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Full Length Article

A conversion-class model for describing fuel conversion in large-scale fluidized bed units

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HIGHLIGHTS

- The use of population balances of fuel classes to model fuel conversion is studied.
- The class discretisation method strongly affects the accuracy of the results.
- A generic discretisation method is proposed and evaluated.
- 6 classes yield errors <1% compared to modelled conversion curves given as input.

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ABSTRACT

Solid fuel conversion in fluidized beds is often modelled with the use of population balances, where the fuel conversion process is divided into a number of classes based on for example fuel particle size. The present work investigates and evaluates different methods for the discretisation of the fuel conversion process into classes, as well as the number of classes necessary to yield a satisfactory accuracy. A discretisation method, which defines classes based on the conversion degree (rather than size or density) and that is valid for all conversion regimes, is proposed. The results show that application of the proposed class division method for modelling biomass gasification in a fluidized bed gives an accuracy that is up to ten times higher than that given by a distribution with equally large classes. For all three conversion processes of biomass gasification (drying, pyrolysis, and char gasification), discretisation into 6 classes is sufficient to yield errors of around 1%, when compared to the continuous conversion curves given as input to the conversion class discretisation model (generated by a particle model in the present work). In line with this, when the conversion class model is used in a semi-empirical 1D model of indirect biomass gasification, the resulting char conversion in the gasifier does not change significantly when more than 3–6 char conversion classes are used.

1. Introduction

Fluidized bed (FB) units are widely used in the energy sector to convert solid fuels into heat, electricity, and gaseous products, owing to their excellent fuel flexibility, relatively good gas-fuel mixing, and uniform temperature [1,2]. Several applications use the FB technology for energy conversion. Large-scale circulating fluidized bed (CFB) combustion is commonly used for the conversion of solid fuels (coal, biomass, and wastes) [2]. In addition, bubbling fluidized bed (BFB) combustion of biomass and waste is applied in smaller units [3]. FB combustion is also of interest for CO_2 capture technologies, such as oxy-fuel combustion and chemical looping combustion [4,5]. For all these systems, a high degree of fuel conversion is desirable so as to maximise the overall efficiency. The first two stages of fuel conversion, drying and devolatilisation, proceed relatively quickly, so they tend to take place close to the fuel inlet, leading to an uneven distribution of the gas species in large boilers. To deal with this, multiple fuel inlets, the placement of which can be optimised through modelling tools, are commonly used in large-scale units [6–8].

Gasification of solid fuels in FBs has a long history. In the 1920s, Winkler developed the first FB gasifier, designed to convert lignite to gas for the gas engines used in ammonia production [2]. Today, biomass gasification is seen as a promising technology for transforming lignocellulosic materials into climate-neutral transport fuels, such as Fischer-Tropsch diesel, methanol, and substitute natural gas (SNG) [9,10]. Current FB gasification technologies can be categorised as: (1) single fluidized bed gasification (FBG), in which the required heat is provided by burning part of the fuel [10]; or (2)

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Nomenclature

Roman letters

A_j	error of class j (s)
C	constant in polynomial (depends on equation)
c_p	specific heat (J/(kg K))
D_{AB}	binary diffusion coefficient (m^2/s)
D_{eff}	effective diffusivity (m^2/s)
D_F	fuel dispersion coefficient (m^2/s)
k	constant in equation for straight line (s^{-1})
k	thermal conductivity (W/(m K))
m	constant in equation for straight line (–)
m	mass (kg)
m_0	initial mass (kg)
$\dot{m}_j$	mass flow of fuel entering class j (kg/s)
n	degree of polynomial (–)
N_k	number of classes (–)
N_F	total number of classes (–)
N_s	number of polynomial sections (–)
P_k	function for conversion of species k (–)
P_a	polynomial valid for section a (–)
r	radial coordinate (m)
R	conversion rate (s^{-1})
S	source term (depends on equation)
t	time (s)
T	temperature (K)
T_1	initial temperature of surroundings (°C)
T_2	final temperature of surroundings (°C)
u	velocity (m/s)
x	space coordinate (m)
$x_{0,k}$	initial fuel mass fraction of component k (–)
x_k	fuel mass fraction of component k (–)
X	degree of conversion (– or %)
ΔX_j	size of conversion class j (–)
X_j	characteristic conversion degree of class j (–)
Y_i	mass fraction of gas species i ($\%_w$)

Indices

a	polynomial section
BM	bed material
$conv$	conversion
CH	char
F	fuel
f	finish
g	gas
i	gas species
i	polynomial indexing
j	conversion class
k	fuel component (M, V, CH, or F)
lin	linear approximation
M	moisture
q	heat
PM	particle model
s	start
s	solid
tot	total
V	volatiles

Greek letters

ε_{por}	char porosity (–)
ε_k	error for fuel component k (–)
ε_{mf}	voidage at minimum fluidization (–)
$\varepsilon_{+\Delta T}$	error due to change in cell temperature (–)
θ	shrinkage factor (–)
θ_F	cross-flow impact factor (–)
ρ	density/concentration (kg/m^3)
τ	dimensionless time (–)
φ	shrinkage factor (–)
χ	conversion degree in the particle model (–)

Dimensionless numbers

Ar	Archimedes number
Nu	Nusselt number
Pr	Prandtl number
Re_{mf}	Reynolds number at minimum fluidization
Sc	Schmidt number
Sh	Sherwood number

dual FB gasification (DFBG), in which the heat is provided by the bed material circulating between a combustor and a gasifier [9]. In FBG, it is difficult to achieve complete fuel burnout, with a consequent decrease in the overall efficiency of the process [10]. For DFBG, there exists an optimal level of char conversion in the gasification chamber, which depends on the type of fuel used and the desired end-product [11].

Thus, to optimise the degree of fuel conversion for the FB technologies described above, e.g., for upscaling purposes, at the design stage, or when evaluating the use of a new fuel type, it is important to be able to predict the fuel conversion as accurately as possible. For this purpose, modelling is a helpful tool. Modelling can also be used to improve understanding of the processes that are taking place in a FB reactor, to investigate the role of different parameters, and to identify key knowledge gaps that need to be addressed. Moreover, accurate modelling of the fuel conversion process results in more reliable predictions of the temperature profiles and concentration profiles of the different gas species in the reactor, which are also important parameters for reactor design.

Given the vigorous mixing that occurs in fluidized beds, any location of the bottom bed can be, and often is, populated by fuel particles at different degrees of conversion. The most rigorous strategy for dealing with this problem is to model the fuel conversion by tracking the location of each fuel particle (or parcel of particles) by solving its equation of motion (Lagrangian Particle Tracking; LPT). LPT has been used to model fuel conversion in CFB combustors and BFB gasifiers [12–15]. However, in large-scale FB reactors, this approach is associated with a high computational cost given the number of fuel particles, and the formulation of the momentum transfer between the fuel and the bed has not yet been fully established [16]. A less detailed approach is to solve one mass balance for each fuel field (moisture, volatiles and char), while assuming a constant conversion rate for each fuel component. While this approach is mostly used in zero-dimensional models (in which the fuel distribution within the reactor is not solved) [17], it has also been applied in 1- and 3-dimensional models to describe the conversion processes of drying and devolatilisation (while char conversion is described through population balances, see below) [6].

A more affordable method than LPT (in terms of computational cost) that offers greater accuracy than the use of constant conversion rates is to solve a fuel population balance in which different conversion classes are considered. The use of population balances, combined with the assumption that fuel conversion takes place in