

BFB reactor model

Gavin Wiggins and Cornelius Agu

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1 Introduction

This documentation is for the one-dimensional bubbling fluidized bed (BFB) reactor model developed in Python. The model predicts dynamic and steady-state conditions of a BFB reactor. See the sections below for installation and usage information along with discussions of the equations that are utilized by the model. The Python code for the model is open source and available on GitHub at <https://github.com/wigging/bfb-reactor>. An online version of this documentation is hosted at <https://gavinw.me/bfb-reactor/>. This work is inspired by the one-dimensional gasification model published by Agu et al. [1].

2 Installation

A recent version of Python 3 is needed to run the BFB reactor model. The following Python packages are also required: NumPy, SciPy, and Matplotlib. The [Anaconda](#) distribution of Python is recommended for Mac, Linux, and Windows operating systems.

3 Usage

Use the commands shown below to run each model from the terminal.

```
# Run the dynamic model  
$ python dynamic examples/params.json --run
```

```
# Plot results from the dynamic model
$ python dynamic examples/params.json -plot

# Run the steady-state model
$ python steady
```

4 Constants

This section provides equations for the various constants calculated by the model. The dimensionless Archimedes number is calculated as shown in Equation 1.

$$Ar = \frac{d_p^3 \rho_g (\rho_p - \rho_g) g}{\mu^2} \quad (1)$$

5 Reactor configuration

Inlet/outlet flows and geometry of the reactor applicable to the BFB model are shown in Figure 1. Fuel (feedstock) enters at the side of the reactor while the fluidization gas enters at the bottom of the reactor. Products leave at the top of the reactor. The following distance or height parameters from the reactor bottom are utilized by the model: overall reactor height (H), total fluidized bed height (H_f), static bed height (H_s), and distance to the fuel inlet (H_{in}). Also shown in Figure 1 is the staggered grid used by the model for the solid and gas phases. Solid fuel particles are assumed to move in a downward direction while gas moves in an upward direction. Distance between node points on the grid is represented by Δz .

6 Reaction kinetics

The kinetic scheme implemented by the model for biomass pyrolysis is shown in Figure 2. Biomass is the fuel (feedstock) fed to the reactor while volatiles, char, and tar are the pyrolysis products. The kinetic rate constant k for each of the pyrolysis reactions are an Arrhenius form as depicted by Equation 2.

$$k = A \exp\left(-\frac{E}{RT}\right) \quad (2)$$

The steam-biomass gasification reactions and associated rate parameters are given below in Table 1. Molar concentration is represented by $[]$ in mol/m^3 , pressure is p in Pa, and X_c is the char conversion factor. The reaction enthalpy is given as ΔH in kJ/mol and the rate constant r is in $\text{mol}/(\text{m}^3 \cdot \text{s})$.

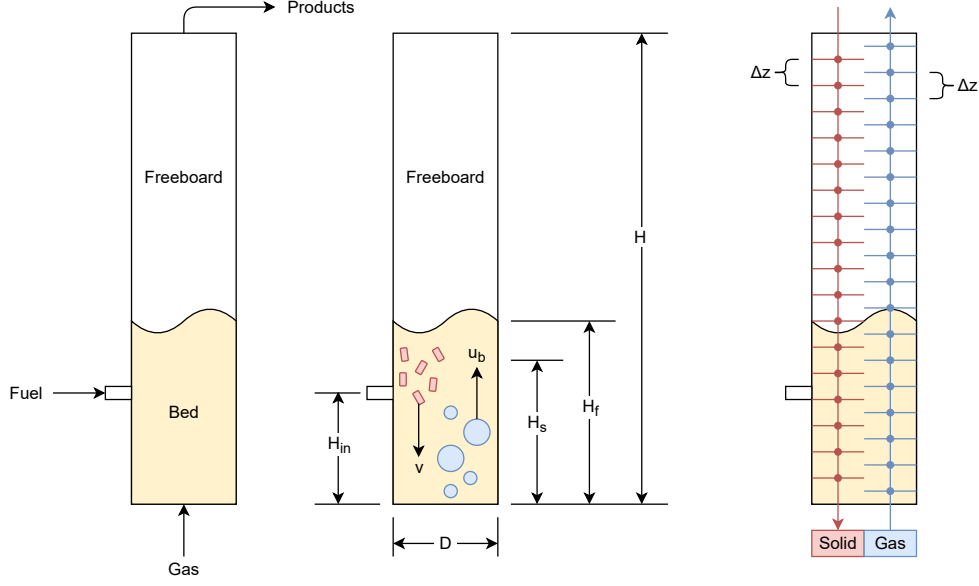


Figure 1: Inlet and outlet flows (left), geometry parameters (center), and one-dimensional grid (right) for the BFB reactor model.

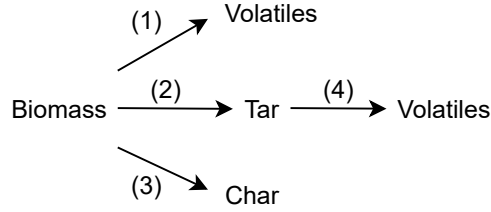


Figure 2: Primary and secondary reactions for biomass pyrolysis.

7 Chemical species mass balance

The rate of change for the solid concentration in a given volume is described by Equation 3. Similarly, the mass balance for each gas species is given by Equation 4 while the gas mixture concentration is given by Equation 5.

$$\frac{\partial \bar{\rho}_{s,j}}{\partial t} = -\frac{\partial(v\bar{\rho}_{s,j})}{\partial z} + S_{s,j} \quad (3)$$

$$\frac{\partial \bar{\rho}_{g,j}}{\partial t} = -\frac{\partial(y_j \dot{m}_g)}{\partial z} + S_{g,j} \quad \text{where} \quad y_j = \frac{\bar{\rho}_{g,j}}{\rho_g} \quad (4)$$

$$\frac{\partial \bar{\rho}_g}{\partial t} = -\frac{\partial \dot{m}_g}{\partial z} + \sum S_{g,j} \quad (5)$$

Table 1: Steam-biomass gasification reactions and rate parameters.

| Item | Reaction | ΔH | Rate constant | Ref. |
|------|--|------------|---|------|
| 5 | $C + H_2O \rightarrow CO + H_2$ | 131 | $r_5 = \frac{k_{5,1}x_{H_2O}}{1/p + k_{5,2}x_{H_2} + k_{5,3}x_{H_2O}}(1 - X_c)[C]$ $k_{5,1} = 1.25 \times 10^5 \exp\left(-\frac{28,000}{T}\right)$ $k_{5,2} = 3.26 \times 10^{-4}$ $k_{5,3} = 0.313 \exp\left(-\frac{10,120}{T}\right)$ | x |
| 6 | $C + CO_2 \rightarrow 2 CO$ | 172 | $r_6 = \frac{k_{6,1}}{1 + \frac{x_{CO}}{k_{6,2}x_{CO_2}}}[C]$ $k_{6,1} = 3.6 \times 10^5 \exp\left(-\frac{20,130}{T}\right)$ $k_{6,2} = 4.15 \times 10^3 \exp\left(-\frac{11,420}{T}\right)$ | x |
| 7 | $C + 2H_2 \rightarrow CH_4$ | -75 | $r_7 = 6.11 \times 10^{-3} \exp\left(-\frac{80,333}{RT}\right)[H_2][C]$ | x |
| 8 | $CO + H_2O \leftrightarrow CO_2 + H_2$ | -41 | $r_8 = 0.278 \exp\left(-\frac{12,560}{RT}\right) \left([H_2O][CO] - \frac{[H_2O][CO]}{k_8} \right)$ $k_8 = 0.022 \exp\left(\frac{34,730}{RT}\right)$ | x |
| 9 | $CH_4 + H_2O \rightarrow CO + 3H_2$ | 206 | $r_9 = 312 \exp\left(-\frac{15,098}{T}\right)[CH_4]$ | x |

8 Fluidization

This section presents equations used to estimate the fluidized state of the BFB reactor. Equations are provided for the bed expansion and minimum fluidization velocity. The current version of the model neglects the effect of the unconverted fuel on the fluidization behavior.

8.1 Minimum fluidization velocity

The minimum fluidization velocity is determined by Equation 6 which relies on Equation 7 for the Reynolds number at minimum fluidization conditions [7].

$$U_{mf} = \frac{Re_{mf} \mu}{\rho_g d_p} \quad (6)$$

$$Re_{mf} = \sqrt{(33.7)^2 + 0.0408 Ar} - 33.7 \quad (7)$$

8.2 Bed expansion

The expanded bed height is estimated using several correlations as defined in this section. The correlations consider bubbling as well as slugging conditions that can occur in the reactor. Correlated parameters a_b and c_b for the bubbling regime are given below while the slugging regime is represented by a_s and c_s . Notice that \log represents the base 10 logarithm [3].

$$a_b = \phi^{1.5}(4.168 - 1.389 \log(Ar)) \quad \log(Ar) < 3.5 \quad (8)$$

$$a_b = \phi^{1.5}(0.329 - 1.156 \times 10^3 Ar^{-0.9}) \quad \log(Ar) \geq 3.5 \quad (9)$$

$$c_b = (1.321 + 8.161 \times 10^4 Ar^{-1.04})^{0.083} \quad \log(Ar) > 0 \quad (10)$$

$$a_s = 0.725 + 0.230 \log(Ar) \quad \log(Ar) < 3.9 \quad (11)$$

$$a_s = 1.184 + 8.962 \times 10^4 Ar^{-1.35} \quad \log(Ar) \geq 3.9 \quad (12)$$

$$c_s = 0.042 + 0.108 \log(Ar) \quad \log(Ar) < 4.0 \quad (13)$$

$$c_s = (0.978 - 1.964 \times 10^2 Ar^{-0.8})^{4.88} \quad \log(Ar) \geq 4.0 \quad (14)$$

When calculating the expanded bed height, the maximum bubble diameter in the bed is restricted by the reactor's bed diameter. This is accounted for by the maximum bubbling diameter to bed diameter ratio at the transition to slugging defined by Equations 15 and 16 where $c_t = c_b/c_s$ and $a_t = 1/(a_s - a_b)$ [4].

$$\left(\frac{\bar{d}_b}{D}\right)_{\max} = \min\left(1, \left(\frac{\bar{d}_b}{D}\right)_{\text{bs}}\right) \quad (15)$$

$$\left(\frac{\bar{d}_b}{D}\right)_{\text{bs}} = 0.848 \left(\frac{U_{mf} \phi^{0.35} c_t^{a_t}}{D}\right)^{0.66} \left[1 - c(\phi^{0.35} c_t^{a_t})^{a-1}\right]^{0.66} \quad (16)$$

The bubble diameter to bed diameter ratios (\bar{d}_b/D) in Equations 17 and 18 are selected based on the Archimedes number [2, 8]. Similarly, the minimum slugging velocity to fluidization ratios (U_{ms}/U_{mf}) in Equations 19 and 20 are also related to the Archimedes number [3, 6].

$$\frac{\bar{d}_b}{D} = 0.848 \left(\frac{U_s}{D} \right)^{0.66} \left[1 - c \left(\frac{U_s}{U_{mf}} \right)^{a-1} \right]^{0.66} \quad \text{for } Ar > 400 \quad (17)$$

$$\frac{\bar{d}_b}{D} = \frac{5.64 \times 10^{-4}}{D H_{mf}} \left[1 + 27.2(U_s - U_{mf}) \right]^{1/3} \left[(1 + 6.84 H_{mf})^{2.21} - 1 \right] \quad \text{for } Ar < 400 \quad (18)$$

$$\frac{U_{ms}}{U_{mf}} = 1 + 2.33 U_{mf}^{-0.027} \left(\phi^{0.35} c_t^{a_t} - 1 \right) \left(\frac{H_0}{D} \right)^{-0.588} \quad \text{for } Ar > 400 \quad (19)$$

$$\frac{U_{ms}}{U_{mf}} = \left(e^{-0.5405 \frac{H_0}{D}} \right) \left(\frac{4.294 \times 10^3}{Ar} + 1.1 \right) + 3.676 \times 10^2 Ar^{-1.5} + 1 \quad \text{for } Ar < 400 \quad (20)$$

The total bed height is based on the bed expansion estimated from the fluidized height and the minimum fluidized height as depicted by Equation 21 shown below. When $\bar{d}_b/D < (\bar{d}_b/D)_{max}$ then the bed expansion is calculated based on bubbling conditions using Equation 22. During slugging conditions, the bed expansion considers the maximum height of the bed in terms of the bed expansion ratio Δe_r as seen in Equation 23 where the height ratios are given in Equations 24 and 25. Finally, Equations 26, 27, and 28 are used to determine the total bed height during fluidization [5, 1, 4, 7].

$$\Delta e = \frac{H_f - H_{mf}}{H_{mf}} = \frac{H_f}{H_{mf}} - 1 \quad (21)$$

$$\Delta e = \left[1 - 0.103(U_s - U_{mf})^{-0.362} \left(\frac{\bar{d}_b}{D} \right) \right]^{-1} - 1 \quad (22)$$

$$\Delta e = \Delta e_r - 1 = \left(\frac{H_{max}}{H_{mf}} \right) \left(\frac{H_f}{H_{max}} \right) - 1 \quad (23)$$

$$\frac{H_{max}}{H_{mf}} = \left[1 - 0.103(U_{ms} - U_{mf})^{-0.362} \left(\frac{\bar{d}_b}{D} \right) \right]^{-1} \quad (24)$$

$$\frac{H_f}{H_{max}} = \left[1 - 0.305(U_s - U_{mf})^{-0.362} D^{0.48} \right]^{-1} \quad (25)$$

$$H_f = H_{mf}(\Delta e + 1) \quad (26)$$

$$H_{mf} = \frac{1 - \epsilon_0}{1 - \epsilon_{mf}} H_0 \quad (27)$$

$$\epsilon_{mf} = \left(\frac{0.071}{\phi} \right)^{1/3} \quad \text{where } \epsilon_{mf} = \max(\epsilon_{mf}, \epsilon_0) \quad (28)$$

8.3 Bubble characteristics

Here for bubble rise velocity u_B in ref Agu 2019b Equation 22.

Here for bubble volumetric flux V_B in ref Agu 2018 Equation 17.

Nomenclature

| | |
|-----------------|---|
| Δe | dimensionless bed expansion [-] |
| ϵ_0 | initial or static bed void fraction [-] |
| ϵ_{mf} | bed void fraction at minimum fluidization [-] |
| μ | dynamic gas viscosity [Pa·s] |
| \bar{d}_b | average bubble diameter [m] |
| ϕ | bed particle sphericity [-] |
| Ar | Archimedes number [-] |
| D | bed diameter [m] |
| d_p | bed particle diameter [m] |
| H_0 | initial or static bed height [m] |
| H_f | total fluidized bed height [m] |
| H_{mf} | bed height at minimum fluidization [m] |
| Re | Reynolds number [-] |
| U_s | superficial gas velocity [m/s] |
| U_{mf} | minimum fluidization velocity [m/s] |
| U_{ms} | minimum slugging velocity [m/s] |

References

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