

BFB reactor model

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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 and usage

A recent version of Python 3 is required 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. After installing Python and the required packages, download or clone the bfb-reactor repository from GitHub. From within the repository, 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
```

3 Constants

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

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

4 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 .

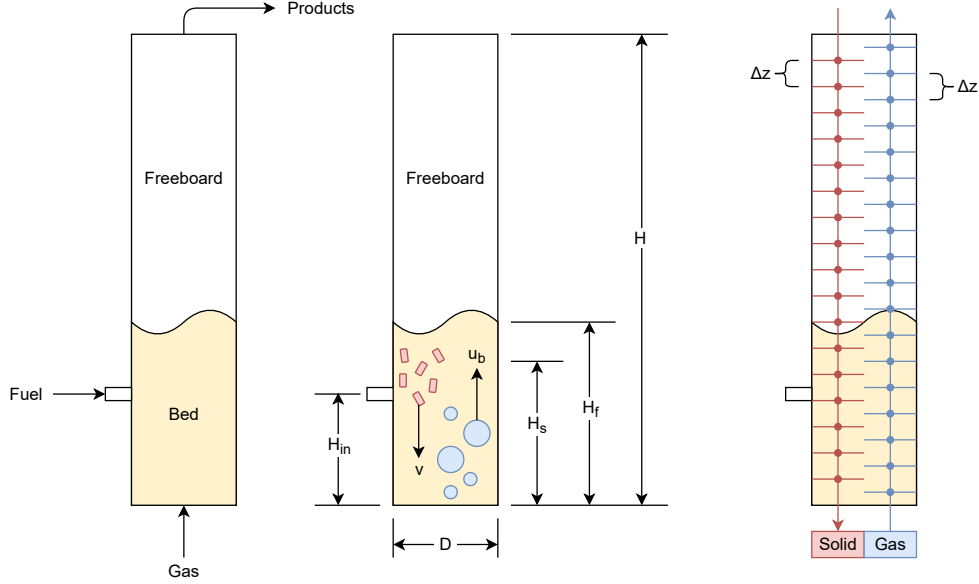


Figure 1: Inlet and outlet flows (left), geometry parameters (center), and one-dimensional grid (right) for the BFB reactor model.

5 Gas phase properties

Mass fractions (Y) for each gas species are calculated using Equation 2 while mole fractions (X) are calculated using Equation 3.

$$Y_i = \frac{\rho_i}{\rho_g} \quad (2)$$

$$X_i = \frac{Y_i/M}{\sum Y_i/M} \quad (3)$$

Gas viscosity for each of the gas phase species is calculated according to Equation 4 where coefficients A , B , and C are provided in Table 1. Thermal conductivity for each gas species is determined using Equation 5 where coefficients A , B , and C are given in Table 2. The heat capacity of each gas species is determined by Equation 6 while the coefficients for A , B , C , D , and E are given in Table 3. These correlations and coefficients are taken from Coker's book on process design [6].

$$\mu = A + B T_g + C T_g^2 \quad (4)$$

$$k = A + B T_g + C T_g^2 \quad (5)$$

$$c_p = A + B T_g + C T_g^2 + D T_g^3 + E T_g^4 \quad (6)$$

Table 1: Viscosity coefficients for different gas species.

Coefficient	CH ₄	CO	CO ₂	H ₂	H ₂ O
A ($\times 10^{-7}$)	3.844	23.811	11.811	27.758	-36.826
B ($\times 10^{-8}$)	4.0112	5.3944	4.9838	2.120	4.290
C ($\times 10^{-11}$)	-1.4303	-1.5411	-1.0851	-0.3280	-0.1620

Table 2: Thermal conductivity coefficients for different gas species.

Coefficient	CH ₄	CO	CO ₂	H ₂	H ₂ O
A ($\times 10^{-2}$)	-0.935	0.158	-1.200	3.951	0.053
B ($\times 10^{-4}$)	1.4028	0.82511	1.0208	4.5918	0.47093
C ($\times 10^{-8}$)	3.318	1.9081	-2.2403	-6.4933	4.9551

Table 3: Heat capacity coefficients for different gas species.

Coefficient	CH ₄	CO	CO ₂	H ₂	H ₂ O
A	34.942	29.556	27.437	25.399	33.933
B ($\times 10^{-3}$)	-39.957	-6.5807	42.315	20.178	-8.4186
C ($\times 10^{-5}$)	19.184	2.0130	-1.9555	-3.8549	2.9906
D ($\times 10^{-8}$)	-15.303	-1.2227	0.39968	3.188	-1.7825
E ($\times 10^{-12}$)	39.321	2.2617	-0.29872	-8.7585	3.6934

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 7.

$$k = A \exp\left(-\frac{E}{RT}\right) \quad (7)$$

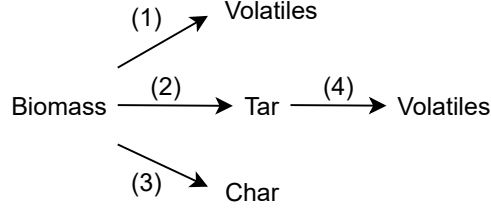


Figure 2: Primary and secondary reactions for biomass pyrolysis.

The steam-biomass gasification reactions and associated rate parameters are given below in Table 4. 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 $\text{mol}/(\text{m}^3 \cdot \text{s})$.

7 Chemical species mass balance

The rate of change for the solid concentration in a given volume is described by Equation 8. Similarly, the mass balance for each gas species is given by Equation 9 while the gas mixture concentration is given by Equation 10.

$$\frac{\partial \bar{\rho}_{s,j}}{\partial t} = -\frac{\partial(v\bar{\rho}_{s,j})}{\partial z} + S_{s,j} \quad (8)$$

$$\frac{\partial \bar{\rho}_{g,j}}{\partial t} = -\frac{\partial(y_j \dot{m}_g)}{\partial z} + S_{g,j} \quad \text{where} \quad y_j = \frac{\bar{\rho}_{g,j}}{\rho_g} \quad (9)$$

$$\frac{\partial \bar{\rho}_g}{\partial t} = -\frac{\partial \dot{m}_g}{\partial z} + \sum S_{g,j} \quad (10)$$

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 11 which relies on Equation 12 for the Reynolds number at minimum fluidization conditions [8].

Table 4: 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

$$U_{mf} = \frac{Re_{mf} \mu}{\rho_g d_p} \quad (11)$$

$$Re_{mf} = \sqrt{(33.7)^2 + 0.0408 Ar} - 33.7 \quad (12)$$

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].

$$a_b = \phi^{1.5}(4.168 - 1.389 \log(Ar)) \quad \log(Ar) < 3.5 \quad (13)$$

$$a_b = \phi^{1.5}(0.329 - 1.156 \times 10^3 Ar^{-0.9}) \quad \log(Ar) \geq 3.5 \quad (14)$$

$$c_b = (1.321 + 8.161 \times 10^4 Ar^{-1.04})^{0.083} \quad \log(Ar) > 0 \quad (15)$$

$$a_s = 0.725 + 0.230 \log(Ar) \quad \log(Ar) < 3.9 \quad (16)$$

$$a_s = 1.184 + 8.962 \times 10^4 Ar^{-1.35} \quad \log(Ar) \geq 3.9 \quad (17)$$

$$c_s = 0.042 + 0.108 \log(Ar) \quad \log(Ar) < 4.0 \quad (18)$$

$$c_s = (0.978 - 1.964 \times 10^2 Ar^{-0.8})^{4.88} \quad \log(Ar) \geq 4.0 \quad (19)$$

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 20 and 21 where $c_t = c_b/c_s$ and $a_t = 1/(a_s - a_b)$ [4].

$$\left(\frac{\bar{d}_b}{D}\right)_{\max} = \min\left(1, \left(\frac{\bar{d}_b}{D}\right)_{\text{bs}}\right) \quad (20)$$

$$\left(\frac{\bar{d}_b}{D}\right)_{\text{bs}} = 0.848 \left(\frac{U_{mf} \phi^{0.35} c_t^{a_t}}{D}\right)^{0.66} \left[1 - c(\phi^{0.35} c_t^{a_t})^{a-1}\right]^{0.66} \quad (21)$$

The bubble diameter to bed diameter ratios (\bar{d}_b/D) in Equations 22 and 23 are selected based on the Archimedes number [2, 9]. Similarly, the minimum slugging velocity to fluidization ratios (U_{ms}/U_{mf}) in Equations 24 and 25 are also related to the Archimedes number [3, 7].

$$\frac{\bar{d}_b}{D} = 0.848 \left(\frac{U_s}{D}\right)^{0.66} \left[1 - c\left(\frac{U_s}{U_{mf}}\right)^{a-1}\right]^{0.66} \quad \text{for } Ar > 400 \quad (22)$$

$$\frac{\bar{d}_b}{D} = \frac{5.64 \times 10^{-4}}{D H_{mf}} \left[1 + 27.2(U_s - U_{mf})\right]^{1/3} \left[(1 + 6.84 H_{mf})^{2.21} - 1\right] \quad \text{for } Ar < 400 \quad (23)$$

$$\frac{U_{ms}}{U_{mf}} = 1 + 2.33 U_{mf}^{-0.027} (\phi^{0.35} c_t^{a_t} - 1) \left(\frac{H_0}{D}\right)^{-0.588} \quad \text{for } Ar > 400 \quad (24)$$

$$\frac{U_{ms}}{U_{mf}} = \left(e^{-0.5405 \frac{H_0}{D}}\right) \left(\frac{4.294 \times 10^3}{Ar} + 1.1\right) + 3.676 \times 10^2 Ar^{-1.5} + 1 \quad \text{for } Ar < 400 \quad (25)$$

The total bed height is based on the bed expansion estimated from the fluidized height and the minimum fluidized height as depicted by Equation 26 shown below. When

$\bar{d}_b/D < (\bar{d}_b/D)_{max}$ then the bed expansion is calculated based on bubbling conditions using Equation 27. 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 28 where the height ratios are given in Equations 29 and 30. Finally, Equations 31, 32, and 33 are used to determine the total bed height during fluidization [5, 1, 4, 8].

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

$$\Delta e = \left[1 - 0.103(U_s - U_{mf})^{-0.362} \left(\frac{\bar{d}_b}{D} \right) \right]^{-1} - 1 \quad (27)$$

$$\Delta e = \Delta e_r - 1 = \left(\frac{H_{max}}{H_{mf}} \right) \left(\frac{H_f}{H_{max}} \right) - 1 \quad (28)$$

$$\frac{H_{max}}{H_{mf}} = \left[1 - 0.103(U_{ms} - U_{mf})^{-0.362} \left(\frac{\bar{d}_b}{D} \right) \right]^{-1} \quad (29)$$

$$\frac{H_f}{H_{max}} = \left[1 - 0.305(U_s - U_{mf})^{-0.362} D^{0.48} \right]^{-1} \quad (30)$$

$$H_f = H_{mf}(\Delta e + 1) \quad (31)$$

$$H_{mf} = \frac{1 - \epsilon_0}{1 - \epsilon_{mf}} H_0 \quad (32)$$

$$\epsilon_{mf} = \left(\frac{0.071}{\phi} \right)^{1/3} \quad \text{where} \quad \epsilon_{mf} = \max(\epsilon_{mf}, \epsilon_0) \quad (33)$$

8.3 Bubble characteristics

Here for bubble rise velocity u_B in Agu 2019b Equation 22. Here for bubble volumetric flux V_B in 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]

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