Documentation for the BFB reactor model

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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://github.com. This work is inspired by the one-dimensional gasification model published by Agu et al. [1].

1 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.

2 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
```

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.

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

4 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.

4.1 Minimum fluidization velocity

The minimum fluidization velocity is determined by Equation 2 which relies on Equation 3 for the Reynolds number at minimum fluidization conditions [7].

$$U_{mf} = \frac{Re_{mf}\, \mu}{\rho_g d_p} \tag{2}$$

$$Re_{mf} = \sqrt{(33.7)^2 + 0.0408 Ar} - 33.7 \tag{3}$$

4.2 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].

$$a_b = \phi^{1.5}(4.168 - 1.389 \log(Ar)) \qquad \log(Ar) < 3.5 \tag{4}$$

$$a_b = \phi^{1.5}(0.329 - 1.156 \times 10^3 Ar^{-0.9}) \qquad \log(Ar) \geq 3.5 \tag{5}$$

$$c_b = (1.321 + 8.161 \times 10^4 Ar^{-1.04})^{0.083} \qquad \log(Ar) > 0 \tag{6}$$

$$a_s = 0.725 + 0.230 \log(Ar) \qquad \log(Ar) < 3.9 \tag{7}$$

$$a_s = 1.184 + 8.962 \times 10^4 Ar^{-1.35} \qquad \log(Ar) \geq 3.9 \tag{8}$$

$$c_s = 0.042 + 0.108 \log(Ar) \qquad \log(Ar) < 4.0 \tag{9}$$

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

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 11 and 12 where $c_t = c_b / c_s$ and $a_t = 1/(a_s - a_b)$ [4].

$$\left(\frac{\overline{d}_b}{D}\right)_{\max} = \min\left(1, \left(\frac{\overline{d}_b}{D}\right)_{\text{bs}}\right) \tag{11}$$

$$\left(\frac{\overline{d}_b}{D}\right)_{\text{bs}} = 0.848\left(\frac{U_{mf}\phi^{0.35}c_t^{a_t}}{D}\right)^{0.66}\left[1 - c(\phi^{0.35}c_t^{a_t})^{a-1}\right]^{0.66} \tag{12}$$

The bubble diameter to bed diameter ratios ($\overline{d}_b/D$) in Equations 13 and 14 are selected based on the Archimedes number [2, 8]. Similarly, the minimum slugging velocity to fluidization ratios (U_{ms}/U_{mf}) in Equations 15 and 16 are also related to the Archimedes number [3, 6].

$$\frac{\overline{d}_b}{D} = 0.848\left(\frac{U_s}{D}\right)^{0.66}\left[1 - c\left(\frac{U_s}{U_{mf}}\right)^{a-1}\right]^{0.66} \quad \text{for} \quad Ar > 400 \tag{13}$$

$$\frac{\overline{d}_b}{D} = \frac{5.64\times10^{-4}}{D\,H_{mf}}\left[1 + 27.2(U_s - U_{mf})\right]^{1/3}\left[(1 + 6.84H_{mf})^{2.21} - 1\right] \quad \text{for} \quad Ar < 400 \tag{14}$$

$$\frac{U_{ms}}{U_{mf}} = 1 + 2.33U_{mf}^{-0.027}\left(\phi^{0.35}c_t^{a_t} - 1\right)\left(\frac{H_0}{D}\right)^{-0.588} \quad \text{for} \quad Ar > 400 \tag{15}$$

$$\frac{U_{ms}}{U_{mf}} = \left(e^{-0.5405\frac{H_0}{D}}\right)\left(\frac{4.294\times10^3}{Ar} + 1.1\right) + 3.676\times10^2 Ar^{-1.5} + 1 \quad \text{for} \quad Ar < 400 \tag{16}$$

The total bed height is based on the bed expansion estimated from the fluidized height and the minimum fluidized height as depicted by Equation 17 shown below. When $\overline{d}_b/D < (\overline{d}_b/D)_{max}$ then the bed expansion is calculated based on bubbling conditions using Equation 18. 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 19 where the height ratios are given in Equations 20 and 21. Finally, Equations 22, 23, and 24 are used to determine the total bed height during fluidization [5, 1, 4, 7].

$$\Delta e = \frac{H_f - H_{mf}}{H_{mf}} = \frac{H_f}{H_{mf}} - 1 \tag{17}$$

$$\Delta e = \left[1 - 0.103(U_s - U_{mf})^{-0.362}\left(\frac{\overline{d}_b}{D}\right)\right]^{-1} - 1 \tag{18}$$

$$\Delta e = \Delta e_r - 1 = \left(\frac{H_{max}}{H_{mf}}\right)\left(\frac{H_f}{H_{max}}\right) - 1 \tag{19}$$

$$\frac{H_{max}}{H_{mf}} = \left[1 - 0.103(U_{ms} - U_{mf})^{-0.362}\left(\frac{\overline{d}_b}{D}\right)\right]^{-1} \tag{20}$$

$$\frac{H_f}{H_{max}} = \left[1 - 0.305(U_s - U_{mf})^{-0.362}D^{0.48}\right]^{-1} \tag{21}$$

$$H_f = H_{mf}(\Delta e + 1) \tag{22}$$

$$H_{mf} = \frac{1-\epsilon_0}{1-\epsilon_{mf}}\, H_0 \tag{23}$$

$$\epsilon_{mf} = \left(\frac{0.071}{\phi}\right)^{1/3} \tag{24}$$

4.3 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]

$\overline{d}_b$ 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

[1] Cornelius E. Agu et al. “Detailed One-Dimensional Model for Steam-Biomass Gasification in a Bubbling Fluidized Bed”. In: *Energy & Fuels* 33.8 (2019), pp. 7385–7397.

[2] Cornelius E. Agu et al. “Investigation of Bubbling Behavior in Deep Fluidized Beds at Different Gas Velocities using Electrical Capacitance Tomography”. In: *Industrial & Engineering Chemistry Research* 58.5 (2019), pp. 2084–2098.

[3] Cornelius E. Agu et al. “Models for Predicting Average Bubble Diameter and Volumetric Bubble Flux in Deep Fluidized Beds”. In: *Industrial & Engineering Chemistry Research* 57.7 (2018), pp. 2658–2669.

[4] Cornelius Emeka Agu. “Bubbling Fluidized Bed Behaviour for Biomass Gasification”. PhD thesis. University of South-Eastern Norway, 2019.

[5] Cornelius Emeka Agu et al. “Improved models for predicting bubble velocity, bubble frequency and bed expansion in a bubbling fluidized bed”. In: *Chemical Engineering Research and Design* 141 (2019), pp. 361–371.

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[7] C.Y. Wen and Y.H. Yu. “A Generalized Method for Predicting the Minimum Fluidization Velocity”. In: *AIChE Journal* 12.3 (1966), pp. 610–612.

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