An open-source one-dimensional model for bubbling fluidized bed reactors

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Workshop on Multiphase Flow Science

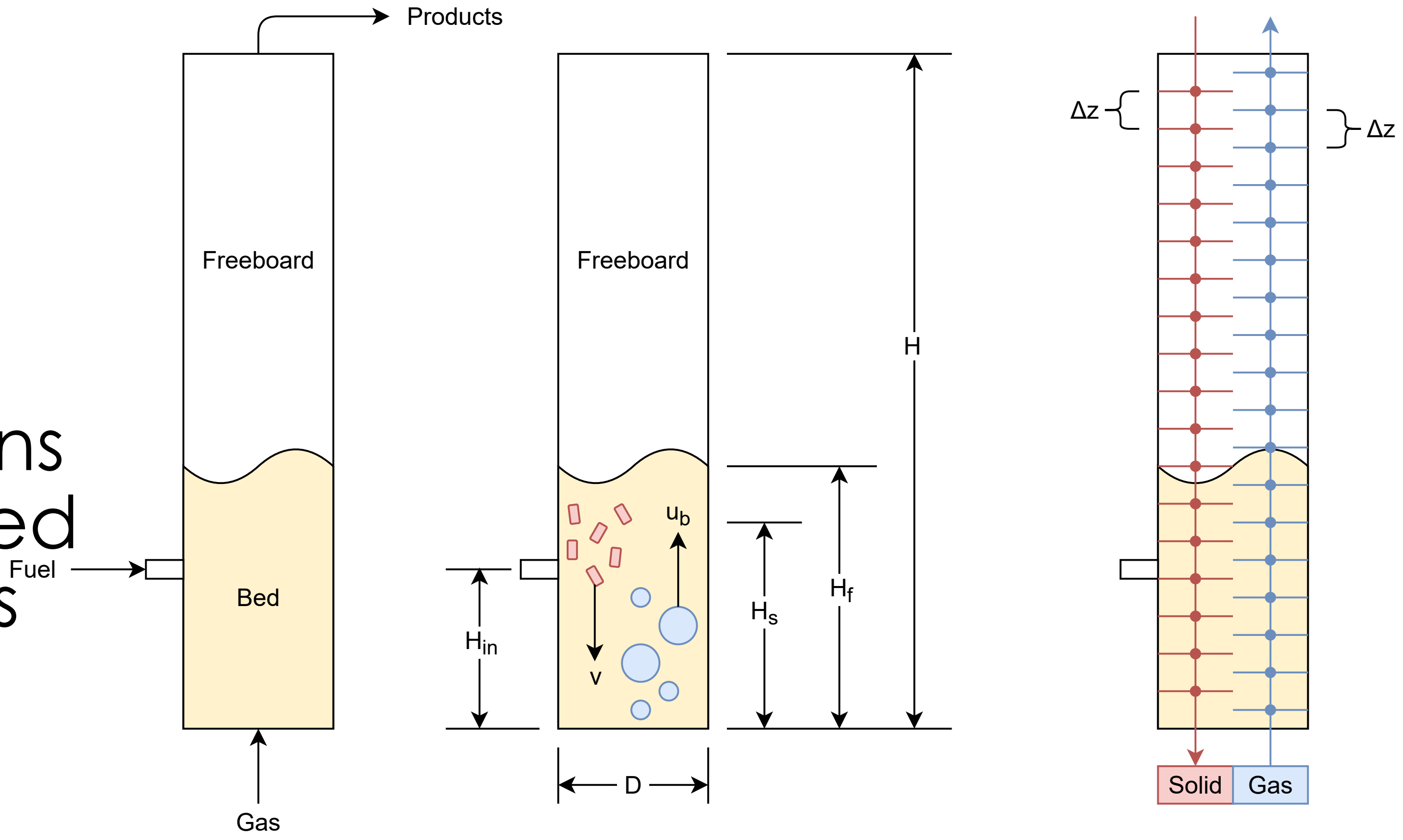
Tuesday, August 3, 2021

Motivation

- Complex hydrodynamic and multiphase characteristics of fluidized bed reactors require expensive and time-consuming resources for CFD/DEM simulations
- Reduced-order models produce efficient results in a timely manner for parameter sweeps, sensitivity analysis, and practical applications
- Open-source code is not available for the abundance of reduced-order models discussed in scientific literature [see refs]
- Scientists and designers must “reinvent the wheel” and develop their own code instead of contributing to existing projects

1D fluidized bed model development

- Fuel inlet defined as distance H_{in} from reactor bottom
- Solid (fuel) particles exhibit downward motion while gas moves upward
- Separate grid for gas and solid phase calculations
- Bed height (H_f) calculations consider static (H_s) and bed voidage at fluidized states
- Net velocity of inert bed particles is considered zero
- No variations in radial direction



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Momentum and energy balance

Solid phase (fuel) momentum

$$\rho_s \frac{\partial v}{\partial t} = -\rho_s v \frac{\partial v}{\partial t} + g\left(\rho_s - \rho_g\right) + F_B' + \beta_{gs}(-u - v) + \beta_{ps}(-v) + v\sum S_{sj}$$

Gas phase momentum

$$\frac{\partial \dot{m}_g}{\partial t} = -\frac{\partial\left(\dot{m}_g \cdot u\right)}{\partial z} + g\left[\epsilon_f\left(1 - \epsilon_f\right)\rho_p - \overline{\rho_g}\right] - \alpha_s \beta_{gs}(-u - v) - \frac{2 f_g \overline{\rho_g}}{D} u \cdot |u| - u\left(\beta_{gp} - \sum S_{gj}\right) - \epsilon_f \frac{dp}{dz}$$

Solid phase (fuel) energy balance

$$\overline{\rho}_s \overline{c}_{ps} \frac{\partial T_s}{\partial t} = -\overline{\rho}_s \overline{c}_{ps} v \frac{\partial T_s}{\partial z} + \frac{6}{d_s} \alpha_s \left[h_{gs}\left(T_g - T_s\right) + \epsilon_s \sigma\left(T_p^4 - T_s^4\right)\right] + h_{ps}\left(T_p - T_s\right) - \left(\sum r_i \Delta H_{ri} + r_{pyr} \Delta H_{pyr}\right)$$

Gas phase energy balance

$$\overline{\rho}_g \overline{c}_{pg} \frac{\partial T_g}{\partial t} = -\overline{\rho}_g \overline{c}_{pg} u \frac{\partial T_g}{\partial t} - \frac{6}{d_s} \alpha_s h_{gs}\left(T_g - T_s\right) - \frac{6}{\phi_p d_p} \alpha_p h_{gp}\left(T_g - T_p\right) - \frac{4}{D} U_a\left(T_g - T_a\right) - \sum\left(r_i \Delta H_{ri}\right)$$

Mass balance and reaction mechanisms

- Concentrations (ρ) are mass based and determined within each discretized volume along the reactor height

Pyrolysis: biomass → volatiles; biomass → tar → volatiles; biomass → char

Solid phase mass balance where j is biomass or char

$$\frac{\partial \bar{\rho}_{sj}}{\partial t} = -\frac{\partial \left(v\bar{\rho}_{sj}\right)}{\partial z} + S_{sj}$$

Gas phase mass balance where j is CH_4, CO, CO_2, H_2, or H_2O

$$\frac{\partial \bar{\rho}_{gj}}{\partial t} = -\frac{\partial \left(y_j \dot{m}_g\right)}{\partial z} + S_{gj} \quad \text{where} \quad y_j = \frac{\bar{\rho}_{gj}}{\bar{\rho}_g}$$

$$\frac{\partial \bar{\rho}_g}{\partial t} = -\frac{\partial \dot{m}_g}{\partial t} + \sum S_{gj}$$

Gasification:

$C + H_2O \rightarrow CO + H_2$

$C + CO_2 \rightarrow 2CO$

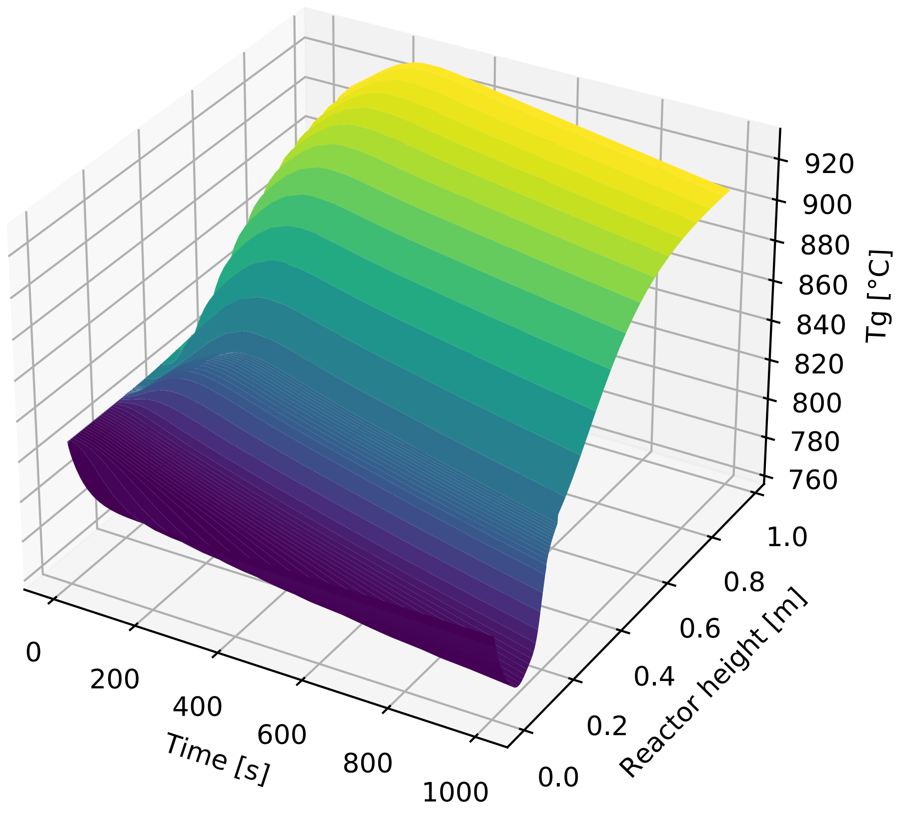
$C + 2H_2 \rightarrow CH_4$

$CO + H_2O \leftrightarrow CO_2 + H_2$

$CH_4 + H_2O \rightarrow CO + 3H_2$

Gasification results

Parameter	Value
Total grid points	100
Initial solid temperature	300 K
Initial gas temperature	1100 K
Gas inlet temperature	1073 K
Bed diameter	0.1 m
Overall reactor height	1 m
Fuel feeding position	0.212 m
Diameter raw biomass particle	6 mm
Sphericity of bed particle	0.72
Diameter of bed particle	0.6 mm
Mass flow rate of biomass	2 kg/hr
and many more...	



Gas temperature (Tg) along reactor height for 1,000 seconds.

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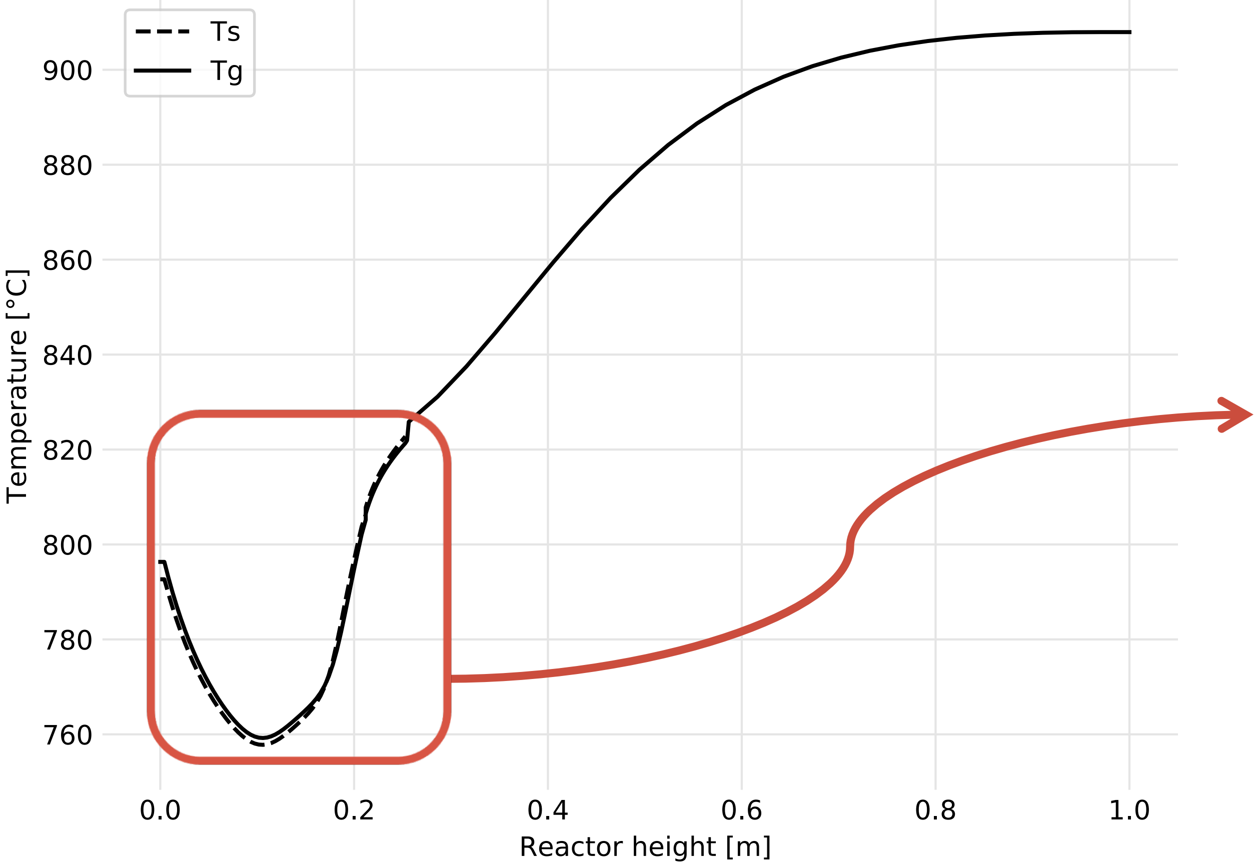
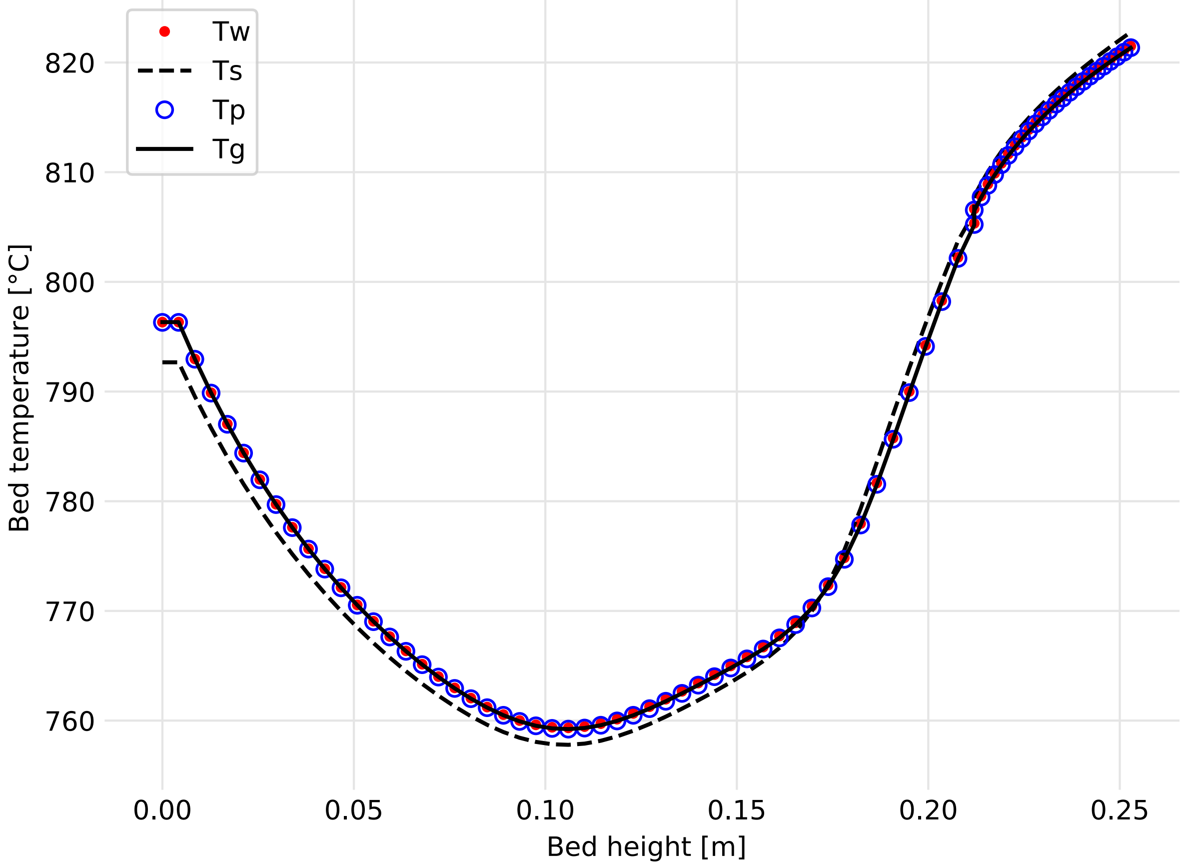
Gasification results

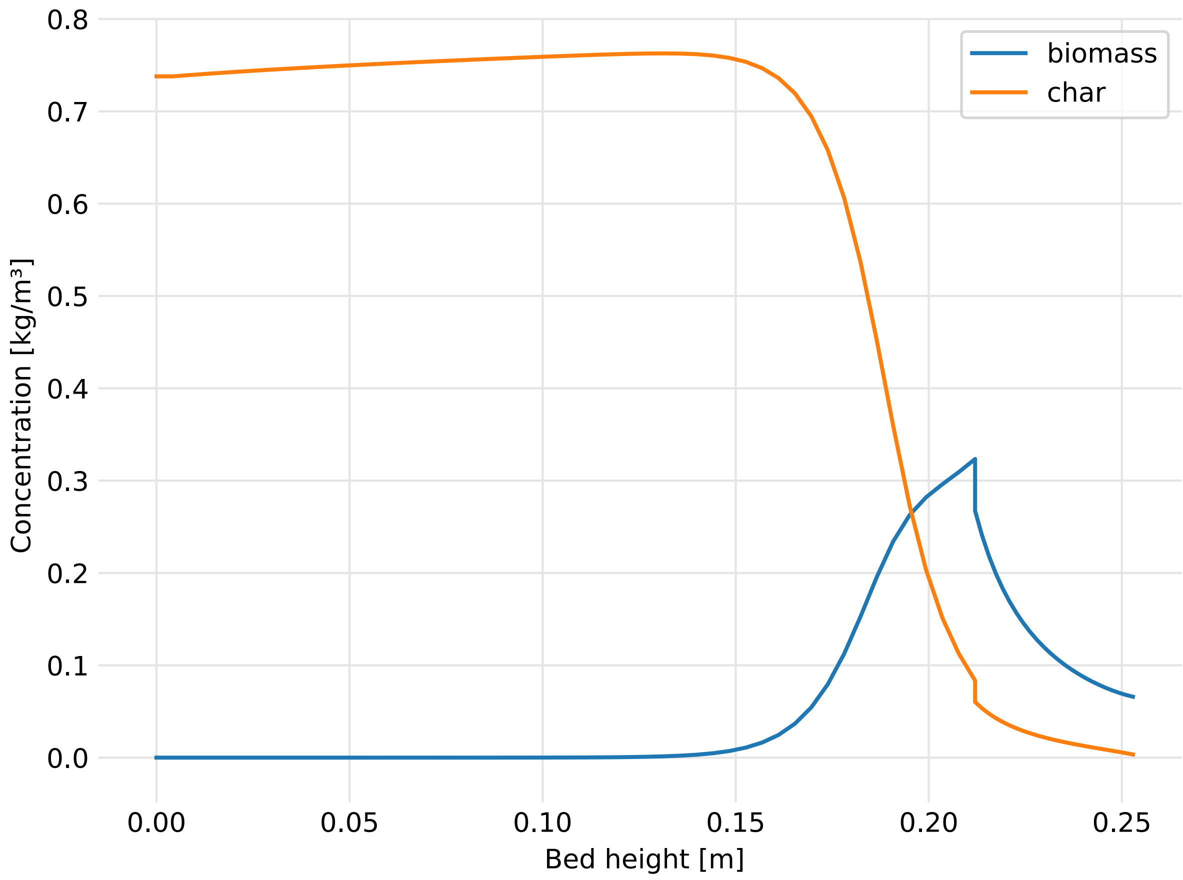


Solid fuel (T_s) and gas (T_g) temperature along reactor at 1,000 s.

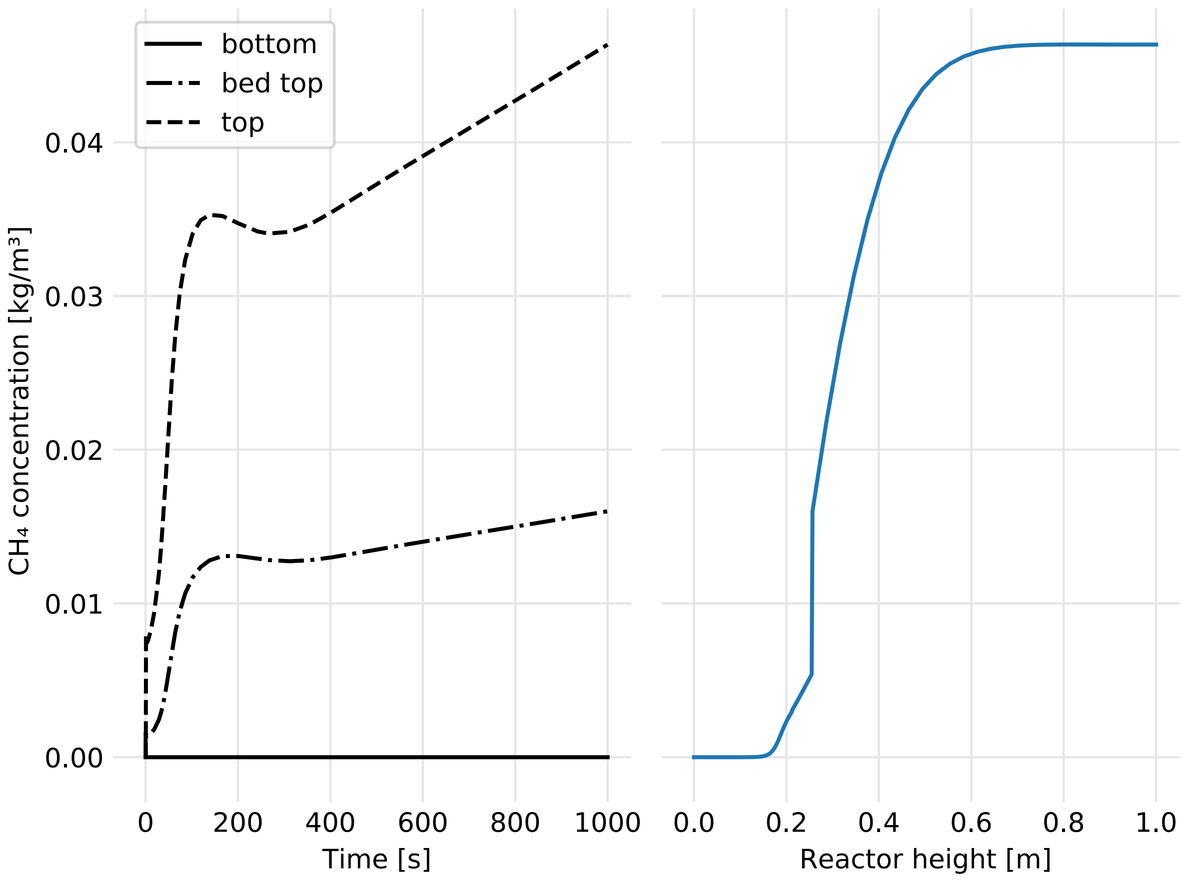


Wall (T_w), solid (T_s), bed (T_p), and gas (T_g) temperatures in the bed at 1,000 s.

Gasification results

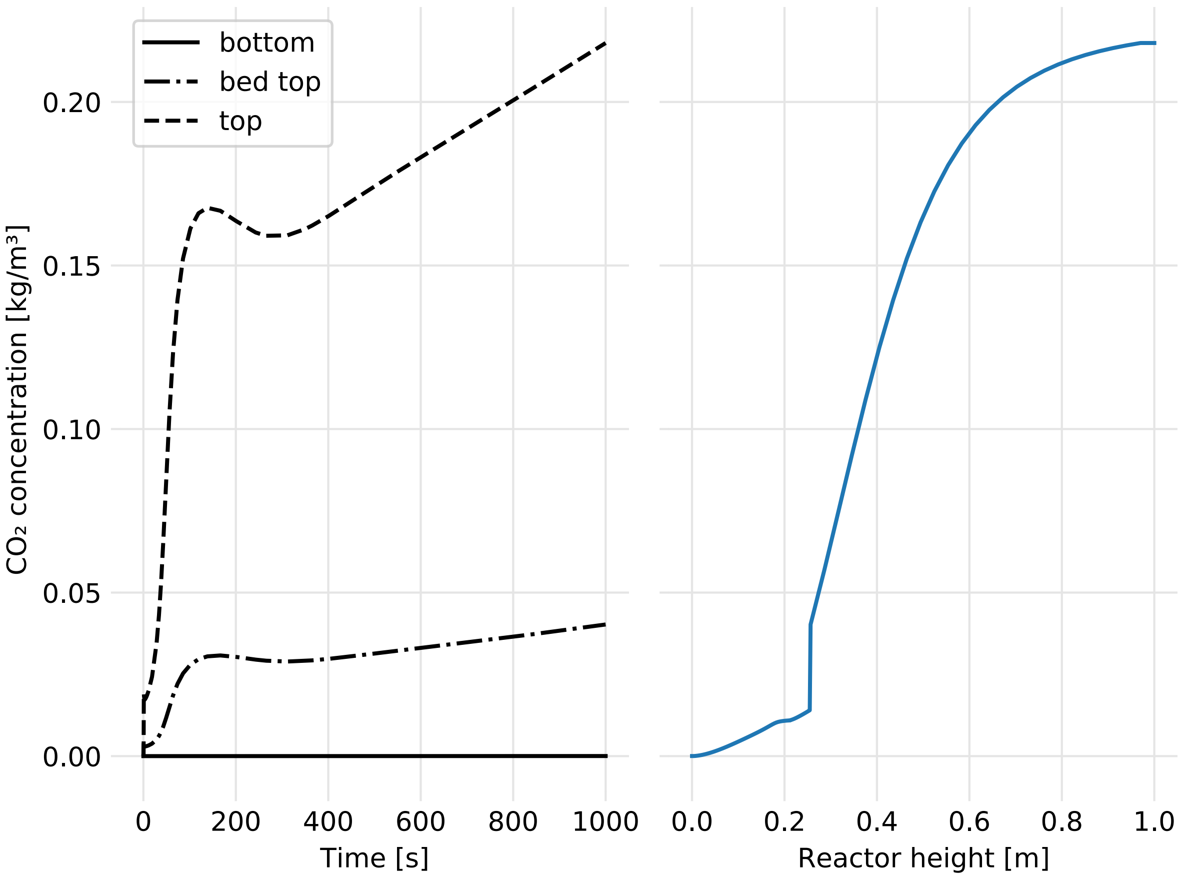


Char and biomass concentrations in the reactor bed at 1,000 s.

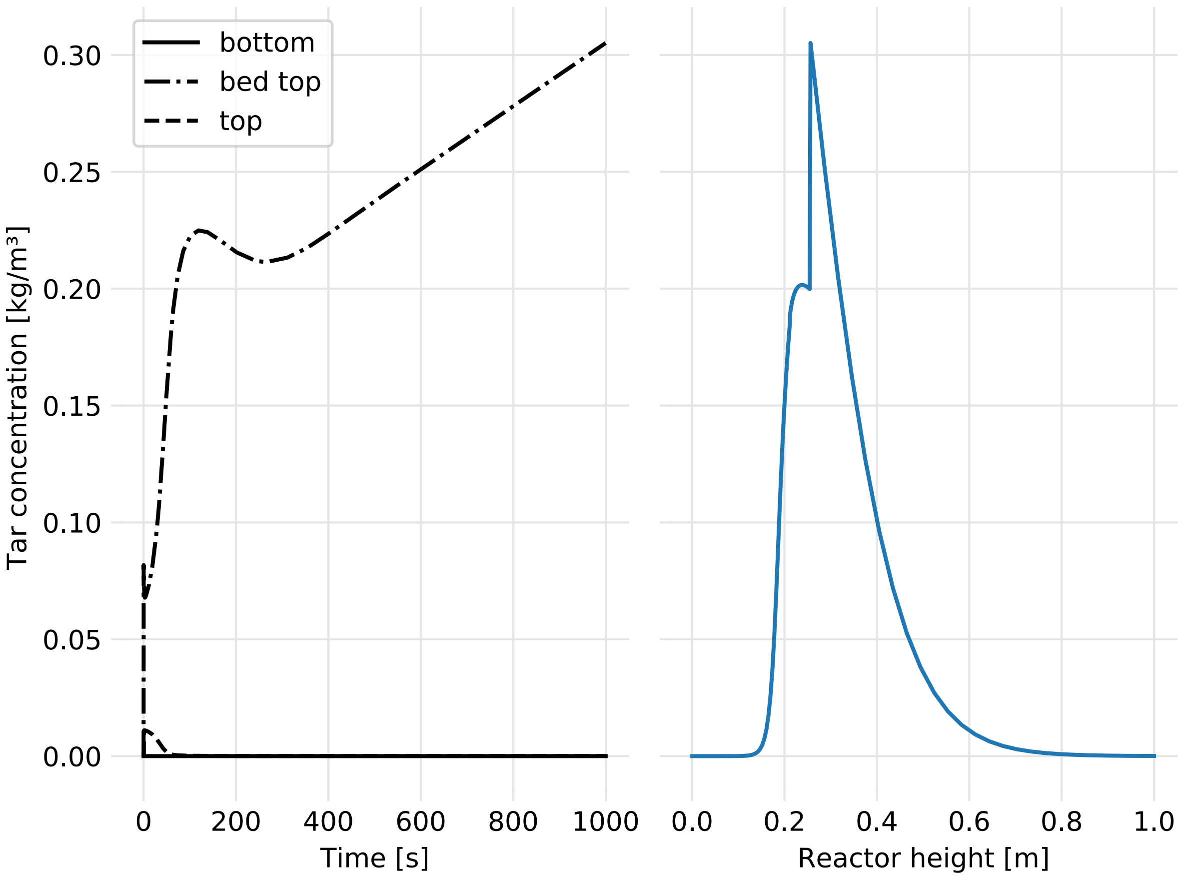


Methane concentration at bed top, reactor bottom, and reactor top (left). Methane concentration along reactor at 1,000 s (right).

Gasification results



Carbon dioxide concentration at bed top, reactor bottom, and reactor top (left). Carbon dioxide concentration along reactor at 1,000 s (right).



Tar concentration at the bed top, reactor bottom, and reactor top (left). Tar concentration along reactor at 1,000 s (right).

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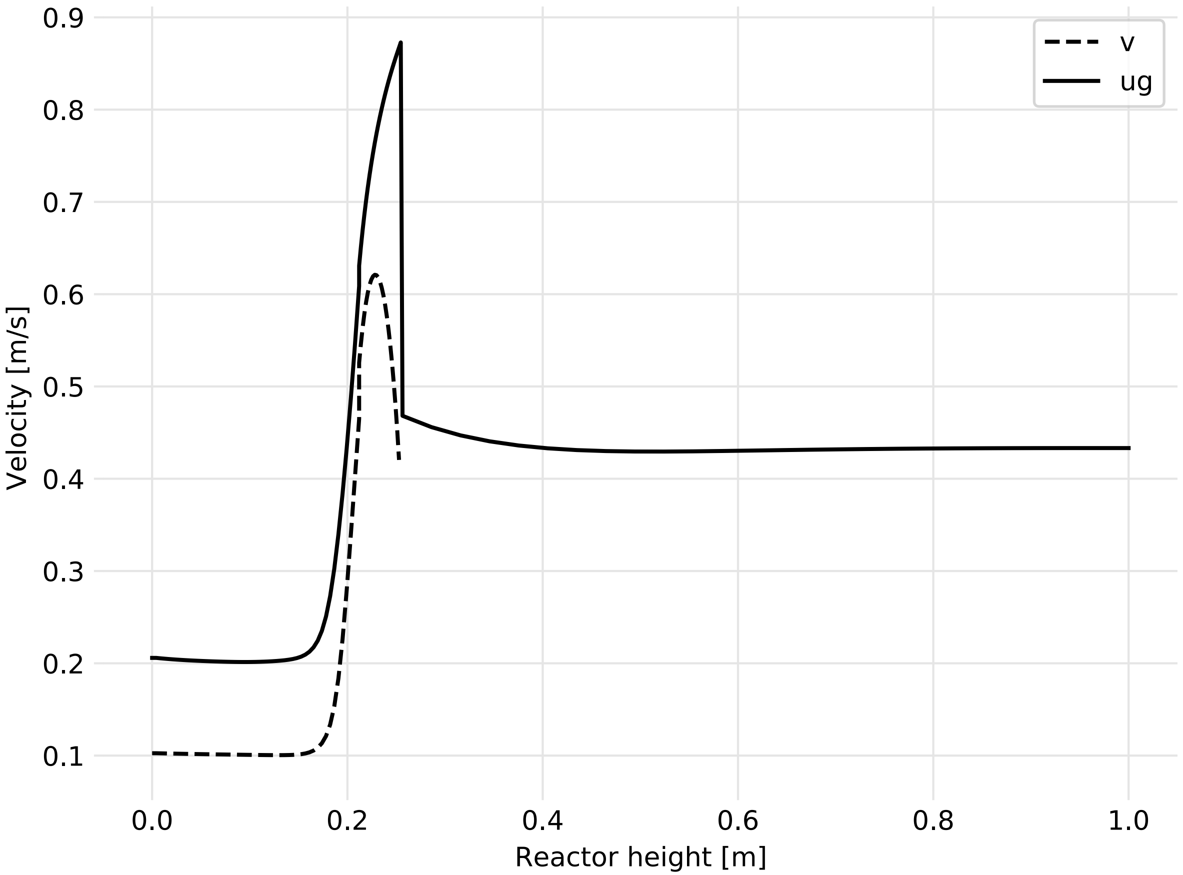
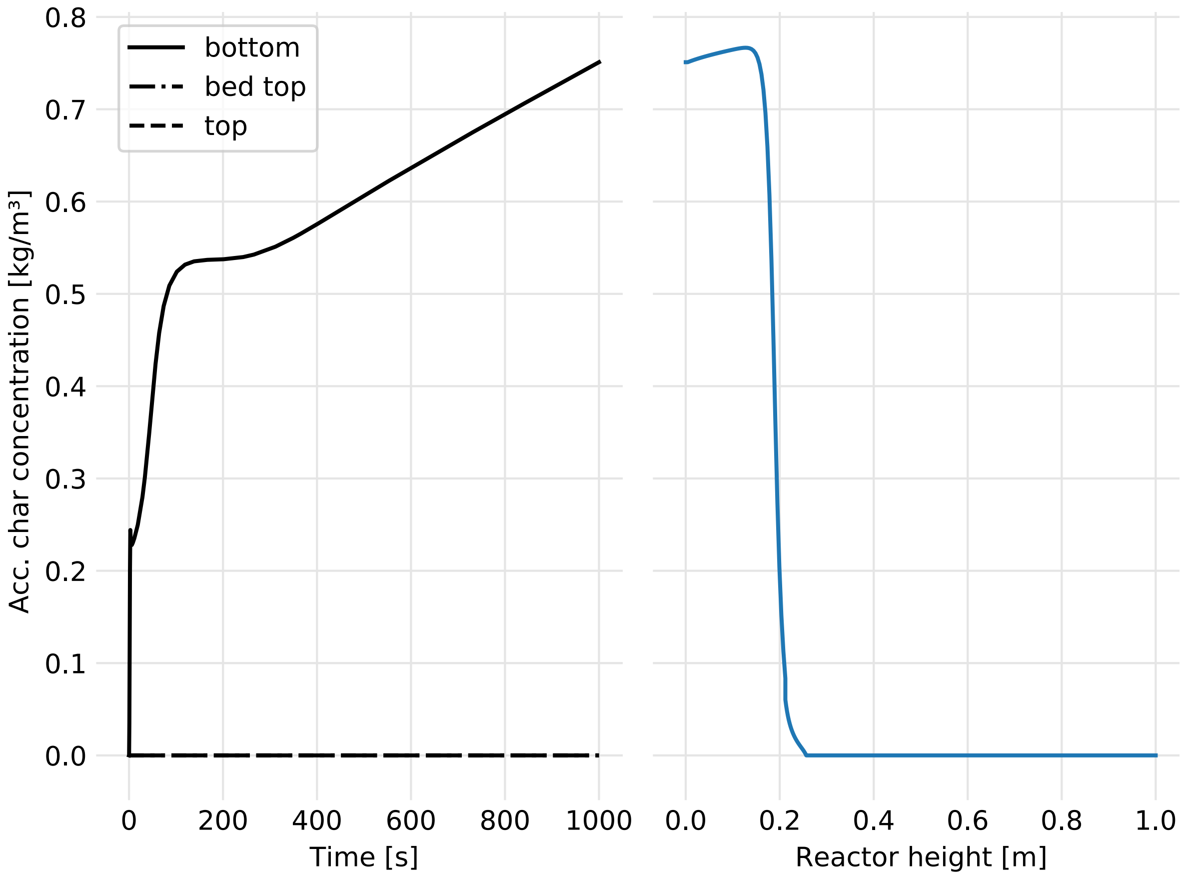
Gasification results



Solid fuel velocity (v) and gas velocity (u) along the reactor at 1,000 s.



Char concentration at the bed top, reactor bottom, and reactor top (left). Char concentration in the reactor at 1,000 s (right).

Next steps

- Release documentation for model equations and code
- Submit code to Journal of Open Source Software (JOSS) https://joss.theoj.org
- Implement pyrolysis (in the works) and combustion features
- Validate model results with experimental data
- Investigate ODE solvers for better performance, currently using SciPy Radau solver (implicit Runge-Kutta)
- Develop fully discretized solution to eliminate dependence on ODE solvers

How to contribute

- Write documentation
- Develop unit tests
- Submit examples and validate with experiments
- Improve existing code base
- Submit issues and feature requests

Python code, examples, and documentation are open source and available on GitHub.

https://github.com/wigging/bfb-reactor

References

See Agu 2019 for more information about the 1D model

1. Cornelius Agu, Christoph Pfeifer, Marianne Eikeland, Lars-Andre Tokheim, and Britt Moldestad. "Detailed One-Dimensional Model for Steam-Biomass Gasification in a Bubbling Fluidized Bed." Energy & Fuels, no. 8, vol. 33, pp. 7385-7397, 2019.

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3. Jannike Solsvik, Zhongxi Chao, and Hugo Jakobsen. "Modeling and simulation of bubbling fluidized bed reactors using a dynamic one-dimensional two-fluid model: The sorption-enhanced steam-methane reforming process." Advances in Engineering Software, vol. 80, pp. 156-173, 2015.

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5. Priyanka Kaushal, Jalal Abedi, and Nader Mahinpey. "A comprehensive mathematical model for biomass gasification in a bubbling fluidized bed reactor." Fuel, vol. 89, no. 8, pp. 3650-3661, 2010.