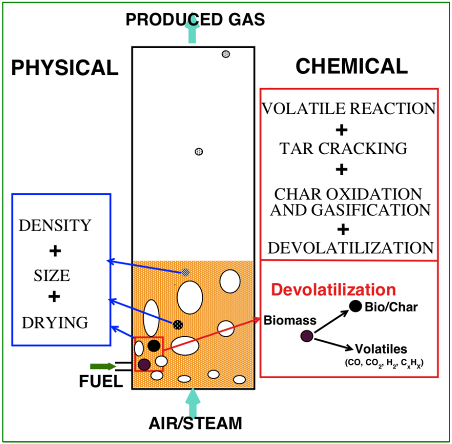
Objectives

- Provide MFIX-based Euler-Euler CFD models for polydisperse, reacting, variable density solid particles
- Facilitate the numerical simulation and scale up of energy systems such as gasifier

Background: Multiphysics & Multiscales



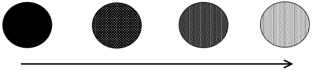




Physical Models

- Spherical particle assumption
- Porosity and moisture modeled
- Uniform conversion model for micro-particles
  - Constant particle diameter (d_p)
  - Variable particle density (ρ_p) with increasing pores
  - Intra-particle transport ignored for micro-particle
- Couple continuity and species equation to update ρ_p

$$\frac{1}{\rho_{apparent}} = \sum_{n=1}^{N} \frac{X_{s,n}}{\left(\rho_n\right)_{true}}$$



Chemical Models

Devolatilization:	Biomass $\rightarrow$ light gas (CO, CO_2, H_2, CH_4) + tar + char + H_2O
Tar reaction:	Tar (g) $\rightarrow$ light gas (CO+ CO_2 + H_2 + CH_4 + H_2O) + inert Tar
Volatile reaction:	
Carbon monoxide oxidation	$CO + 1/2\ O_2 \rightarrow CO_2$
Hydrogen oxidation	$H_2 + 1/2\ O_2 \rightarrow H_2O$
Methane oxidation	$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$
Water-gas shift	$CO + H_2O \leftrightarrow CO_2 + H_2$
Char combustion	
Partial combustion	$C + 1/2\ O_2 \rightarrow CO$
Char gasification:	
Boudouard reaction	$C + CO_2 \rightarrow 2\ CO$
Steam gasification	$C + H_2O \rightarrow CO + H_2$
Hydrogen gasification	$C + 2\ H_2 \rightarrow CH_4$

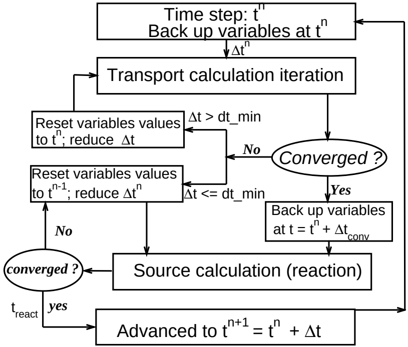
- Reaction rate based on **min**[$k = exp[-E/RT], C(2\bar{S}_{ij}\bar{S}_{ij})^{1/2}$]

Implementation in MFIX-Continuum

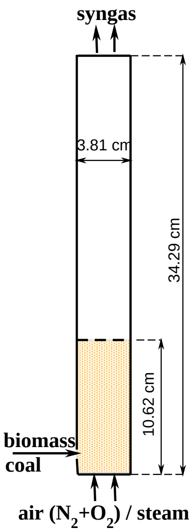
- Time-splitting approach coupling hydrodynamics and kinetics

$$\phi(t) \xrightarrow{\text{transport}} \phi^*(t+\Delta t) \xrightarrow{\text{chemical reaction}} \phi(t+\Delta t)$$

- Synchronized time-step for transport and reaction



A Lab-scale Fluidized-bed Reactor



Simulation Conditions

Phase	Species (n)	X_n	T (K)	ϵ_g, ϵ_{sm} bed, freeboard	ρ_{true} (g/cm^3)	d (cm)
gas (g)	N_2	1	1123	0.41, 1	EOS[a]	-
	O_2	0				
	light gas[b]	0				
	tar[c]	0				
solid ($s1$)	sand	1	1123	0.59, 0	2.649	0.05
solid ($s2$)	biomass[d]	1	300	0, 0	0.585	0.05
	moisture	0			0.649	
	char	0			0.45	
	ash	0			0.45	
	void	0			same as gas	

[a] quation of state for an ideal gas

[b] includes CO, CO_2, H_2O, H_2, CH_4

[c] includes active tar and inert tar

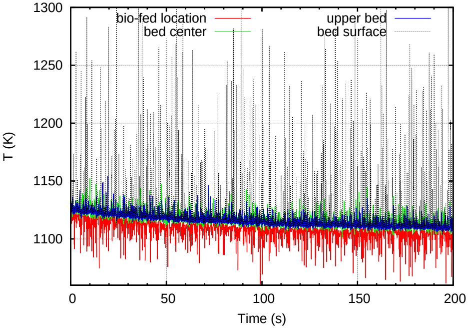
[d] air fuel ratio ($\dot{m}_{air}/\dot{m}_{biomass}$) is 1.5

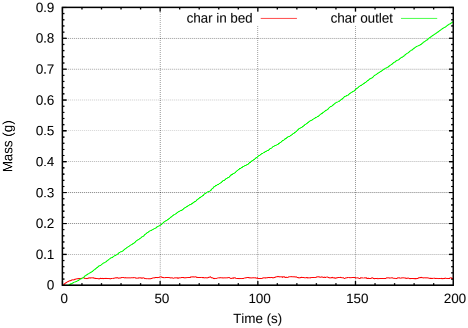
Simulation Cases

Cases	air/biomass ratio	biomass moisture (wt%)
	0.4	0
	0.8	0
base	1.5	0
	2.1	0
	1.5	15
	1.5	25

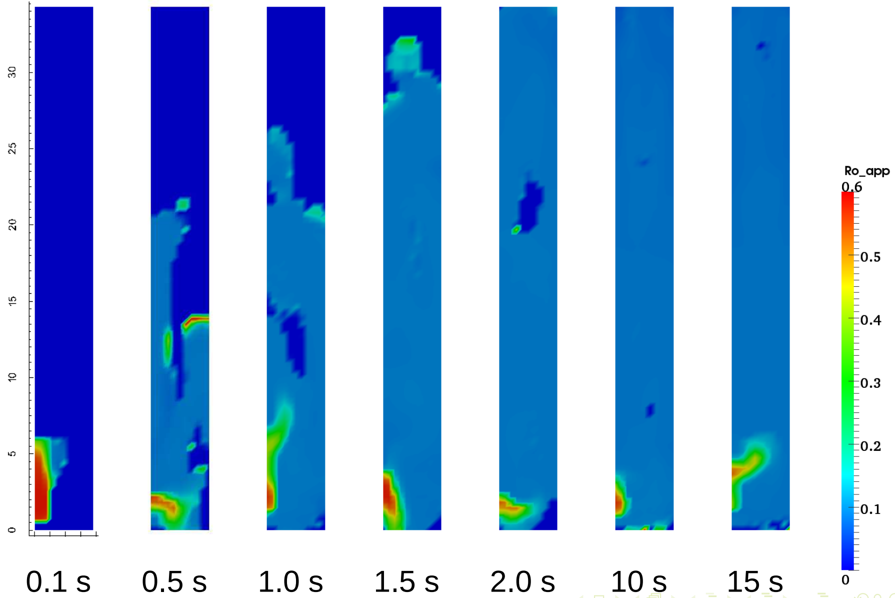
Convergency History

- Gas Temperature and mass inside reactor

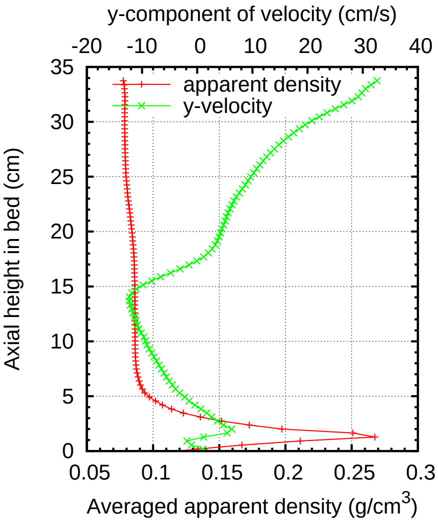


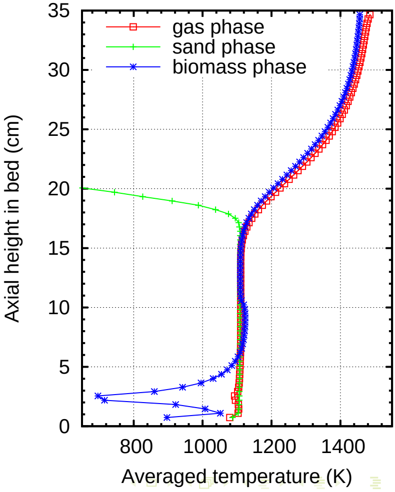


Biomass Apparent Density

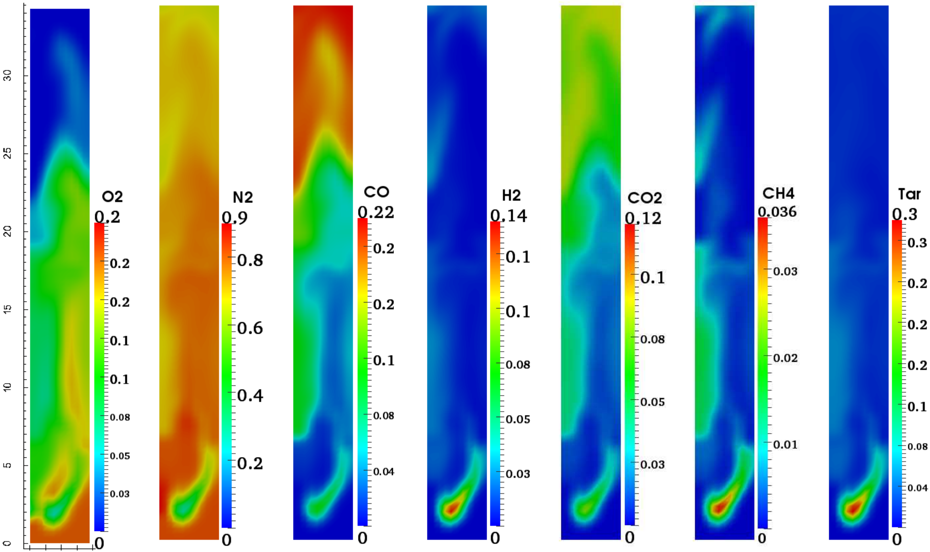


Time- and Spatial-Averaged Density and Temperature (160-200 s)



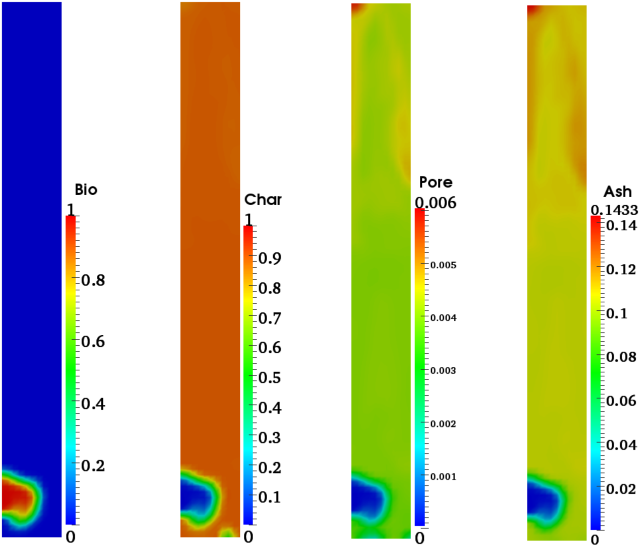


Gas Molar Fraction @180 s



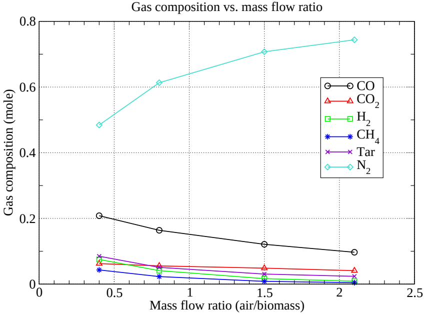
O_2 N_2 CO H_2 CO_2 CH_4 Tar

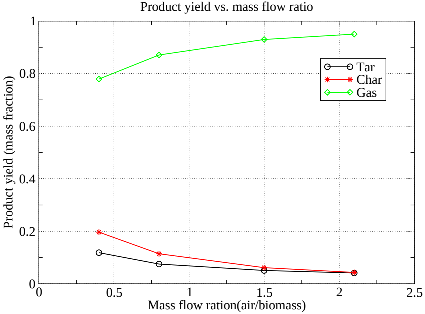
Biomass Mass Fraction @180 s



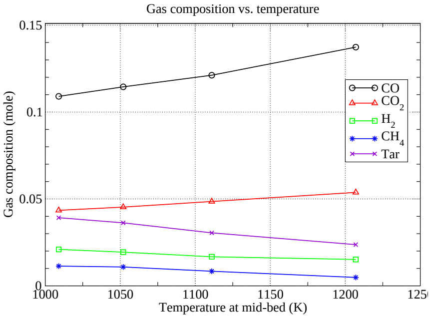
Bio Char Pore Ash

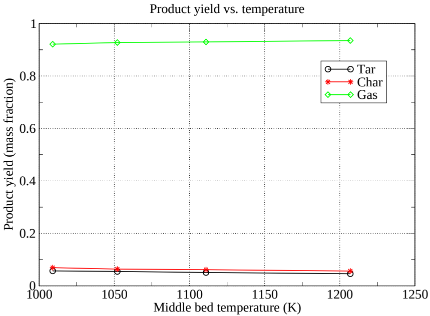
Mass Flow Ratio (Air/Biomass)



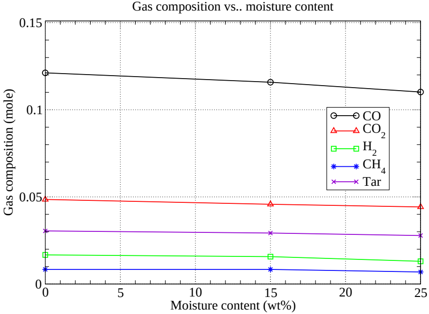


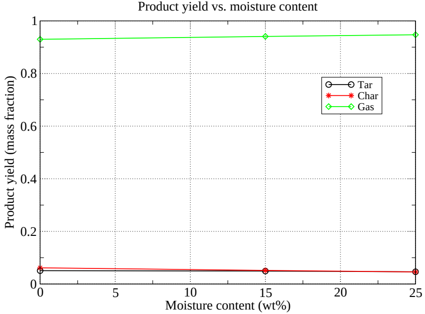
Bed Temperature





Moisture Content





Summary

- Variable particle density implemented for modeling bio-particle transport
- Biomass (wood) gasification kinetics implemented
- The model captures the key features of gasification
- Different conditions tested

Acknowledgement

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