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Review

Mathematical modelling and simulation approaches of agricultural residues air gasification in a bubbling fluidized bed reactor

D.A. Nemtsov, A. Zabaniotou*

Department of Chemical Engineering, Faculty of Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece

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Abstract

Agricultural residues (agro-biomass) can produce energy by thermochemical conversion. Gasification is becoming one of the best clean technologies for power production. Thermochemical process of gasification sets free the solid fuel inherent energy and converts the solid phase into a mixture of gases (producer gas or syngas) that carries a percentage of this energy. Fluidized bed reactors may be used for biomass gasification offering many advantages such as: (1) the superior mixing properties and (2) the enhanced heat transfer rates between the gas and the particles as well as between the particles and the heat exchanger surfaces. In this paper gasification process applied to agricultural residues is reviewed by means of modelling. Description of various stages of the biomass gasification in a fluidized bed is made and the whole spectrum of problems from the processes in an individual biomass particle (drying, pyrolysis, fragmentation and charl burning) to the global mass transfer and chemical processes in a fluidized bed reactor and freeboard is presented. The paper discusses also the specific problems arising from using agricultural residues as raw material and recommends further experimental studies necessary for process optimisation and for scale up. Extensive investigation of gasification plant behaviour depending on various operating parameters is always required in order to support the optimisation procedure and mathematical models are helpful to reduce the temporal and financial efforts.

Keywords: Modelling; Simulation; Agricultural residues; Gasification; Bubbling fluidized bed; Single fuel particle

1. Introduction

Biomass is important in energy conversion processes due to its favourable status with respect to greenhouse gas emissions. Biomass fuels available for gasification include charcoal, wood and wood waste (branches, twigs, roots, bark, wood shavings and sawdust) as well as a multitude of agricultural residues (maize cobs, coconut shells, coconut husks, cereal straws, rice husks, cotton ginning, olive kernels, stalks, etc.). Because those fuels differ greatly in their chemical, physical and morphological properties, they make different demands on the method of gasification and consequently require different reactor designs or even gasification technologies. It is for this reason that, during a century of gasification experience, a large number of different gasifiers has been developed and marketed, all types geared towards handling the specific properties of a typical fuel or range of fuels.

Giving the important role that agricultural residues and lignocellulosic biomass gasification can play not only in bioenergy production but also for second generation biofuels and hydrogen production, modelling of their thermochemical process is helpful in developing successful and efficient gasification commercial plants. However, biomass particles have unusual properties which make them difficult to fluidize and handle.

Fluidized beds have been applied widely in processes involving gasification, pyrolysis and combustion of a wide range of particulate materials including biomass. Advantages of fluidization include high heat transfer, uniform and controllable temperatures, favourable gas–solid contacting and the ability to handle a wide variation in particulate properties [1].

In the recent years, research and literature has predominantly concentrated on practical applications and experience in fluidization equipment, designed and fabricated to carry out biomass gasification, pyrolysis and combustion processes. There is an extensive literature on the kinetics of devolatilization and

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* Corresponding author at: University Box 455, 54124, University Campus, Greece. Tel.: +30 2310 996274; fax: +30 2310 996209.

E-mail address: sonia@cheng.auth.gr (A. Zabaniotou).

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Nomenclature

a	pre-exponential factor (s/mm^n)
a'	ratio of the volume of emulsion transported upward behind a bubble (volume of wake) to the volume of a bubble
A_p	particle surface (m^2)
A_t	furnace cross-section (m^2)
c_v	solids volume fraction (m^3/m^3)
C_c	char concentration (kg/m^3)
C_i	gas concentration species i (kmol/m^3)
CDe	drag coefficients,
d_p	particle diameter (m)
d_{p1}	the mean diameter of the sand particles
d_{p2}	the mean diameter of the biomass particles
d_G	diameters of the coarse particles
d_p	diameters of the fine particles
D	dispersion coefficient (m^2/s)
D_{eff}	effective dispersion coefficient (m^2/s)
D_{hyd}	hydraulic diameter (m)
E	is the activity energy (27.76 kcal/kmol)
f_d	dense phase volume fraction
f_{wg}	is a reactivity parameter which is dependent on char
F	convective flux (kg/s, kmol/s)
F_F	net flow in the upward direction
g	gravitational constant
Gs	solids recirculation rate based on riser cross-section (kg/(m^2 s))
h	height above distributor (m)
H_{bz}	height of bottom zone (m)
j	dispersive flux per unit area (kmol/(m^2 s))
J	dispersive flux (kg/s, kmol/s)
k·a	exchange coefficient lean/dense phase (1/s)
k_0	surface reaction rate constant (m/s)
k_f^E	is the equilibrium constant of reaction j.
k_{conv}	convective exchange coefficient (1/s)
k_{ig} & a	exchange coefficient suspension/bubble phase (1/s)
k_f	fragmentation constant (1/s)
k_g	mass transfer coefficient (m/s)
K	char combustion rate constant (m/s)
$K_{eq.\,wg}$	an equilibrium constant
l	depth of the orifice up to which particle spilling occurs
L	length (m)
Lx	riser dimension in x-reaction (m)
Ly	riser dimension in y-reaction (m)
m	mass (kg)
m'	mass flux (kg/s)
M	molar mass (kmol/kg)
n	amount of substance (kmol)
$n^{\cdot}$	molar flux of substance (kmol/s)
p	split factor char combustion
p_i	partial pressure of component i (atm)
P	probability
PT	total pressure (atm)
q_3	particle mass density function (1/mm)
Q	local sources of potential flow field (kg/(m^3 s), kmol/(m^3 s))
Q_3	cumulative mass distribution
r	reaction rate based on unit phase volume (kg/(m^{3}s), kmol/(m^{3}s))
$r_{A,c}$	reaction rates per unit volume of the cloud phase
$r_{A,e}$	reaction rates per unit volume of the emulsion phase
r_p	particle radius (m)
R	reactive flux (kg/s, kmol/s)
$R_{hom,\,GF,\,j}$	reactive flux of gas phase in freeboard
sF	width of feed chute (m)
sr	width of solids return chute (m)
t	time (s)
T	temperature (K)
Ts	grade efficiency for strand separation
Tv	grade efficiency for vortex separation
u	gas velocity (m/s)
U	net gas flux (m^3/s)
U_0	superficial gas velocity (m/s)
Uc	critical velocity for complete fluidization
U_G	axial component of the superficial gas velocity (m/s)
v	solids velocity (m/s)
wc	char weight fraction of bed material
w_1	the mass of sand particles
w_2	the mass of biomass particles
x, y, z	space coordinates (m)
xu	volatile weight fraction of fuel (kg/kg raw)
xw	water weight fraction of fuel (kg/kg raw)
X	mass fraction of the volatile matter in the coal on a dry and ash-free basis

Greek letters

β	damping factor
ε	porosity
ε_b	bubble phase volume fraction
ε_{sp}	porosity of suspension phase
Δd_{pi}	width of size class i (m)
ΔP_b	pressure drop across the bed (kPa)
$\Delta P_{b,mf}$	pressure drop across the bed at minimum fluidization velocity (kPa)
ΔP_d	pressure drop across the distributor (kPa)
ΔP_{ds}	pressure drop caused by stagnant zones (kPa)
$\Delta P_{d,z}$	excess pressure drop required by non-operating orifice (kPa)
φ	carbon weight fraction of char
μ	solids load of gas flux (kg/m^3)
ν	kinematic viscosity (m^2/s)
Θ	mechanism factor char combustion
Φ_g	gas flow potential (m^3/(ms))

Φ_s	solids flow potential (kg/(ms))
$\rho^{\cdot}$	local sources (kg/(m s))
ρ	density (kg/m^3)
τ	mean residence time (s)
τ	viscous shear stress
ξ	mass fraction
ψ	constant relating the bubble diameter

Subscripts or superscripts

0	start
*	bulk phase
b	bubble phase
bz	bottom zone
c	char
C	carbon
conv	convective
cyc	cyclone
d	dense phase
e	entry condition
eff	effective
ex	exchange
f	fragmentation
F	feed
g	gas
gh	gas horizontal
G	critical
h	horizontal
i	species i, particle class i
in	incoming
int	intermediate
p	particle
R	return leg inlet
s	solids
sc	stand coarse
sf	standfine
sh	solids horizontal
slip	gas-solid slip
sp	suspension phase
t	terminal settling
top	riser's top
up	upper dilute and splash zones
v	volatile
vc	vortex corse
vf	vortex fine
w	water
wv	water plus volatiles
x, y, z	x-, y-, z-direction

Abbreviations

ASPEN	Flowsheeting package from ASPEN TECH
BFB	Bubbling Fluidized Bed Combustion
CFB	Circulating Fluidized Bed
CFBC	Circulating Fluidized Bed Combustion
CSTR	Continuous Stirred Tank Reactor
daf	dry and ash free
FBC	Fluidized Bed Combustion
PSD	Particle Size Distribution
RTD	Residence Time Distribution
ODE	Ordinary Differential Equation

gasification. Much of it is directed at the early moving bed and fluidized bed gasifiers. The application of fluidization in biomass gasification is well suited because of the non-homogeneous biomass nature and the surface area contact between the solid and the gas phase. The efficient mixing in a fluidized bed creates isothermal conditions into the gasifier, which also lead to better control of emissions due to the lower operating temperatures. Interactions that also occur in the fluidized bed gasifier depend mainly on the hydrodynamics and involve several phenomena including: (a) chemical reactions, (b) heat transfer, (c) mass transfer, (d) size reductions of particles and even (e) attrition of particles and bed material.

The traditional approach necessary to establish commercial plant technology is based on comprehensive experimental investigations, progressing from a laboratory scale test unit to a pilot scale plant, before building a full-scale commercial demonstration plant. For process optimisation, an extensive investigation of the plant behaviour depending on various operating parameters is required for each scale up step. To support this optimisation procedure, mathematical models are helpful to reduce the temporal and financial efforts. Pre-condition is a reliable simulation tool, which includes the mathematical formulation of all important chemical and physical processes by describing their dependency on operating parameters and their interdependencies [2]. However, only limited research has been performed to model those complex systems including also the hydrodynamics of biomass particles. The developments of numerical models for fluidized-bed gasification (FBG) documented in the literature [3–10,2,11–24] are devoted mainly for coal and less for biomass. Even though, biomass in comparison to coal is made up not only of lignin but also of cellulose, hemi cellulose, each one having its own thermal behaviour and making the modelling more difficult, the modelling approaches used for coal can serve for biomass gasification modelling as well.

Ma et al. [14] developed a steady-state model which involved instantaneous devolatilization of *coal* at the top of the gasifier (freeboard region) and char combustion and gasification in the fluidized bed. Chejne and Hernandez [6] developed a comprehensive mathematical model to predict the behaviour of *coal* combustion and gasification on stacks in non-stationary operation. Sett and Bhattacharya [20] developed a mathematical model for the behaviour of a fluidised-bed charcoal gasifier, taking into account fluidised-bed hydrodynamic conditions, chemical reaction rates, mass diffusion rates, and the conservation of mass and energy. The model was solved numerically using an IBM 3083 mainframe computer. Ross et al. [25,18] modified their one-dimensional numerical isothermal model of a fluidised-bed *coal* gasifier in order to simulate the performance of a laboratory-scale gasifier.

A new numerical model based on the two-fluid model (TFM) including the kinetic theory of granular flow (KTGF) and complicated reactions has been developed by Zhang et al. [26] to simulate *coal* gasification in a bubbling fluidized bed gasifier (BFBG). The collision between particles was described by KTGF. The *coal* gasification rates were determined by combining Arrhenius rate and diffusion rate for heterogeneous reactions or turbulent mixing rate for homogeneous reactions. The flow behaviours of gas and solid phases in the bed and freeboard could be predicted, which were not easy to be measured through the experiments.

Hamel and Krumm [11] have developed a mathematical model for simulation of gasification processes of solid fuels in atmospheric or pressurised bubbling fluidised beds incorporating bed and freeboard hydrodynamics, fuel drying and devolatilization, and chemical reaction kinetics is presented. The model has been used to simulate four bubbling fluidised bed gasifiers, described in literature, of different scales from atmospheric laboratory scale up to pressurised commercial scale, processing brown *coal*, *peat* and *sawdust*. The gasifiers have been operated within a wide range of parameters using air, air steam or oxygen steam as gasification agent, operating with or without recirculation of fines at operating pressures up to 2.5 MPa. The simulation results for overall carbon conversion, temperature and concentrations of gaseous species agreed sufficiently well with published experimental data.

Corella and Sanz [27,28], at the Universities of Zaragoza and Madrid (Spain) started to study the modelling of fluidized bed biomass gasifiers in the mid-1980s. More recently Corella et al. [29], discussed the reaction network existing in a CFB biomass gasifier and the problems associated with the accuracy of the kinetic equations needed for the existing complex reaction network. Further, Corella et al. [29], presented a model for bubbling fluidized bed (BFB) *biomass* gasifiers, gasifying with pure steam. That model identified the four main, for modelling purposes, chemical reactions among the reaction network existing in the gasification process. With only four kinetic parameters, the model predicted quite well the BFB gasifier. Finally, Corella and Sanz [27,28] have presented a whole model for CFBBGs. Such model is 1-dimensional and for steady state. The model has a semi rigorous character because of the assumptions that had to be introduced by lack of accurate knowledge in some parts of the modelling.

De Souza-Santos [7] developed a comprehensive mathematical model and commercially available computer program performing a comprehensive simulation of fluidized-bed equipment (CSFB Version 3.5), to use as a tool for engineering design and operation optimisation, by predicting the behaviour of a real unit during steady-state operation. His model is regarded as complete and it includes the conservation equations for the emulsion phase and bubbles, empirical equations for hydrodynamics, and it is also includes a through mass balance which considers that both drying and volatilisation are not instantaneous. Jiang and Morey [12] developed one-dimensional, steady state, numerical model for a fluidized bed biomass gasifier. The gasifier model consisted of a fuel pyrolysis model, an oxidation model, a gasification model and a freeboard model which were validated with experimental results. Haggerty and Pulsifer [10] used the reaction model together with three different reactor models (a) plug-flow, (b) complete-mixing and (c) bubble-assemblage, where the bubble-assemblage model represents a valid alternative when modelling fluidized-bed gasifiers. Marias et al. [15] developed a mathematical model for the fluidized-bed incineration process using the waste composed of *wood*, cardboard and *polyvinyl chloride*. Aarsen et al. [3] model treated an isothermal fluidized bed as two separate zones, the oxidation zone at the bottom and the gasification zone at the top. Fuel pyrolysis took place at such a fast rate that only pyrolysis yields, which were assumed to vary with bed temperature, were needed. Mukosei et al. [16] examined the problem of the mathematical simulation of heterogeneous processes in a fluidized-bed reactor.

These works and other more recent ones such as the work by He and Rudolph [30] proposed a new approach to the modelling of gross gas–solids flow through the riser in a circulating fluidized-bed system. This approach differs from the previous ones, which are found to be theoretically incorrect based on a fundamental analysis of the riser process hydrodynamics. Panopoulos et al. [31] used the simple way of approaching the biomass gasification modelling by predicting thermodynamic equilibrium composition through Gibbs free energy minimisation calculations for the C, H, and O atoms of the fuel and the gasification agent mixture.

Samuilov et al. [19] developed a mathematical model for the gasification in carbon dioxide of a *single carbon particle*. The porous structure of the particle, diffusion processes, the gasification processes on the pore surface according to the Langmuir–Hinshelwood model, and reactions on active carbon sites were taken into account. Deen et al. [32] reviewed the use of *discrete particle models* (DPMs) for the study of the flow phenomena prevailing in fluidized beds.

EU under the program JOULE JOR3-CT98-0232 has funded a project entitled ‘Biomass gasification modelling for energy systems’ in the direction to reduce its CO_2 emissions and to fulfil commitments made according to Kyoto protocol. This project aimed to develop a comprehensive macroscopic model of *lignocellulosic biomass* gasification using the circulating fluidised bed process. The proposed approach included in the model the heterogeneous fluid dynamics and the finite and competing kinetic rates at all stages of the CFB reactor. The main frame of the model was gasification-oriented instead of gasifier-oriented, to maximise the flexibility and to ensure the applicability of the model to any design of CFB gasifier.

In relation to the increased need for modelling and simulation of bioenergy systems and mainly gasification and pyrolysis ones and the importance directed at improving the modelling of biomass fluidization hydrodynamics, which are critical to successful design and operation of fluidized bed processes, the present study aims to review the main approaches in modelling of biomass gasification with incorporation of hydrodynamics.

In order to design and scale up a bubbling fluidised bed reactor, which is the ultimate purpose of the research program this study makes part, the understanding of the interaction between chemical and physical phenomena during agricultural residues gasification, the determination of the overall rate of the reaction and mainly the establishment of reliable scaling up rules and optimization of the design of reactors are of fundamental importance. The experimental work of the project includes study of olive kernel (a residue from olive oil production) in the bubbling fluidised bed pilot scale reactor. In a next study the available experimental results will be used to validate the modelling and simulation approach.

2. Modelling approaches

By reviewing the literature, two categories of modelling approaches have been distinguished and presented: those dealing with the discrete biomass particle and those simulating the reactor.

2.1. Modelling of a single fuel particle [DPM]

Solid fuel particles, regardless of their fuel properties, undergo several processes before and during the burning process. These include (a) heating-up, (b) drying, (c) devolatilization and (d) primary fragmentation combustion of the volatiles and the residual char with or without secondary char fragmentation and attrition. Knowledge of the kinetics of drying and devolatilization in combination with the fluid dynamics is important for a better interpretation of variations in operation behavior using moist fuel. Temperature profile, is decisively affected by the vertical location of water evaporation and volatile release.

Deen et al. [32] reviewed the use of discrete particle models (DPMs) for the study of the flow phenomena prevailing in fluidized beds. They gave an outlook for the use of DPMs for the investigation of various chemical engineering problems in the area of fluidization and not only of biomass. DPMs describe the gas-phase as a continuum, whereas each of the individual particles is treated as a discrete entity. The DPMs accounts for the gas–particle and particle–particle interactions. Furthermore, the use of the discrete particle model (DPM) enables the simultaneous ‘measurement’ of several properties, such as the gas and particle velocities, and the porosity, which is difficult if not impossible to achieve by direct experimentation. Provided that computer models possess sufficient predictive capabilities, they have the additional advantage over experiments that several design options and operation conditions can be tested with relative ease.

2.1.1. The timing of drying and volatile release

Heating rates in fluidized beds are very high. Therefore the short heating-up phase can be neglected safely and it can be assumed that drying commences at the time the fuel particle enters the combustor. To calculate simultaneous fuel drying and devolatilization of fuel particles, the model proposed by Agarwal et al. [33] can be applied. Assuming that drying takes place at a boundary moving from the outer surface to the centre of the particle, an unsteady-state heat conduction equation in spherical coordinates with a convective boundary condition is solved analytically. The determined temperature profile in the dried shell is used in a numerical integration over the volume of particle to calculate the volatile release using a non-isothermal fuel decomposition kinetic. The amount of volatile matter released is calculated using the distributed activation energy model. The heat conduction equation in one-dimensional spherical coordinates with appropriate initial and boundary conditions is presented in Agarwal et al. [33] also suggests that between 10 and 90% devolatilization, the extent of devolatilization, X, may be considered as linear with respect to the final temperature. With the presented equation, it is possible to estimate the rate of devolatilization of large fuel particles.

Other models have been developed for devolatilization, which give the rate, volatile yield and composition of the products. The three most widely used are these developed by [34–36]. The models yield relatively comparable results. One of the commonly used model is the Chemical Percolation Devolatilization (CPD) model of Solomon et al. [37] which describes the importance to gasification of tar yields and the effect of pressure on volatile yields.

A very general and often applied approach to determine the volatile release time is the empirical power law relation, which correlates the devolatilization time t_{v} in seconds to the particle diameter d_{p} in millimeters [38].

$$t_{\mathrm{v}}(d_{\mathrm{p}}) = a d_{\mathrm{p}}^{n} \tag{1}$$

The pre-exponential factor a and the exponent n are usually determined by fitting experimental data. Ross et al. [38] have compiled numerous data on the devolatilization time from the literature and proposed numerical values of $a = 4.4\ \mathrm{s/mm}^{n}$ if d_{p} is inserted in mm and $n = 1.2$, respectively.

Then moist fuel is combusted the time required for completing the volatile release could be significantly prolonged due to the superimposed drying process. In order to quantify the effect of the moisture content an empirical correlation was derived from measured data published by Ross et al. [38].

$$\frac{t_{\mathrm{v}}\mathrm{dried}}{t_{\mathrm{v}}\mathrm{wet}} = 0.28 + 0.72\ \exp\left(-\frac{x_{\mathrm{w}}}{0.41}\right) \tag{2}$$

Any possible influences of the surrounding gas and solids on the devolatilization time are neglected. For reasons of simplification a constant volatile release rate is assumed during the whole devolatilization process.

2.1.2. Primary fragmentation

Primary fragmentation concerns big particles. During the devolatilization process the so-called primary fragmentation occurs. The fuel particle bursts most likely due to thermal shock and pressure build-up of released volatile gases inside the particle. An approach often found in literature [39] to quantify the fragmentation probability P_{f} is given in:

$$P_{\mathrm{f}}(d_{\mathrm{p}}) = 1 - \exp(-k_{\mathrm{f}} t_{\mathrm{v}} d_{\mathrm{p}}) \tag{3}$$

where the fragmentation constant has a value of $k_{\mathrm{f}} = 0.11\ 1/\mathrm{s}$. This correlation results in an almost 100% probability for large fuel particles to break up, whereas small particle classes do not undergo fragmentation. Experiments have shown that during devolatilization this breakage occurs such that the fuel particles fall apart into few large particles. To describe this behavior

Table 1
Values of a_1 and a_2 for calculation of minimum fluidization velocity U_{mf}

Reference	a_1	a_2
Babu et al. [90]	25.25	0.0651
Grace [91]	27.2	0.0408

it can be assumed that the fragments of a mother particle with diameter d_{p} are evenly distributed to the smaller particle classes on a number basis. If the fragments are assumed to be spherical and to be of the same density, the distribution of the fragment particle diameter $d_{\mathrm{p,\,f}}$ on a number basis could be converted to the required particle mass density function of the fragments [39].

$$q_{3,\mathrm{f}}(d_{\mathrm{p,f}}) = \frac{4d_{\mathrm{p,f}}^3}{d_{\mathrm{p}}^4} \tag{4}$$

The exact timing of primary fragmentation is not well known. Preliminary model calculations with fragmentation either at the beginning or at the end of the devolatilization have hardly shown any influence on the final volatile source distributions at the end of the devolatilization process. In the following primary fragmentation is simply assumed to take place just at the end of the volatile release process.

2.1.3. Char particle burn-out

After the devolatilization step is completed the volatile-free char particles which consist mainly of fixed carbon and ash, start to burn. Since in a fluidized bed the char particles are colliding frequently with other sand and char particles as well as with the reactor walls one might assume that due to this mechanical stress the ash layer is stripped off from the particles. Hence, the *shrinking particle model* has been chosen to describe the char oxidation process. In this model for heterogenous gas–solid reactions one must distinguish at least between mass transfer phenomena from and to the burning particle and oxidation reactions taking place on the particle surface. In analogy to the mass transfer a limited heat transfer could also result in non-equilibrium between the conditions of a single particle and the surrounding bed. Usually, burning particles exhibit an excess temperature compared to the bed temperature. This, in turn, influences the surface reaction rate and has to be taken into account as well [39] (Table 1).

2.1.4. Mass transfer to the particle

The film resistance at the surface of the char particle depends on numerous factors such as the relative velocity between char particle and fuel gas, the size of the particle and the fuel gas properties. For the special conditions prevailing in fluidized beds these factors have been considered and were lumped together in empirical correlations for the Sherwood number Sh from which the mass transfer coefficient k_{g} can be derived, Table 2, Eq. (9).

For a non-moving sphere the Sherwood number achieves the theoretical value of 2. However, in the turbulent environment of a fluidized bed the gas boundary layer of a single particle is supposed to decrease and hence larger Sherwood numbers could be expected [40].

According to the description of the flow structure we have to distinguish between correlations for Sh applicable to the solid rich bottom bed and those developed for the upper dilute region with comparable low solids concentrations. In the dense bottom zone correlations might be applicable which are proposed for stationary fluidized beds. Generally a constant Sherwood number of 3.5 has been applied for the bottom bed and in the upper dilute zone also the approach shown in Table 2, Eq. (10) can been applied [40].

For fine particles this correlation results in values for the Sherwood number close to the theoretical values of a single free falling particle.

2.1.5. Surface reaction and shrinking rate

Once the oxygen of the combustion air has reached the particle surface, the carbon of the char particles is either oxidized to CO or to CO_2, Table 3, (R-1), (R-2).

According to the researchers [40] a third possible gas–solid reaction, i.e. the gasification of char carbon by CO_2 to form carbon monoxide, can be neglected since the temperatures in fluidized bed combustors are usually not sufficiently high for this gasification reaction. Therefore the two equations can be summarized by introducing a mechanism factor Θ which describes the ratio of carbon monoxide to carbon dioxide produced, Table 3, (R-3). The valid value for Θ is around 1, representing complete oxidation to CO_2, and 2 for complete carbon monoxide production, respectively. To quantify the molar ratio of CO to CO_2 produced a splitting factor p is introduced which is linked to the stoichiometric factor Θ. Table 3, Eq. (7).

Table 2
Fundamental equations for biomass particle gasification

No.	Description	Equation	Reference
(1)	Heat conduction equation in one-dimensional spherical coordinates	$\frac{\partial T}{\partial t} = \frac{a}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)$	Agarwal et al. [33]
(2)	Initial conditions	$T_{(\mathrm{r,o})} = T_{\mathrm{o}}$	Agarwal et al. [33]
(3)	Boundary conditions	$k_{\mathrm{s}}\frac{\mathrm{d}T}{\mathrm{d}r} \rvert= h(\mathrm{To} - \mathrm{Ts})$	Agarwal et al. [33]
(4)	Boundary conditions	$\frac{\mathrm{d}T}{\mathrm{d}r}\rvert_{r=o} = 0$	Agarwal et al. [33]
(5)	Fractional average devolatilization	$X_{\mathrm{avg}} = \frac{3}{R_0^3}\int_0^{Ro} Xr^2\,\mathrm{d}r$	Agarwal et al. [33]
(6)	Initial conditions T_{U1} is the temperature at which devolatilization begins	$X = 0,0 \quad T \leq T_{\mathrm{U1}}$	Agarwal et al. [33]
(7)	Initial and Boundary conditions	$X = \frac{T-T_{\mathrm{U1}}}{(T_{\mathrm{U2}}-T_{\mathrm{U1}})T_{\mathrm{U1}}} < T < T_{\mathrm{U2}}$	Agarwal et al. [33]
(8)	Boundary conditions T_{U2} the temperature at which it is complete	$X = 1,0 \quad T \geq T_{\mathrm{U2}}$	Agarwal et al. [33]
(9)	Sherwood number	$Sh = \frac{k_{\mathrm{g}}d_{\mathrm{p}}}{D_{\mathrm{eff}}}$	
(10)	Sherwood number and in the upper dilute zone	$Sh = 2\varepsilon + 0.69\sqrt[3]{Sc}\sqrt{\frac{Re}{\varepsilon}}$	Luecke et al. [40]

Table 3
Kinetic equations of biomass particle gasification

No.	Description	Reaction/Equation	Reference
Surface reaction and shrinking rate			
(R-1)	Solid–gas	$C + O_2 \rightarrow CO_2$	De Souza-Santos [7]
(R-2)	Solid–gas	$C + 1/2O_2 \rightarrow CO$	De Souza-Santos [7]
(R-3)	Solid–gas	$O_2 + \Theta C \rightarrow 2(\Theta - 1)CO + (2 - \Theta)CO_2$	Luecke et al. [40]
Volatiles burn-off			
(R-4)	Gas–gas	$CH_4 + 3/2O_2 \rightarrow CO_2 + 2H_2O$	De Souza-Santos [7]
(R-5)	Gas–gas	$H_2 + 1/2O_2 \rightarrow H_2O$	De Souza-Santos [7]
(R-6)	Gas–gas	$CO + 1/2O_2 \rightarrow CO_2$	De Souza-Santos [7]
(7)	Splitting factor	$p = \frac{\dot{n}_{CO}}{\dot{n}_{CO_2}} = \frac{2(\Theta-1)}{2-\Theta}$	De Souza-Santos [7]
(8)	Particle temperature T_p at combustion conditions	$p = 2500 \ \exp\left(\frac{-6240K}{T_p}\right)$	De Souza-Santos [7]
(9)	Molar consumption of char carbon and oxygen	$\frac{dn_c}{dt} = \Theta \frac{dn_{O_2}}{dt} = -\Theta K A_p C^*_{O_2}$	De Souza-Santos [7]
(10)	Mass conversion of char carbon into carbon monoxide and carbon dioxide	$\frac{dm_c}{dt} = M_c \frac{dn_c}{dt} = \phi \frac{dm_c}{dt}$	De Souza-Santos [7]
(11)	Mass reduction rate of a particle	$\frac{dm_c}{dt} = \frac{dV}{dt}\rho_c = 4\pi r_p^2 \frac{dr_p}{dt}\rho_c = A_p \frac{dr_p}{dt}\rho_c$	De Souza-Santos [7]
(12)	Shrinking rate of a single particle	$\frac{dr_p}{dt} = -\frac{M_C \Theta}{\phi \rho_c} K C^*_{O_2}$	De Souza-Santos [7]
(13)		$\frac{d}{dt}(d_p) = -2 \frac{M_C \Theta}{\phi \rho_c} K C^*_{O_2}$	De Souza-Santos [7]
(14)	Reaction rate for the methane	$-r_{CH_4} = 50.122 \times 10^{10} \frac{1}{s} \left(\frac{m^3}{kmol}\right)^{0.5} \exp\left(\frac{-24157\,K}{T}\right) C^{0.7}_{CH_4} C^{0.8}_{O_2}$	De Souza-Santos [7]
(15)	Reaction rate for the hydrogen	$-r_{H_2} = 10.318 \times 10^{13} \frac{K^{1.5}}{s} \left(\frac{m^3}{kmol}\right)^{1.5} T^{-1.5} \ \exp\left(\frac{-3430\,K}{T}\right) C^{1.5}_{H_2} C_{O_2}$	De Souza-Santos [7]
(16)	Reaction rate for the CO	$-r_{CO} = 4.6 \times 10^{13} \frac{1}{s} \left(\frac{m^3}{kmol}\right) \exp\left(\frac{-15088}{T}\right) C_{CO} \sqrt{C_{O_2} \times C_{H_2O}}$	De Souza-Santos [7]
(17)	The composition of the volatiles	$\xi_{i,v} = \xi_{i,F} \frac{1}{x_v} - \xi_{i,c} \frac{1}{1-x_v}$	De Souza-Santos [7]

An important parameter influencing Θ is the particle temperature T_p at combustion conditions, Table 3, Eq. (8).

If the stoichiometric split of carbon to carbon monoxide and carbon dioxide, respectively, is known, the consumption of oxygen could be directly linked to the molar consumption of carbon.

For the char conversion on the particle surface a reaction order of unity with respect to oxygen has been assumed. Furthermore, the surface reaction rate is proportional to the external particle surface A_p available, Table 3, Eq. (9).

The conversion of char carbon into carbon monoxide and carbon dioxide results in a loss of particle mass which can be easily correlated with the molar consumption of carbon Table 3, Eq. (10).

Since a char particle does not completely consist of carbon, the actual transient char reduction is obtained by multiplying the carbon reduction rate with the carbon content $\varphi = m_C/m_c$ of the char particle. This implies a constant char composition and, hence, a proportional release of O, H, N and S atoms with C atom oxidation. The actual composition of the char must be determined experimentally, and is an input for the combustor model. With the further assumptions of a constant particle density and an ideal spherical shape the mass reduction rate can be related to a volume reduction rate, and further to a reduction rate of the particle radius r_p, Table 3, Eq. (11).

The shrinking rate of a single particle can be determined either on the basis of the particle radius, or on the basis of the particle diameter, respectively, Table 3, Eqs. (12) and (13).

The shrinking rate, i.e. the reduction of the particle radius with time, is the link between reaction rate and population balance.

2.1.6. *Volatiles burn-off*

Next to the burn-out of the char particles the oxidation of the released volatile species has to be considered. Basically, the volatiles can be released as any of the eight gas species considered in the overall combustor model, i.e. CO, CO_2, CH_4, H_2, H_2O, O_2, SO_2 and N_2.

On a stoichiometric basis the further oxidation of CO, CH_4 and H_2, is described in Table 3, (R-4), (R-5), (R-6).

The reaction rates for the methane and hydrogen oxidation are taken from De Souza-Santos [7], without any further fitting, Table 3, Eqs. (14) and (15). Methane represents the sum of unburned hydrocarbons. Since the volatiles are the only source of methane its spatial distribution indicates the extent of volatile mixing.

The carbon monoxide oxidation equation in Table 3, Eq. (16) considers the lower reaction rate of homogenous combustion reactions in fluidized beds compared to reactions in the solids-free space. In the case of carbon monoxide one must consider that not only the volatile matter, but also char is a possible source.

2.1.7. *The composition of the volatiles*

The mass of volatiles released in the time t_v must be split up into the single gas species considered in the combustor model, i.e. CO, CO_2, CH_4, H_2, H_2O, O_2, SO_2 and N_2. The net volatile mass flux released is assumed to equal the fuel feed flux times its volatile content as determined by the proximate analysis. Based on the elementary analysis of the initial fuel and the residual char the mass fractions ξi of carbon, hydrogen, oxygen, nitrogen and sulphur (i = C, H, O, N, S) which end up in the volatiles shown in Table 3, Eq. (17).

2.2. *Modelling the fluidized bed reactor*

The main objective of a present model is to combine the kinetics of drying and devolatilization, the chemistry of the reactions and hydrodynamic parameters mathematically to arrive at equations that are useful in estimating the performance and the size of the reactor.

Generally speaking, when creating a fluidized bed gasification model it is convenient to divide the whole process into several sub-models. The sub-models can be treated and solved separately with the aim to approach the whole process in a realistic way. A fluidized-bed reactor can be divided into three main sections: (1) the fluidizing gas entry or distributor section at the bottom, essentially a perforated metal plate that allows entry of the gas through a number of holes; (2) the fluidized-bed itself, which, unless the operation is adiabatic, includes heat transfer surface to control T; (3) the freeboard section above the bed, essentially empty space to allow disengagement of entrained solid particles from the rising exit gas stream [41].

Luecke et al. [40] on the other hand divide a circulating FB gasifier into four regions: (a) the bottom region with high solid volume concentrations, where the flow domain is subdivided into a suspension phase and a bubble phase with an upwards gas flow; (b) splash zone which has the same structure as the upper dilute zone but with higher solid volume concentrations and therefore with higher solids mass fluxes; (c) the upper dilute region where the flow is subdivided into an upward flowing lean suspension (lean phase) and descending clusters (dense phase); (d) fully developed zone which is modeled as a simple continuous stirred-tank reactor with an infinitely small height.

2.2.1. *Distributor section*

The gas distributor type plays a major role in the establishment of uniform gas flux throughout the cross section of the reactor. The main design factor of distributor is the resistance which appears across its area. The distributor resistance also depends on the type, the free open area and the gas flow through it.

De Souza-Santos [42] provides mathematic equations for several types of gas distributors such as perforated plate, porous plate, and perforated tubes or flutes.

Siegel [43] developed more general approach which incorporates pressure drop ratio of a distributor section and fluidized bed.

$$\frac{\Delta P_{\mathrm{d}}}{\Delta P_{\mathrm{b}}} = \frac{1}{n}\left(\frac{U_{\mathrm{mf}}}{U_{\mathrm{t}}}\right)^{1/\bar{n}} \frac{1}{(1-\varepsilon_{\mathrm{mf}})} \tag{5}$$

where

$$\frac{U}{U_{\mathrm{t}}} = \varepsilon^{\bar{n}} \tag{6}$$

The criterion U/U_{t} is function of the Archimedes number [41]

$$Ar = \frac{g\rho_{\mathrm{g}}(\rho_{\mathrm{p}}-\rho_{\mathrm{g}})d_{\mathrm{p}}^3}{\mu_{\mathrm{g}}^2} \tag{7}$$

$$Ar < 10^3 : Re_{\mathrm{mf}} = 6.1 \times 10^{-4} Ar$$

$$U_{\mathrm{mf}} = 0.00061 \frac{g(\rho_{\mathrm{p}}-\rho_{\mathrm{g}})d_{\mathrm{p}}^2}{\mu_{\mathrm{g}}} \tag{8}$$

$$Ar > 10^7 : Re_{\mathrm{mf}} = 0.202 Ar^{0.5}$$

$$U_{\mathrm{mf}} = 0.20\sqrt{\frac{g(\rho_{\mathrm{p}}-\rho_{\mathrm{g}})d_{\mathrm{p}}}{\rho_{\mathrm{g}}}} \tag{9}$$

Since multiorifice distributors are most used in the full-scale FB gasifiers. Baskakov et al. [44] suggested critical resistance at the distributor for fluidization uniformity.

$$\frac{U_{\mathrm{c}}}{U_{\mathrm{mf}}} = \sqrt{1+\frac{\Delta P_{\mathrm{ds}}}{\Delta P_{\mathrm{b}}}} \tag{10}$$

$$\Delta P_{\mathrm{ds}} = \frac{P_{\mathrm{s}}(1-\varepsilon)gd_0}{4\phi}\left[1-\frac{7}{3}\sqrt{\phi}+\frac{4l}{d_0}\right] \tag{11}$$

$$\Delta P_{\mathrm{d}} = \frac{\rho_{\mathrm{g}}U_{\mathrm{c}}^2}{2\phi^2} \tag{12}$$

2.3. *Fluidized bed reactor*

Fluidization occurs when a gas is forced to flow vertically through a bed of particles at such a rate that the buoyed weight of the particles is completely supported by the drag force imposed by the fluid. The particles are then able to move relative to one another. The bed of the fluidized reactor is composed mainly from two phases: (a) emulsion and (b) bubbles.

2.3.1. *Hydrodynamics models*

The hydrodynamics models of fluidization can be categorized in three main classes based on the phases accounted in the reactor single, two and three phase [45]. Single-phase models are too simplistic to be of practical use, while three-phase models tend to be relatively complicated. It should be noted that three-phase models despite their accurate results do not show any significant improvements over the two-phase models since the model predictions are more sensitive to the reaction kinetics than to hydrodynamic parameters.

The two-phase approach considers the fluidized bed reactors to consist of two phases: (a) emulsion and (b) bubbles. The model proposes a separate governing equation for each phase and mass interchange between them. Most of the reactions occur in the emulsion phase since it is combination of the solid and gases. Due to high circulation of the particles in the emulsion phase a high homogeneity of particle composition and the temperature throughout the bed can be achieved. Bubbles on the other hand grow in size from the distributor to the top of the bed. *Bubble wake*, created from small particles located in the emulsion phase,

Table 4
Fundamental equations for biomass gasification in fluidized bed reactor

No.	Description	Equation	Reference
(1)	Minimum fluidisation velocity	$U_{\mathrm{mf}} = \left(\frac{\mu_0}{d_{\mathrm{p}} p_{\mathrm{g}}}\right)\left(\left[(25.25)^2 + \frac{0.0651 d_{\mathrm{p}}^3 g_{\mathrm{p}}(p_{\mathrm{s}} - p_{\mathrm{g}})g}{\mu_{\mathrm{f}}^2}\right]^{1/2} - 25.25\right)$	Grace [91]
(2)	Or Minimum fluidisation velocity	$U_{\mathrm{mf}} = \left(\frac{\mu_{\mathrm{o}}}{d_{\mathrm{p}} p_{\mathrm{g}}}\right)((27.2^2 + 0.0408Ar)^{1/2} - 27.2)$	Grace [91]
(3)	Mass transfer coefficients (Interstitial mass transfer rate to particle surface)	$k_{\mathrm{g}} = \frac{D_{\mathrm{g}}}{d_{\mathrm{p}}}\left(2\varepsilon_{\mathrm{mf}} + 0.69(Sc)^{1/3}\left(\frac{Re}{\varepsilon_{\mathrm{b}}}\right)^{1/2}\right)$	Grace [91]
(4)	Interphase mass transfer coefficients	$k_{\mathrm{BE}} = \frac{U_{\mathrm{mf}}}{3} + \sqrt{\frac{4 D_{\mathrm{G}} \varepsilon_{\mathrm{mf}} U_{\mathrm{b}}}{\pi d_{\mathrm{b}}}}$	Grace [91]
(5)	The interfacial area between bubble and emulsion phases per unit bed volume is	$a_{\mathrm{B}} = \frac{6\varepsilon_B}{d_{\mathrm{b}}}$	Grace [91]
(6)	Johnson's kinetics for char gasification (Rate of the $\mathrm{j_{tb}}$ reaction per unit volume of particle is)	$r_{\mathrm{Egj}} = \frac{\varepsilon_{\mathrm{s}} \rho_0 f_0}{m w_{\mathrm{c}}} r(X) g_j(T_{\mathrm{p}} P_{\mathrm{t}})(\mathrm{kmol\ m^{-3}\,s^{-1}})$	Grace [91]
(7)		$r(X) = \frac{\mathrm{d}X}{\mathrm{d}t} = M_{\mathrm{c}}(1 - X)^{2/3}\ \exp(-aX^2)$	Grace [91]
(8)		$g_j(T_{\mathrm{p}}, p_i) = \frac{\exp(4704/T_{\mathrm{p}})}{60}(k_j)$	Grace [91]
(9)	The Johnson kinetic parameters are	$a = \frac{52.5 p_{\mathrm{H_2}}}{1+54.3 p_{\mathrm{H_2}}} + \frac{0.521 p_{\mathrm{H_2}}^{0.5} p_{\mathrm{H_2O}}}{1+0.707 p_{\mathrm{H_2}} + 0.5 p_{\mathrm{H_2}}^{0.5} p_{\mathrm{H_2O}}}$	Grace [91]
(10)		$k_1 = \frac{\exp(9.0201-17613/T)(1-(p_{\mathrm{CO}} p_{\mathrm{H_2}}/p_{\mathrm{H_2O}} K_{\mathrm{eq1}}))}{[1+\exp(-22.216+24881/T)(1/p_{\mathrm{H_2O}}+16.35(p_{\mathrm{H_2}}/p_{\mathrm{H_2O}})+43.5(p_{\mathrm{co}}/p_{\mathrm{H_2O}}))]}$	Grace [91]
(11)		$k_2 = \frac{\exp(2.6741-18375/T)(1-(p_{\mathrm{CH_4}}/p_{\mathrm{H_2}}^2 K_{\mathrm{eq2}}))}{[1+p_{\mathrm{H_2}}\ \exp(1-10.452+11097/T)]}$	Grace [91]
(12)		$k_3 = \frac{p_{\mathrm{H_2}}^{0.5} p_{\mathrm{H_2O}}\ \exp(12.4663-24746/T_{\mathrm{p}})(1-(p_{\mathrm{CH_4}} p_{\mathrm{CO}}/p_{\mathrm{H_2}} P_{\mathrm{H_2O}} K_{\mathrm{eq3}}))}{[1+\exp(-6.6696+8.443/T_{\mathrm{p}})(p_{\mathrm{H_2}}^{0.5}+0.85 p_{\mathrm{CO}}+18.62(p_{\mathrm{CH_4}}/p_{\mathrm{H_2}}))]^2}$	Grace [91]
(13)		$\log_{10} K_{\mathrm{eq1}} = 7.49 - 7070/T$	Grace [91]
(14)		$\log_{10} K_{\mathrm{eq2}} = -5.373 + 47723/T$	Grace [91]
(15)		$K_{\mathrm{eq3}} = K_{\mathrm{eq2}} K_{\mathrm{eq2}}$	Grace [91]

bursts in to the freeboard section when bubble reaches the top of the bed [45].

Among the two-phase models [46,47,48], the *bubbling bed model* proposed by Kunii and Levenspiel [49] and the *bubble assemblage model* proposed by Kato and Wen [50] have received the most attention (Tables 4 and 5).

Kunii and Levenspiel [49] modified the original version of the two-phase model provided by Toomey and Johnstone [46] by considering cloud-wake phase in addition to the bubble and the emulsion phases. The model incorporates two distinct resistances one from the bubble phase to the cloud-wake phase, and the other from the cloud-wake phase to the emulsion phase. The model assumes that: (a) the bubble are at one size and evenly distributed in the bed; (b) bubble gas stays with the bubble, recirculating and penetrating at a small distance into the emulsion; (c) each bubble drags along with it a wake of solids; (d) the emulsion stays at minimum fluidization conditions, while the relative velocity of gas and solids remain unchanged. State equations for the *bubbling bed model* are presented in Table 6.

Kato and Wen [50] in their *bubble assemblage model* improve the previous models by taking into consideration the change of the bubble size with height in the bed (Tables 7 and 8). The following assumptions were made:

- A fluidized bed may be represented by *n* compartments in a series. The height of each compartment is equal to the size of each bubble at the corresponding bed height.
- Each compartment is considered to consist of a bubble phase and an emulsion phase. The gas flows through the bubble phase, and the emulsion phase is considered to be completely mixed within the phase.
- The void space within the emulsion phase is considered to be equal to that of the bed at the incipient fluidizing conditions. The upward velocity of the gas in the emulsion phase is U_{e}.

Table 5
Kinetic parameters and rate expressions for reactions of FB biomass gasification

No	Description	Equation	Reference
(1)	Homogeneous water-gas shift reaction	$r_j = k_j C_{\mathrm{H_2O}} C_{\mathrm{CO}} - \frac{k_{\mathrm{J}}}{k_{\mathrm{J}}^{\mathrm{E}}} C_{\mathrm{CO_2}} C_{\mathrm{H_2}}$	
(2)	Catalytic water-gas shift reaction	$r_j = f_{\mathrm{wg}} k_{\mathrm{t}} P_{\mathrm{T}}\left(p_{\mathrm{co}} - \frac{p_{\mathrm{H_2}} p_{\mathrm{CO_2}}}{p_{\mathrm{H_2O}} K_{\mathrm{eq.wg}}}\right)$	Yan et al. [23]
(3)		$k = 1.26 \times 105\ \exp(-E/RT)$	Yan et al. [23]
(4)	Rate expressions for the simultaneous combustion of Hz and CO	$r_{\mathrm{CO}} = k_{\mathrm{CO}} C_{\mathrm{CO}}^2 C_{\mathrm{CO_2}}$ $r_{\mathrm{H_2}} = k_{\mathrm{H_2}} C_{\mathrm{H_2}}^2 C_{\mathrm{CO_2}}$	Yan et al. [23]
(5)		$k_{\mathrm{CO}}/k_{\mathrm{H_2}} = 0.35$	Yan et al. [23]
(6)	The rate constant in the rate expressions above is	$k_{\mathrm{CO}} = 2.4601 \times 10^{-12}\ \exp\left(-\frac{21137}{T} + 24.74414\right) T^3$	Yan et al. [23]

Table 6
State equations for the two-phase model

No	Description	Equation	Reference
(1)	Bubble velocity	$u_{\mathrm{b}} = (U - U_{\mathrm{mf}}) + 0.711(gd_{\mathrm{b}})^{0.5}$	Kunii and Levenspiel [49]
(2)	Bed fraction in bubbles	$\delta = \frac{(U-[1-\delta-\alpha\delta]U_{\mathrm{mf}})}{u_{\mathrm{b}}} \cong \frac{U-U_{\mathrm{mf}}}{u_{\mathrm{b}}}$	Kunii and Levenspiel [49]
(3)	Bed fraction in clouds	$\beta = \frac{3\delta(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}{u_{\mathrm{br}}-(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}$	Kunii and Levenspiel [49]
(4)	Bed fraction in wakes	$\omega = \alpha\delta$	Kunii and Levenspiel [49]
(5)	Bed fraction in downflowing emulsion including clouds	$\bar{\omega} = 1 - \delta - \alpha\delta$	Kunii and Levenspiel [49]
(6)	Downflow velocity of emulsion solids	$u_{\mathrm{s}} = \frac{\alpha\delta u_{\mathrm{b}}}{1-\delta-\alpha\delta}$	Kunii and Levenspiel [49]
(7)	Rise velocity of emulsion gas	$u_{\mathrm{e}} = \frac{U_{\mathrm{mf}}}{\varepsilon_{\mathrm{mf}}} - u_{\mathrm{s}}$	Kunii and Levenspiel [49]
(8)	Interchange of gas between bubble and cloud is	$K_{\mathrm{bc}} = 4.5\frac{U_{\mathrm{mf}}}{d_{\mathrm{b}}} + 5.85\frac{D^{0.5}g^{0.25}}{d_{\mathrm{b}}^{1.25}}$	Kunii and Levenspiel [49]
(9)	Interchange of gas between cloud and emulsion	$K_{\mathrm{ce}} = 6.78\left(\frac{\varepsilon_{\mathrm{mf}}Du_{\mathrm{b}}}{d_{\mathrm{b}}^{3}}\right)^{0.5}$	Kunii and Levenspiel [49]

Table 7
State equations of two-phase model

No	Description	Equation	Reference
(1)	Mole balance for species A in the emulsion phase	$\frac{\mathrm{d}C_{\mathrm{Ao}}}{\mathrm{d}z} = \frac{R_{\mathrm{Ao}}(1-\varepsilon_{\mathrm{mf}})p_{\mathrm{s}}(1-\delta)+K_{\mathrm{be}}\delta(C_{\mathrm{Ab}}-C_{\mathrm{Ao}})}{U_{\mathrm{mf}}(1-\delta)}$	Mostoufi et al. [51]
(2)	Mole balance for species A in the bubble phase	$\frac{\mathrm{d}C_{\mathrm{Ab}}}{\mathrm{d}z} = -\frac{\mathrm{K}_{\mathrm{be}}(C_{\mathrm{Ab}}-C_{\mathrm{Ao}})}{U_{\mathrm{b}}}$	Mostoufi et al. [51]
(3)	Mean concentration of species A	$C_{\mathrm{A}} = \frac{U_{\mathrm{mf}}(1-\delta)}{U_{\mathrm{o}}}C_{\mathrm{Ae}} + \frac{U_{\mathrm{b}}\delta}{U_{\mathrm{o}}}C_{\mathrm{Ab}}$	Mostoufi et al. [51]
(4)	Bubble fraction	$\delta = \frac{U_{\mathrm{o}}-U_{\mathrm{mf}}}{U_{\mathrm{b}}-U_{\mathrm{mf}}}$	Mostoufi et al. [51]
(5)	Average bed voidage	$\varepsilon = (1 - \delta)\varepsilon_{\mathrm{mf}} + \delta$	Mostoufi et al. [51]

- The bubble phase is assumed to consist of spherical bubbles surrounded by spherical clouds. The voidage within the cloud is assumed to be the same as that in the emulsion phase,
- Gas interchange takes place between the two phases.
- The bubbles are considered to grow continuously while passing through the bed until they reach the maximum stable size, or reach the diameter of the bed column.
- The bed is assumed to be operating under isothermal conditions since the effective thermal diffusivity and the heat transfer coefficient are large.

State equations for the Bubble Assemblage Model are presented in Table 9, Sett and Bhattacharya [20] used the *Bubble Assemblage Model* to simulate Fluidised-Bed Charcoal Gasifier. They described a riser as a several different regions which can be treated as a continuous flow stirred tank (CFST) reactor with the temperature and composition the same at every point within the bubble and the emulsion phase. In order to model the charcoal FB gasifier, Sett and Bhattacharya [20] made the following assumptions; (a) the emulsion phase voidage and velocity are constant at $\varepsilon_{\mathrm{mf}}$ and U_{mf} respectively; (b) bubbles are spherical; (c) the cloud and wake portions of the bubble are lumped with the emulsion phase, and bubbles are free of solids; (d) certain fraction of solids is carried up with the rising bubbles which has been treated as an adjustable parameter in their model.

De Souza-Santos [7] in his comprehensive model of fluidized bed boilers and gasifiers uses a modification of the two-phase model, which includes the cloud region in the emulsion phase. The emulsion phase can be departed from the minimum fluidization condition. Also he suggested that the conceptual separation of the cloud region is unnecessary.

Mostoufi et al. [51] in their work summarize three different hydrodynamic models for predicting the performance of the fluidized bed. The models are (1) Simple Two-Phase Model (STP) (2) Dynamic Two-Phase Structure Model (DTP) and (3) Plug-Flow Model (PF).

Ross et al. [18] have improved their one-dimensional numerical isothermal model of a fluidised-bed coal gasifier by

Table 8
State equations for the dynamic two-phase structure model

No	Description	Equation	Reference
(1)	Mole balance for species A in the emulsion phase	$\frac{\mathrm{d}C_{\mathrm{Ae}}}{\mathrm{d}z} = \frac{R_{\mathrm{Ae}}(1-\varepsilon_{\mathrm{e}})p_{\mathrm{s}}(1-\delta)+K_{\mathrm{be}}\delta(C_{\mathrm{Ab}}-C_{\mathrm{Ae}})}{U_{\mathrm{o}}(1-\delta)}$	Mostoufi et al. [51]
(2)	Mole balance for species A in the emulsion phase	$\frac{\mathrm{d}C_{\mathrm{Ab}}}{\mathrm{d}z} = \frac{Rb(1-\varepsilon_{\mathrm{e}})p_{\mathrm{s}}+K_{\mathrm{be}}\delta(C_{\mathrm{Ab}}-C_{\mathrm{Ae}})}{U_{\mathrm{b}}}$	Mostoufi et al. [51]
(3)	Mean concentration of species A	$C_{\mathrm{A}} = \frac{U_{\mathrm{e}}(1-\delta)}{U_0}C_{\mathrm{Ae}} + \frac{U_{\mathrm{b}}\delta}{U_{\mathrm{o}}}C_{\mathrm{Ab}}$	Mostoufi et al. [51]
(4)	Average emulsion voidage	$\varepsilon_{\mathrm{e}} = \varepsilon_{\mathrm{mf}} + 0.00061\ \exp\left(\frac{U_0-U_{\mathrm{mf}}}{0.262}\right)$	Mostoufi et al. [51]
(5)	Average bubble voidage	$\varepsilon_{\mathrm{b}} = 0.784 - 0.139\ \exp\left(\frac{U_{\mathrm{o}}-U_{\mathrm{mf}}}{0.272}\right)$	Mostoufi et al. [51]
(6)	Bubble fraction	$\delta = 1 - \exp\left(-\frac{U_{\mathrm{o}}-U_{\mathrm{mf}}}{0.62}\right)$	Mostoufi et al. [51]
(7)	Emulsion velocity	$U_{\mathrm{e}} = \frac{U_{\mathrm{o}}-\delta U_{\mathrm{b}}}{1-\delta}$	Mostoufi et al. [51]
(8)	Average bed voidage	$\varepsilon = (1 - \delta)\varepsilon_{\mathrm{e}} + \delta\varepsilon_{\mathrm{b}}$	Mostoufi et al. [51]

Table 9
State equations for the bubble assemblage model

No.	Description	Equation	Reference
(1)	Bubble size	$d_{\mathrm{b}} = 0.14\rho_{\mathrm{p}} d_{\mathrm{p}} \left(\frac{U}{U_{\mathrm{mf}}}\right) h + d_{\mathrm{o}}$	Cooke et al. [92]
(2)		$d_{\mathrm{o}} = 0.025 \frac{[6(U-U_{\mathrm{mf}})/(n_{\mathrm{o}}\pi)]^{0.4}}{g^{0.2}}$	Cooke et al. [92]
(3)	Maximum stable bubble size	$d_{\mathrm{b,t}} = \left(\frac{u_{\mathrm{t}}}{0.711}\right)^2 \frac{1}{g}$	Davidson and Harrison [47]
(4)	Diameter of the bubbles and that of clouds	$\left(\frac{d_{\mathrm{c}}}{d_{\mathrm{b}}}\right)^3 = \frac{u_{\mathrm{br}}+2(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}{u_{\mathrm{br}}-(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}, \quad u_{\mathrm{br}} \geq \frac{U_{\mathrm{mf}}}{\varepsilon_{\mathrm{mf}}}$	Davidson and Harrison [47]
(5)	Bubble velocity	$u_{\mathrm{b}} = (U - U_{\mathrm{mf}}) + 0.711(g d_{\mathrm{b}})^{0.5}$	Davidson and Harrison [47]
(6)	Bed expansion, based	$\frac{L-L_{\mathrm{mf}}}{L_{\mathrm{mf}}} = \frac{U-U_{\mathrm{mf}}}{0.711(g d_{\mathrm{b,a}})^{0.5}}$	Davidson and Harrison [47]
(7)	Average bubble diameter of the bed	$d_{\mathrm{b,a}} = 0.14\rho_{\mathrm{p}} d_{\mathrm{p}} \frac{U}{U_{\mathrm{mf}}} \frac{L_{\mathrm{mf}}}{2} + d_{\mathrm{o}}$	Davidson and Harrison [47]
(8)	Voidage of the bed (a) condition	$1 - \varepsilon = \frac{L_{\mathrm{mf}}}{L}(1 - \varepsilon_{\mathrm{mf}}), \quad h \leq L_{\mathrm{mf}}$	Davidson and Harrison [47]
(9)	Voidage of the bed (b) condition	$1 - \varepsilon = \frac{L_{\mathrm{mf}}}{L}(1 - \varepsilon_{\mathrm{mf}}) - 0.5 \frac{L_{\mathrm{mf}}(1-\varepsilon_{\mathrm{mf}})(h-L_{\mathrm{mf}})}{2L(L-L_{\mathrm{mf}})}, \quad L_{\mathrm{mf}} \leq h \leq L_{\mathrm{mf}} + 2(L - L_{\mathrm{mf}})$	Davidson and Harrison [47]
(10)	Superficial gas velocity in emulsion phase	$\frac{U_{\mathrm{e}}}{U_{\mathrm{mf}}} = 1 - \frac{\varepsilon_{\mathrm{mf}} a' \theta u_{\mathrm{b}}}{U_{\mathrm{mf}}(1-\theta-\alpha'\theta)}, \quad \theta = \frac{L-L_{\mathrm{mf}}}{L}$	Davidson and Harrison [47]
(11)	Overall mass interchange coefficient per unit volume of gas bubbles	$F_{\mathrm{D}} = F_{\mathrm{o}} + K'M$	Davidson and Harrison [47]
(12)	The model neglects gas interchange due to adsorbed gas on interchanging particles	$F_{\mathrm{d}} = F_{\mathrm{o}} = \frac{0.11}{d_{\mathrm{b}}}$	Davidson and Harrison [47]
(13)	The height of the initial compartment immediately above the distributor	$\Delta h_1 = \frac{d_{\mathrm{o}}+(\psi\,\Delta h_1+d_{\mathrm{o}})}{2}$	Kato and Wen [50]
(14)	The above height written differently	$\Delta h_1 = \frac{2d_{\mathrm{o}}}{2-\psi}$	Kato and Wen [50]
(15)	Constant relating the bubble diameter	$\psi = 0.14\rho_{\mathrm{p}} d_{\mathrm{p}} \frac{U}{U_{\mathrm{mf}}}$	Kato and Wen [50]
(16)	The height of the second compartment	$\Delta h_2 = 2d_0 \frac{2+\psi}{(2-\psi)^2}$	Kato and Wen [50]
(17)	The height of the *n*th compartment	$\Delta h_{\mathrm{n}} = 2d_0 \frac{(2+\psi)^{n-1}}{(2-\psi)^n}$	Kato and Wen [50]
(18)	Number of bubbles in the nth compartment	$N = \frac{6S(\varepsilon-\varepsilon_{\mathrm{mf}})}{\pi(\Delta h_{\mathrm{n}})^2(1-\varepsilon_{\mathrm{mf}})}$	Kato and Wen [50]
(19)	Volume of cloud in the nth compartment	$V_{\mathrm{cn}} = \frac{N\pi(\Delta h_{\mathrm{n}})^3}{6} \frac{3(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}{u_{\mathrm{br}}-U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}}}$	Kato and Wen [50]
(20)	Total volume of the bubble phase (bubble and cloud) and that of the emulsion phase in the nth compartment	$V_{\mathrm{cn}} = \frac{N\pi(\Delta h_{\mathrm{n}})^3}{6} \frac{u_{\mathrm{br}}+2(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}{u_{\mathrm{br}}-U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}}}$	Kato and Wen [50]
(21)	Volume of emulsion phase at the nth compartment	$V_{\mathrm{en}} = S\,\Delta h_{\mathrm{n}} - V_{\mathrm{bn}}$	Kato and Wen [50]
(22)	The gas interchange coefficient based on unit volume of bubble phase (bubble and cloud)	$F'_{\mathrm{on}} = F_{\mathrm{on}} \frac{u_{\mathrm{br}}-(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}{u_{\mathrm{br}}+2(U_{\mathrm{mf}}/\varepsilon_{\mathrm{mf}})}$	Kato and Wen [50]
(23)	The material balance for the gaseous reactant around the *n*th compartment becomes, for the bubble phase	$(\mathrm{SUC}_{\mathrm{A,b}})_{n-1} = [F'_{\mathrm{on}} V_{\mathrm{b}}(C_{\mathrm{A,b}} - C_{\mathrm{A,e}})]_n + (r_{\mathrm{A,c}} V_{\mathrm{c}})_n + (\mathrm{SUC}_{\mathrm{A,b}})_n$	Kato and Wen [50]
(24)	The material balance for the gaseous reactant around the *n*th compartment becomes, for the emulsion phase	$[F'_{\mathrm{on}} V_{\mathrm{b}}(C_{\mathrm{A,b}} - C_{\mathrm{A,e}})]_n = (r_{\mathrm{A,c}} V_{\mathrm{c}})_n$	Kato and Wen [50]

considering the non-isothermal behaviour of gases and heat transfer mechanisms in the fluidised-bed. Their model is based on *two-phase theory* of bubbling fluidised bed [47]. An important resulting feature of the modelling work is the consideration of the "*net flow*" term from the emulsion phase to the bubble phase in the model conservation equations.

The formulation of the isothermal two-phase fluidised bed gasifier model with the "*net flow*" term has been described in detail previously by Yan et al. [23,24].

Jiang and Morey [12] provided a model of the fluidized bed biomass gasifier based on *two-phase* fluidization theory. The model involves concentrations of eight gas species, each of which is described with a system of two differential equations, one for the bubble phase and the other for the dense phase.

Fiaschi and Michelini [8] used a *two-phase* model as a basis for their study, with a dense phase (gas plus solid particles) and a bubble phase (mainly gaseous with much lower solid matter). The two-phase reactor is modelled as the sum of several elemental reactors of dz thickness. The related differential equations are solved versus the temperature and the syngas composition, along the gasifier axis, for both dense and bubble phases.

2.3.2. Minimum fluidization velocity

The minimum fluidization velocity $U_{\rm mf}$ is one of the basic design parameters to estimate fluidization conditions in the reactor. Ergun [52] developed equations which are referenced the most in the literature [45,42] in the field of fluid–solid flows.

$$U_{\rm mf} = \frac{N_{Re,\rm mf}\mu_{\rm G,av}}{d_{\rm p,av}\rho_{\rm G,av}} \qquad (13)$$

$$N_{Re,\rm mf} = (a_1^2 + a_2 N_{Ar})^{1/2} - a_1 \qquad (14)$$

$$N_{Ar} = \frac{g d_{\rm p,av}^3 \rho_{\rm G,av}(\rho_{\rm P,av} - \rho_{\rm G,av})}{\mu_{\rm G,av}^2} \qquad (15)$$

Values of a_1 and a_2 referred in the literature are shown in Table 1.

Wen [53] correlation is considered as most widely used to predict the effects of temperature and pressure on minimum fluidization velocity.

$$U_{\rm mf} = \frac{\mu}{\rho_{\rm g} d_{\rm p}}\left[\frac{33.7^2 + 0.0408 d_{\rm p}^3 \rho_{\rm g}(\rho_{\rm p} - \rho_{\rm g})g}{\mu^2}\right]^{0.5} \qquad (16)$$

For small particles

$$U_{\rm mf} = \frac{d_{\rm p}^2 (p_{\rm p} - p_{\rm g})g}{1650\mu}, \quad Re_{\rm p,mf} < 20 \qquad (17)$$

For large particles

$$U_{\rm mf}^2 = \frac{d_{\rm p}(p_{\rm p} - p_{\rm g})g}{24,5\rho_{\rm g}}, \qquad Re_{\rm p,mf} > 1000 \qquad (18)$$

Some references have been found in the literature about the minimum fluidization velocities of sand/biomass mixtures, however none of conventional equations were able to give reliable predictions [54–57].

The effects of temperature and pressure on fluidized-bed systems cannot be considered independently of particle size. Whether temperature and pressure have an effect on a system depends strongly on particle size. In addition, the type of interaction between gas and solids, i.e. whether the interaction is due to momentum or drag, determines if gas viscosity has an effect upon the system Yang (1998).

Rao et al. [57] concluded that the minimum fluidization velocity of biomass/sand mixtures is increased with increasing biomass weight fraction, as well as with increasing sand density and particle size. Therefore they determined new correlations based on Wen [53] equations for small particles ($N_{\rm Re,mf} < 20$).

$$U_{{\rm mf},m} = \frac{d_{\rm peff}^2 (p_{\rm eff} - p_{\rm g})g}{1650\mu_{\rm g}} \qquad (19)$$

$$p_{\rm eff} = k\frac{w_1 p_1 + w_2 p_2}{w_1 + w_2} \qquad (20)$$

$$d_{\rm peff}^2 = k\left[d_{\rm p1}\left[\left(\frac{\rho_1}{\rho_2}\right)\left(\frac{d_{\rm p2}}{d_{\rm p1}}\right)^{w2/w1}\right]\right]^2 \qquad (21)$$

$$k = 20 d_{\rm p1} + 0.36 \qquad (22)$$

Kozanoglu et al. [58] concluded for large particle fluidization that when the absolute pressure is decreased, the minimum fluidization velocity is increased, whereas the bed voidage at minimum fluidization was practically unaffected. The prediction of $U_{\rm mf}$ was correlated to:

(a) for rounded particles (sphericity > 0.8)

$$Re_{\rm mf} = \left[\left(\frac{0.982}{Knp + 0.0155}\right)^2 + 0.0546 Ar\right]^{1/2} - \frac{0.982}{(Knp + 0.0155)} \qquad (23)$$

(b) for angular particles (0.5 < sphericity_0.8)

$$Re_{\rm mf} = \left[\left(\frac{1.397}{Knp + 0.0158}\right)^2 + 0.0650 Ar\right]^{1/2} - \frac{1.397}{(Knp + 0.0158)} \qquad (24)$$

where $Knp = \lambda/{\rm d}p$ is the Knudsen number, with λ being the mean free path.

Suarez and Beaton [59] suggest that the minimum fluidization velocity of coffee husks in a small cold-model column equipped with a perforated plate distributor can be predicted by following equations.

$$U_{\rm mf} = 0.19\,{\rm e}^{0.305 d_{\rm p}} \qquad (25)$$

$$u_{\rm t} = 1.55\,{\rm e}^{0.081 d_{\rm p}} \qquad (26)$$

Yang et al. [60] provided a graphical method for predicting of minimum fluidization velocity at elevated pressure and temperature. The procedure includes experimental determination of

U_{mf} and then the data is located on a curve of constant $\varepsilon_{\mathrm{mf}}$ on a plot of:

$$[(Re)_{\varepsilon}^{2}(C_{\mathrm{D}})_{\varepsilon}]_{\mathrm{mf}}^{1/3} \quad \text{vs.} \quad [(Re)_{\varepsilon}/(C_{\mathrm{D}})_{\varepsilon}]_{\mathrm{mf}}^{1/3} \tag{27}$$

Cobbinah et al. [61] determined new correlation for low-velocity hydrodynamic regimes between the minimum fluidization velocity of the fine particles and a critical value of superficial gas velocity.

$$Re_{\mathrm{mc}} = \frac{\rho_{\mathrm{g}} d_{\mathrm{p}} U_{\mathrm{mc}}}{\mu_{\mathrm{g}}} = 4.331 \times 10^{-3} Ar^{0.732} \left(\frac{d_{\mathrm{G}}}{d_{\mathrm{p}}}\right)^{1.322} \tag{28}$$

2.3.3. Particle terminal velocity

De Souza-Santos [42] provides us equations for terminal velocity $U_{\mathrm{T,\,av}}$ of single near spherical particle of diameter d_{p}. These equations can be applied only in systems with high void fractions (above 0.8).

$$U_{\mathrm{T}} = \frac{d_{\mathrm{p}}^{2}(p_{\mathrm{p}} - p_{\mathrm{g}})g}{18\mu_{\mathrm{g}}}, \quad Re \leq 2 \tag{29}$$

$$U_{\mathrm{T}} = \left[\frac{d_{\mathrm{p}}^{1,6}(p_{\mathrm{p}} - p_{\mathrm{g}})g}{13.9\rho_{\mathrm{g}}^{0.5}\mu^{0.6}}\right]^{0.71}, \quad 2 < Re \leq 500 \tag{30}$$

$$U_{\mathrm{T}} = \left[\frac{3.03 d_{\mathrm{p}}(p_{\mathrm{p}} - p_{\mathrm{g}})g}{\rho_{\mathrm{g}}}\right]^{0.5}, \quad Re > 500 \tag{31}$$

2.3.4. Bed Voidage

The bed voidage is defined as the fraction of the total volume, which is occupied by gas, therefore:

$$\varepsilon = \frac{V_{\mathrm{m}}}{V} \tag{32}$$

where V is the total volume of the fluidized bed and V_{m} is volume of fluidized bed occupied by the media (gas, bubbles, emulsion phase) [42].

The fluidized-bed voidage at minimum bubbling conditions $\varepsilon_{\mathrm{mb}}$ is increased by temperature [62] and pressure [63].

Kmiec [64] determined correlation for dense-phase voidage:

$$\varepsilon_{\mathrm{d}} = \frac{(18Re_{\mathrm{p}} + 2.7Re_{\mathrm{p}}^{1.687})^{0.209}}{\mathrm{Ga}^{0.209}} \tag{33}$$

Wen [53] provided empirical equation for void fraction at minimum fluidization.

$$\varepsilon_{\mathrm{mf}} = \left(\frac{1}{14\phi_{\mathrm{A}}}\right)^{1/3} \tag{34}$$

Delvosalle and Vanderschuren [65] determined correlation of the void fraction in the emulsion phase:

$$\varepsilon_{\mathrm{E}} = \varepsilon_{\mathrm{mf}}\left(\frac{U_{\mathrm{E}}}{U_{\mathrm{mf}}}\right)^{1/6.7} \tag{35}$$

The bed expansion factor is:

$$\varepsilon = 1 - \frac{1 - \varepsilon_{\mathrm{mf}}}{f_{\mathrm{b\,exp}}} \tag{36}$$

2.3.5. Bubbles in fluidized bed

Fluidized bed is to be considered stable when it is not bubbling and unstable when bubbling. There is generally two theories which explain instability of the bed; (a) Interparticle Force Theory, proposed by Rietema et al. [66] and; (b) Hydrodynamic Theory of fluidized bed, proposed by Foscolo and Gibilaro [67].

The *Interparticle Force Theory* suggests that in the elasticity of bed interpartical forces are playing the major role. The equation which shows when the fluidized bed become unstable (starts to bubble) shown hereafter.

$$\frac{\rho_{\mathrm{p}}^{3} d_{\mathrm{p}}^{4} g^{2}}{\mu^{2}\mathrm{M}_{\mathrm{mb}}} = \left[\frac{150(1 - \varepsilon_{\mathrm{mb}})}{\varepsilon_{\mathrm{mb}}^{2}(2 - 2\varepsilon_{\mathrm{mb}})}\right]^{2} \tag{37}$$

The left side of equation is smaller of a right side when the bed is stable. The bed becomes unstable (bubbling) when the right side is bigger than left side.

Foscolo and Gibilaro [67] in their Hydrodynamic Theory postulated that a fluidized bed is composed of two interpenetrating fluids. The gas and solid phases are considered as continuous fluid phases. The stability of the fluidized bed depends upon relative velocities of dynamic (u_{ε}) and kinetic (u_{e}) waves which are created due to voidage disturbances in the bed.

$$u_{\mathrm{e}} = n u_{\mathrm{t}}(1 - \varepsilon)\varepsilon^{n-1} \tag{38}$$

$$u_{\mathrm{e}} = \sqrt{\frac{3.2 g d_{\mathrm{p}}(1 - \varepsilon)(\rho_{\mathrm{p}} - \rho_{\mathrm{g}})}{\rho_{\mathrm{p}}}} \tag{39}$$

If (u_{ε}) is greater than (u_{e}) then the bed will be stable, otherwise it will be unstable (bubbling).

2.3.6. Mass and solid fractions of solids

The mass fraction of particles kind m (f_m) among all other solid species ($m = 1$–n) is easily calculated De Souza-Santos [42]:

$$f_m = \frac{F_{\mathrm{LD},m}}{\sum_{m=1}^{n} F_{\mathrm{LD},m}} \tag{40}$$

and the volume fraction can be calculated from

$$f_m = \frac{F_{\mathrm{LD},m}/\rho_{\mathrm{p},m}}{\sum_{m=1}^{n}(F_{\mathrm{LD},m}/\rho_{\mathrm{p},m})} \tag{41}$$

2.3.7. Mass balances inside the FB riser

A general form which any kind of mass conservation balance follows is given Patankar [68]:

$$\frac{\partial}{\partial t}C_i + \mathrm{div}(uC_i) = \mathrm{div}(D_{i,\mathrm{eff}}\,\mathrm{grad}\,C_i) + r_i \tag{42}$$

In analogy to the single particle approach and its division into a devolatilization and a subsequent char combustion step two types of mass balances concerning the solid phase can be described. The first type covers the fuel dispersion during the gasification process, while the second one results in a char population balance under steady-state conditions. Simultaneously to the char balance the steady-state gas balances have to be solved, since both local gas and local char concentrations are linked by the combustion reaction rates.

2.3.8. Gas balances in the riser bottom zone

Due to the large cross-sectional area of industrial combustion chambers and because of the very shallow bottom bed with a height less than 1 m, horizontal gas mixing in the bottom region is neglected [69]. Thus, vertical convection is the dominating transport mechanism for the gas. The bubble phase is assumed to be free from solid particles. The mass exchange coefficient k_{ig} between the bubble and suspension phases is calculated [70]. Because of the increase of bubble size and velocity, the bubble volume fraction is decreasing with height. This is leading to a convective exchange flux between the phases which is taken into account by introducing the coefficient $k_{\mathrm{conv,\,bz}}$. The balance for a gas species i in the bubble phase hold then:

$$0 = \frac{\partial(u_0 - u_{\mathrm{sp}}(1-\varepsilon_b))c_{i,\mathrm{b}}}{\partial z} + k_{ig}a(C_{i,\mathrm{b}} - C_{i,\mathrm{sp}}) + k_{\mathrm{conv,bz}}C_{i,\mathrm{b}} - \varepsilon_{\mathrm{b}}r_{i,\mathrm{b}} \tag{43}$$

with the boundary conditions at the gas distributor

$$z = 0 : C_{i,\mathrm{b}} = C_{i,0} \tag{44}$$

For a gas species i in the suspension phase we obtain a similar equation:

$$o = u_{\mathrm{sp}}\frac{\partial((1-\varepsilon_{\mathrm{b}})C_{i,\mathrm{sp}})}{\partial z} - k_{ig}a(C_{i,\mathrm{b}} - C_{i,\mathrm{sp}}) - k_{\mathrm{conv,bz}}C_{i,\mathrm{b}} - (1-\varepsilon_{\beta})r_{i,\mathrm{sp}} \tag{45}$$

$$z = 0 : C_{i,\mathrm{sp}} = C_{i,0} \tag{46}$$

The equations for the single gas species are linked to each other and to the char balance by the reaction rates $i_{i,\mathrm{b}}$ and $r_{i,\mathrm{sp}}$, respectively.

2.3.9. Gas mass balance in the upper dilute and splash zones

Horizontal dispersion J as well as horizontal convection Fx and Fy plays a great role in the upper dilute and splash zones. The dispersion coefficient Dg is assumed to be equal in the x and y directions, respectively. The vertical gas convection fluxes Fz of the dilute and dense phases have opposite orientations. It is also assumed that the solid volume concentration in the dense phase is higher than in the lean phase. This leads to different reaction rates R in both phases and thus to a difference in the concentrations of the gaseous species, which causes a mass transfer V_{ex} between the dense and the lean phase [40]. The mass transfer is governed by the product of the mass transfer coefficient k based on unit mass transfer area and the volume specific mass transfer area a between the two phases. A correlation for k & a can applied in the model calculations [71]. It must be noted that the flow conditions are changing with height in the upper dilute zone, leading to a lateral convective exchange flux between the dense and the lean phase occurs. The convective exchange flux is considered in the mass balance by introducing the transfer coefficient k_{conv}. The final mass balance for the gas species i in the lean phase and its boundary conditions are then given by

$$\begin{aligned} -(1-f_{\mathrm{d}})r_{i,l} - (1-f_{\mathrm{d}})\dot{\rho}_{i,l} - ka(C_{i,l} - C_{i,\mathrm{d}}) - k_{\mathrm{conv}}C_{i,l} &= D_{\mathrm{g,up}}(1-c_{v,l})\left(\frac{\partial}{\partial x}\left((1-f_{\mathrm{d}})\frac{\partial C_{i,l}}{\partial x}\right)\right. \\ &\quad \left. + \frac{\partial}{\partial y}\left((1-f_{\mathrm{d}})\frac{\partial C_{i,l}}{\partial y}\right)\right) - \frac{\partial}{\partial x}(u_{l,x}(1-f_{\mathrm{d}})(1-c_{v,l})C_{i,l}) \\ &\quad - \frac{\partial}{\partial y}(u_{l,y}(1-f_{\mathrm{d}})(1-c_{v,l})C_{i,l}) \\ &\quad - \frac{\partial}{\partial z}(u_{l,z}(1-f_{\mathrm{d}})(1-c_{v,l})C_{i,l}) \end{aligned} \tag{47}$$

$$\begin{aligned} &x = 0, L_x : \frac{\partial C_{i,l}}{\partial x} = 0 \quad y = 0, L_y : \frac{\partial C_{i,l}}{\partial y} = 0 \\ &z = H_{\mathrm{bz}} : C_{i,l} = \bar{C}_{i,\mathrm{spb}} \end{aligned} \tag{48}$$

The dilution of the other components is accounted for by an increased gas flux which results in increased gas velocities.

The dense phase is assumed to be dispersed in the continuous lean phase therefore no horizontal mass fluxes can occur and the mass balance can be simplified with the following boundary conditions:

$$z = H_{\mathrm{riser}} : C_{i,\mathrm{d}} = \bar{C}_{i,\mathrm{top}} \tag{49}$$

The distribution of the upward gas velocity in the lean phase $u_{l,z}$ over the cross-sectional area is changing with height such that the profile is flattening out [72].

The flow potential $\Phi_{\mathrm{g,\,up}}$ of the overall gas balance over one control volume look like follows:

$$0 = \dot{Q}_{g,\mathrm{up}}(x,y) + \frac{\partial^2 \Phi_{\mathrm{g,up}}}{\partial x^2} + \frac{\partial^2 \Phi_{\mathrm{g,up}}}{\partial y^2} \tag{50}$$

There is also an intermediate gas mass balance between the bottom zone and the splash zone has to be formulated. The *potential flow theory* will be used again, by modifying the general Eq. (47).

$$\dot{Q}_{\mathrm{g,int}}(x,y) = \frac{\partial}{\partial z}(f_{\mathrm{d}}u_{\mathrm{d},z}(1-c_{v,\mathrm{d}}) + (1-f_{\mathrm{d}})u_{l,z}(1-c_{v,l})|_{H_{\mathrm{bz}}} - u_{\mathrm{o}}) \tag{51}$$

2.3.10. Fuel distribution balance

Solid fuel particles enter the combustor in the FB bottom zone. Upon entering the reactor a solid fuel particle starts to dry and simultaneously looses its volatile matter. During this time the fuel particle will already be spread over the cross-sectional area of the bed by dispersion and convection. The volatiles are assumed to be released in the bottom zone only, and since in this zone ideal mixing of the solids is assumed in vertical direction, i.e. z direction, the balance is limited to two dimensions only, i.e. the x and y direction [40].

For modelling purposes the char fraction of the entering fuel is balanced only. Since the char is assumed to start burning only after complete devolatilization, the balance does not include any reaction terms and the transient distribution process is described by:

$$\frac{\partial C_{\mathrm{F,c}}}{\partial t} = D_{\mathrm{s,bz}}\frac{\partial^2 C_{\mathrm{F,c}}}{\partial x^2} + D_{\mathrm{s,bz}}\frac{\partial^2 C_{\mathrm{F,c}}}{\partial y^2} - \frac{\partial^2}{\partial x^2}(u_{\mathrm{bz},x}C_{\mathrm{F,c}}) - \frac{\partial^2}{\partial y^2}(u_{\mathrm{bz},y}C_{\mathrm{F,c}}) \tag{52}$$

This balance has to be solved for each particle size separately. The initial conditions for the size fraction in the interval (d_{p}, $d_{\mathrm{p}} + d(d_{\mathrm{p}})$) at $t_{\mathrm{o}} = 0$ are a fuel char field of $C_{\mathrm{F,\,c}}(x, y, d\mathrm{p}, i, t = 0) = 0$ at any position combined with an initial feed impulse at the feed chute only [40]:

$$t_0 = 0 : u_{\mathrm{bz},x}C_{\mathrm{F,c}}(1-\varepsilon_{\mathrm{b}})|_{y\mathrm{F}} = -\frac{m_{\mathrm{F}}(1-x_{\mathrm{u0}}-x_{\mathrm{w0}})(Q_3(\dot{d}_{\mathrm{p}}+d(d_{\mathrm{p}})))-Q_3(d_{\mathrm{p}})}{s_{\mathrm{F}}H_{\mathrm{bz}}} \tag{53}$$

2.3.11. *Slagging Wall Model*

Slagging of hot mineral matter on the gasifier walls is important for good gasifier operation. The slag properties and heat transfer through the walls of the gasifier can be predicted by the gas flow field (e.g., gas composition, gas temperature, incident heat transfer, and particle deposition rate).

The equations used to describe the slag layer are the conservation equations for momentum, energy, and mass mentioned in Bockelie et al. [88]. Since inertial forces and the pressure gradient are negligible for a falling film at low Reynolds number with a free surface, the equation of motion (*x*-direction) for the slag layer is simply

$$\frac{\partial \tau}{\partial y} = \rho g \tag{54}$$

A number of empirical correlations relating the viscosity of a slag to its composition and temperature have been reported in the literature. These include the correlations published in refs. [73–75].

The flow behavior of coal slags has been described in ref. [74]. Briefly, coal slag's exhibit Newtonian flow at high temperatures where slag viscosity decreases with increase in temperature.

2.4. *Freeboard section*

Above the bubbling bed there is a region known as *freeboard*. The main function of the *freeboard* is to serve as a space for disengaging of particles carried by the gas flow. Therefore the cross-sectional area at the freeboard should always be larger than the bed section.

The *freeboard* also consist of so-called "*splash zone*", near the surface of bubbling bed where a considerable amount of solids is present [45].

2.4.1. *Entrainment*

Entrainment from fluidized beds is affected by temperature and pressure. Increasing system pressure increases the amount of solids carried over with the exit gas because the drag force on the particles increases at higher gas densities. Increasing gas viscosity also increases the entrainment rate from fluidized beds because the drag force on the particles increases with increasing gas viscosity [76].

Kunii and Levenspiel [45] presented correlation of the entrainment at the top of the bed:

$$F_{Y,m,l,z=z_{\mathrm{D}}} = 3.07\times 10^{-9} S^2 d_{\mathrm{B},z=z_{\mathrm{D}}} p_{\mathrm{G}}^{3.5} g^{0.5} \times \frac{(U_{\mathrm{G}}-U_{\mathrm{G,mf}})^{2.5}_{z=z_D}}{\mu_{\mathrm{G}}^{2.5}} f_m w_{m,l} \tag{55}$$

The rate of the elutriation is given in ref. [77]:

$$F_{\mathrm{X},m,l} = [\rho_m(1-e_{\mathrm{F},m,l})(U_{\mathrm{G}}-u_{\mathrm{T},m,l})S]\times w_{m,l} \tag{56}$$

where the mass fraction *w* of particles *m* at level *l* is the value found in the bed at steady-state condition and not at the feeding position.

Similar to the bed section, area and volume relations are necessary for computations regarding the freeboard section.

The void fraction in the freeboard is given by:

$$\varepsilon_{\mathrm{F},m,l} = \left[1 + \frac{a_{\mathrm{e},m,l}(U_{\mathrm{G}}-u_{\mathrm{T},m,l})^2}{2gd_{\mathrm{D}}}\right]^{-1/4.7} \tag{57}$$

$$\frac{a_{\mathrm{e},m,l}\rho_{m,l}}{d_{m,l}^2}\left(\frac{\mu_{\mathrm{G}}}{\rho_{\mathrm{G}}}\right)^{2.5} = 5.17(N_{Re,m,l})^{-1.5}d_{\mathrm{D}}^2, \quad \frac{N_{Re,m,l} \le 2.38}{d_{\mathrm{D}}} \tag{58}$$

$$\frac{a_{\mathrm{e},m,l}\rho_{m,l}}{d_{m,l}^2}\left(\frac{\mu_{\mathrm{G}}}{\rho_{\mathrm{G}}}\right)^{2.5} = 12.3(N_{Re,m,l})^{-1.5}d_{\mathrm{D}}^2, \quad \frac{N_{Re,m,l} > 2.38}{d_{\mathrm{D}}} \tag{59}$$

$$N_{Re,m,l} = \frac{\rho_{\mathrm{G}}(U_{\mathrm{G}}-u_{\mathrm{T},m,l})_z d_{m,l}}{\mu_{\mathrm{G}}} \tag{60}$$

An alternative estimation of void fraction at each point was proposed by De Souza-Santos [42]:

$$\varepsilon_{\mathrm{F}} = \frac{F_{\mathrm{GF}}/\rho_{\mathrm{GF}}}{(F_{\mathrm{GF}}/\rho_{\mathrm{GF}}) + \sum_{m=1}^{3}(F_{\mathrm{SF},m}/\rho_{\rho,m})} \tag{61}$$

The available surface area of each solid species can be calculated by

$$\frac{\mathrm{d}A_{\mathrm{PF},m}}{\mathrm{d}z} = \frac{6}{d_{p,m}} f''_m(1-\varepsilon_{\mathrm{F}})S_{\mathrm{F}} \tag{62}$$

2.4.2. *Transport disengaging height*

After reaching a certain height in the freeboard, the upward flow of particles or entrainment no longer decreases (or decreases very slowly). Therefore, no matter how high the freeboard, the entrainment remains practically constant. This is called *transport disengaging height* (*TDH*) and is defined as the height at which the derivative of entrainment flow against height is just 1% of its value at the top of the bed. TDH is a fundamental parameter during the design of fluidized beds [77].

$$z_{\mathrm{TDH}} = z_{\mathrm{D}} + \frac{1}{a_\gamma} \ln\left(\frac{F_{\gamma, z=z_{\mathrm{D}}}}{0.01 F_x}\right) \tag{63}$$

Kunii and Levenspiel [45] provided correlation between entrainment $F_{\gamma,m,\mathrm{b}}$ and elutriation $F_{X,m,\mathrm{b}}$ rates and height of the freeboard $(z - z_{\mathrm{d}})$ below TDH.

$$F_{Y,m,l} = F_{X,m,l} + (F_{Y,m,l,z=z_{\mathrm{d}}} - F_{X,m,l}) \exp[-a_\gamma(Z - Z_{\mathrm{D}})] \tag{64}$$

2.4.3. *Mass and energy balances*

Hereafter the set of differential equations for the mass flow of gas and each solid species ($m = 1$–n) is shown by De Souza-Santos [42]:

$$\frac{\mathrm{d}F_{\mathrm{F},j}}{\mathrm{d}z} = \sum_{m=1}^{3}\left(R_{\mathrm{her,SF},m,j}\frac{\mathrm{d}A_{\mathrm{PF},m}}{\mathrm{d}z}\right) + R_{hom,\mathrm{GF},j}\frac{\mathrm{d}V_{\mathrm{GF}}}{\mathrm{d}z} 1 \le j \le 1000 \tag{65}$$

The assumption of plug flow regime as well as axial flow direction for the solid particles in the freeboard was made. The first term on the right side of the equation refers to solid particles ($m = 1$–3) and the second term to the gas phase.

The energy balance for the gas phase in the freeboard is shown:

$$F_{\mathrm{GF}}c_{\mathrm{GF}}\frac{\mathrm{d}T_{\mathrm{GF}}}{\mathrm{d}z} = \frac{\mathrm{d}V_{\mathrm{GF}}}{\mathrm{d}z}\left[-R_{\mathrm{QGF}} + \sum_{m=1}^{3}(R_{\mathrm{CSFG},m} + R_{\mathrm{hSFGF},m}) - R_{\mathrm{CGFTF}} - R_{\mathrm{GFWF}}\right] \tag{66}$$

The energy balance for the solid phase in the freeboard is shown:

$$F_{\mathrm{SF},m}c_{\mathrm{SF},m}\frac{\mathrm{d}T_{\mathrm{SF},m}}{\mathrm{d}z} = \frac{\mathrm{d}V_{\mathrm{SF},m}}{\mathrm{d}z}\left[-R_{\mathrm{QSF},m} - (R_{\mathrm{CSFGF},m} + R_{\mathrm{hCSFGF},m}) \times \frac{\mathrm{d}V_{\mathrm{GF}}/\mathrm{d}z}{\mathrm{d}V_{\mathrm{SF},m}/\mathrm{d}z} - R_{\mathrm{RSFTF},m} - \sum_{n=1}^{3}(R_{\mathrm{RSFSF},m,n})\right] \quad 1 \le m \le 3 \tag{67}$$

2.4.4. *Catalytic reactions in the freeboard*

Yates and Rowe [78] made an assumption that the freeboard contained perfectly mixed, equally dispersed particles derived from bubble wakes. The fraction of wake particles ejected, f' was a model parameter. The governing equation of the model was proposed as:

$$-\frac{\mathrm{d}C_{A,\mathrm{cell}}}{\mathrm{d}t} = \frac{k_{\mathrm{g}}A_{\mathrm{p}}}{V_{\mathrm{cell}}}(C_{\mathrm{Ah}} - C_{\mathrm{Ap}}) \tag{68}$$

$$V_{\mathrm{cell}} = \frac{3V_{\mathrm{p}}}{f'(1-\varepsilon_{\mathrm{mf}})}\frac{U - U_{\mathrm{mf}}}{U - u_{\mathrm{t}}} \tag{69}$$

$$Sh = \frac{k_{\mathrm{g}}d_{\mathrm{p}}}{D} = 2 + 0.69 Sc^{0.33} Re_t^{0.5} \tag{70}$$

$$Sc = \frac{\mu}{\rho_{\mathrm{g}} D} \tag{71}$$

$$Re_{\mathrm{t}} = \frac{u_{\mathrm{t}} d_{\mathrm{p}} \rho_{\mathrm{g}}}{\mu} \tag{72}$$

3. Computational tools

There are several comprehensive modeling tools for modeling of combustion and gasification systems. One of them is a GLACIER Computational Fluid Dynamic (CFD) code *REI Models* which is capable to model: (a) a turbulent flow mechanics, (b) radiation and convective heat transfer, (c) wall slag surface properties, (d) chemical reactions and (e) particle/droplet dynamics.

A CFX package CFX International [79] represents a powerful tool which can be used in gasifier design and analysis. Recently, this package was used to simulate the flow and reaction in an entrained flow biomass gasifier [34].

The Morgantown Energy Technology Center (METC) developed the MFIX (Multiphase Flow with Interphase eXchanges) (FORTRAN based) model *MFIX (Multiphase Flow with Interphase eXchanges)*, which is a general-purpose hydrodynamic model that describes chemical reactions and heat transfer in dense or dilute fluid–solids flows. MFIX has the following capabilities: (a) mass and momentum balance equations for gas and multiple solids phases, (b) a gas phase and two solids phase energy equations, (c) an arbitrary number of species balance equations for each of the phases (d) granular stress equations based on kinetic theory and frictional flow theory, (e) a user-defined chemistry subroutine; three-dimensional Cartesian or cylindrical coordinate systems, (f) non uniform mesh size, (g) impermeable and semi permeable internal surfaces, (i) user-friendly input data file and (k) multiple, single-precision, binary, direct-access, output files that minimize disk storage and accelerate data retrieval; and extensive error reporting.

On the other hand process simulators, such as *ASPEN* (Advanced System for Process Engineering), are widely used to evaluate the performance, emissions, and costs of integrated gasification combined cycle (IGCC) systems. Panopoulos et al. [31] have simulated allothermal biomass gasification in conjunction with high temperature solid oxide fuel cell, with general purpose process simulation software *ASPEN*. The model was built, to predict the main product gas composition including methane and char as well as the external heat required to drive the process. In all cases, the *Redlich–Kwong–Soave* cubic equation of state method was used for the properties estimation. Biomass was treated as non-conventional component. Existing unit operation models were combined with *FORTRAN* calculator blocks to model the performance of the four subsections. Tarud [80] has developed a model for the gasification unit at the National Renewable Energy Laboratory using *ASPEN* simulation software. The model was designed for a feed of poultry litter and was also run with a feed of wood. De Jong et al. [81] simulated the mass, energy and species balances in the pressurised bubbling fluidized bed gasifier using plug-flow reactor model, of the *ASPEN* simulation software. The system of *ODEs*, which come from the model where numerically solved using *GEARS* algorithm. Frey and Bharvirkar [82] created desktop model utilizing *ASPEN* simulation software and *FORTRAN* subroutines to evaluate the effects of alternative assumptions regarding process performance and cost for integrated gasification combined cycle (IGCC) system with hot gas cleanup. The *ASPEN* simulation model was used to estimate mass and energy balances for all major process areas, whereas the cost model was implemented as *FORTRAN* subroutines. The model generates 100 sets of outputs, using regression analysis, based upon 100 different values for each of the 12 user-specified input assumptions in *ASPEN* flow sheet. NREL (National Renewable Energy Laboratory) has also published technical reports [83] on modelling of process integration effects and economics of a final product from biomass gasification, utilizing ASPEN simulation software.

4. Discussion of the particularities of agricultural residues gasification modelling

The traditional approach necessary to establish commercial plant technology is based on comprehensive experimental investigations, progressing from a laboratory scale test unit to a pilot scale plant, before building a full-scale commercial demonstration plant. For process optimisation, an extensive investigation of the plant behaviour depending on various operating parameters is required for each scale up step. To support this optimisation procedure, mathematical models are helpful to reduce the temporal and financial efforts. Pre-condition is a reliable simulation tool, which includes the mathematical formulation of all important chemical and physical processes by describing their dependency on operating parameters and their interdependencies [2]. However it must be pointed out that the modelling of the above processes are at the earlier stages giving poor results due to complexity of the problem and often leads to trial and error solutions. The difficulty arises when the simultaneous solution of heat and mass transfer equations, multiphase flow, complex geometries along with general assumptions are involved.

Regarding the wide range of operation parameters of a gasification plant and the specific parameters devoted to the raw material which usually are avoided, modelling, simulation and validation efforts are needed in order not to limit the validity and flexibility of the model.

Up to now, many gasifiers for agricultural residues have been designed and tested at different scales, but still they remain in demonstration scale. This situation is mainly due to the fact that design of such reactors is quite complex and relevant information is needed particularly when agro biomass is concerned.

Atmospheric bubbling fluidised bed gasifiers have proven to be reliable with a variety of feedstocks at pilot scale and commercial applications in the small to medium scale up to about 25 MW. They are limited in their capacity size range as they have not been scaled up significantly [84].

Although, previous literature has predominantly concentrated on practical applications and experience in fluidization equipment, designed and fabricated to carry out biomass gasification, pyrolysis and combustion processes, limited research has been performed to investigate the hydrodynamics of biomass particles in such systems.

Looking at the international literature concerning the comprehensive study of agricultural residues gasification in fluidised bed reactors, someone could notice that there is a need of furthermore research and modelling due to the lack of deep analysis and interpretation of some important issues and lack of experimental data needed to be incorporated into the models. Some of the above are the following:

1. Fuel characteristics impacts on the operation of the fluidised bed reactors.
2. Fluidisation aspects.
3. Fluidisation of non-uniform biomass particles.
4. Multiphase aspects.
5. Interaction of mixing non-uniform biomass with bed particles.
6. Pyrolysis step and charcoal formation.
7. Tar formation and destruction.
8. Individual kinetic parameters for the pyrolysis and gasification reactions of the different lignocellulosic material and fuel chars. Kinetic parameters valid for different bed materials or fuel ashes are not available. Thus, an extrapolation of the kinetic model studied for biomass is necessary.

4.1. Fuel characteristics

Agro-biomass/agricultural residues are derived from cultivations developed for food or industry purposes (olive, cotton, rice, etc.) and recently as well as in the future by energy crops, and it is made up of a mixture of several components such as cellulose, lignin, hemicelluloses, extractives and inorganics, each one behaving differently under thermochemical conversion. The elementary and ultimate analysis of agricultural biomass performed in our laboratory leads to a mean molecular formula, which is valid for a wide variety of sources and could be presented with the molecular type of $C_{45}H_6O_{40.}$ Agro-biomass/agricultural residues mean global composition is relatively constant; whatever is the origin of the residue, with a molar H/C ratio close to 8.8. Their average moisture, ash and volatiles content is respectively 6.6%, 5.6% and 76.5% [89].

Each type of gasifier will operate satisfactorily with respect to stability, gas quality, efficiency and pressure losses only within certain ranges of the fuel properties of which the most important are:

- energy content;
- moisture content;
- volatile matter;
- ash content and ash chemical composition;
- reactivity;
- size and size distribution;
- bulk density;
- charring properties.

Before choosing a gasifier for any individual fuel, it is important to ensure that the fuel meets the requirements of the gasifier or that it can be treated to meet these requirements. Practical tests are needed if the fuel has not previously been successfully gasified.

The choice of a fuel for gasification will in part be decided by its heating value. The heating value of the gas produced by any type of gasifier depends at least in part on the moisture content of the feedstock. The amount of volatiles in the feedstock determines the necessity of special measures (either in design of the gasifier or in the layout of the gas cleanup train) in order to remove tars from the product gas in engine applications. Ashes can cause a variety of problems. Slagging or clinker formation in the reactor can be caused by melting and agglomeration of ashes. If no special measures are taken, slagging can lead to excessive tar formation and/or complete blocking of the reactor. Slagging occurs depends on the ash content of the fuel, the melting characteristics of the ash, and the temperature pattern in the gasifier. Local high temperatures in voids in the fuel bed in the oxidation zone, caused by bridging in the bed, may cause slagging even using fuels with a high ash melting temperature. For gasification purposes the melting behaviour of the fuel ash should be determined in both oxidating and reducing atmospheres.

The reactivity is an important factor determining the rate of reduction of carbon dioxide to carbon monoxide in a gasifier. Reactivity influences the reactor design insofar as it dictates the height needed in the reduction zone. It is well known that the reactivity of char can be improved through various processes such as steam treatment (activated carbon) or treatment with lime and sodium carbonate.

Another interesting point is the assumed positive effect on the rate of gasification of a number of elements which act as catalysts. Small quantities of potassium, sodium and zinc can have a large effect on the reactivity of the fuel.

Excessively large sizes of particles or pieces give rise to reduced reactivity of the fuel, resulting in startup problems and poor gas quality, and to transport problems through the equipment. A large range in size distribution of the feedstock will generally aggravate the above phenomena.

Fuels with high bulk density are advantageous because they represent a high energy-for-volume value. Consequently these fuels need less bunker space for a given refuelling time. Low bulk density fuels sometimes give rise to insufficient flow under gravity, resulting in low gas heating values and ultimately in burning of the char in the reduction zone [85].

4.2. Fluidisation aspects

Whereas there has been considerable effort to develop new biomass gasification, combustion, pyrolysis and bio-conversion processes, relatively few authors have characterized the relevant flow characteristics of biomass particles in fluidized beds or investigated measures that could assist in resolving flow issues. Flow is complex given the heterogeneous nature of the particles, turbulence of the fluidizing fluid, complex geometries, simultaneous heat and mass transfer, and rapid gas release during devolatilization [1].

However, little work has been done to understand the fluidization mechanics of biomass itself, or of mixtures of biomass and inert particles. It generally appears to be assumed that the design and operation of equipment involving biomass materials can be based on conventional fluidization knowledge and methodologies.

4.3. Fluidisation of non uniform biomass particles

The agricultural biomass particles or pieces are commonly non-standard – large in size, extreme in shape (e.g. long and thin as with stems or fibres), wet and pliable – relative to normal particulate matter handled in chemical, mineral and pharmaceutical operations. These differences are often critical, making it difficult, or even impossible, to handle, feed or process biomass particles. Biomass particles are difficult to fluidize due to their peculiar shapes, sizes and densities In particular, there is very little knowledge of how fluidized bed hydrodynamics and related properties are affected by such characteristics as extreme particle sizes and shapes, moisture content and compressibility.

Since the hydrodynamics are critical to successful design and operation of fluidized bed processes, it is important to undertake research directed at improving the characterization and modelling of various species of agro-biomass fluidization hydrodynamics [1].

In contrast to coal and woody biomass which have been studied in the past, a lignocellulosic biomass particle has unusual properties which make them difficult to fluidize and handle. The limited work that has been reported on biomass fluidization primarily treats means of achieving fluidization, mixing and segregation. Most of the work has been in low-velocity fluidized beds, although circulating fluidized beds are also important [1].

For this purpose, in our previous study [86] the conceptual design and preliminary hydrodynamic study of an agro biomass (olive kernel) in a bench gasification fluidized bed reactor has presented.

Further research is needed to provide general understanding of interactions among heterogeneous particles and guidance on conditions that can lead to viable and sustainable processes.

4.4. Multiphase aspects

As known, the phenomena governing the gasification of a particle are both chemical and physical. Depending on the operational conditions the process may be controlled by the chemical or the physical phenomena or both. In addition and especially concerning bubbling bed fluidized bed reactors, although considerable progress has been made in utilizing biomass in them, characterization of the multiphase flow aspects is weak, leading to trial and error ad hoc solutions. There has been little work of a comprehensive or fundamental nature which could provide more general rules or delineate principles helpful in resolving multiphase flow issues.

Further research is needed to provide a general understanding of interactions among heterogeneous particles and guidance on conditions most likely to lead to viable and sustainable processes.

4.5. Mixing

In the bubbling fluidized bed, a binary system of particles is present. In this binary system one particle specie is biomass and the other is bed particles. This corresponds to the mixing/segregation of biomass particles in a bubbling fluidized bed. Large differences in size and density between biomass and bed or even catalytic particles lead to a non-uniform distribution of biomass particles within the bed. There are a number of studies on mixing and segregation of particles of different size and/or different density in fluidized beds. However, little has been reported in literature on solids mixing and segregation for cases when the particles are injected from above the dense bed, as would correspond to the injection of fuel particles above the bed in a fluidized bed reactor. Many of the applications involve biomass particles co-fluidized with much denser and more regular particles such as sand. Interaction and mixing of the species then become major issues.

Most reported work has been empirical and directed to a single binary, seeking operating conditions that allow fluidized bed reactors to function [87].

4.6. Pyrolysis step and charcoal formation

During biomass pyrolysis a charcoal layer is developed at the surface of the particle. Since the thermal conductivity of the char is less than that of wood the heat transfer through this layer becomes limiting for the rate of pyrolysis of the interior biomass particle. The medium properties (porosity, permeability, density, mass diffusivity, specific heat capacity and thermal conductivity), the volume occupied by the solid (wood and char) and consequently the total volume of the particle, also changes continuously. As a result of the chemical restructuring during pyrolysis, the density of the char increases. The temperature profile of the particle changes due to increased density and decreased distance across the pyrolysis region. The product yield is also affected by the thinner and hotter char layer.

To investigate those alterations, a more detailed knowledge of the pore size distribution in the charcoal is required [89].

Concerning charcoal, the identification of the mechanisms or parameters limiting the production of charcoal with high reactivity with respect to its heterogeneous oxidation during the gasification is necessary.

4.7. Tar destruction and bed material

Concerning tar formation, a better understanding of the mechanisms of tar from blignocellulosic biomass formation and destruction is needed. This complex process takes into account the solid morphology (porosity, specific surface, tortuosity, etc.), heat and mass transfers in the particle and intrinsic charcoal reactivity.

The bed material in the fluidised bed reactor is of great importance because it can play a dual role in the gasification as heat transfer and as catalyst for the tar destruction. The formation of tar can be a problem during biomass gasification process. To get a low tar content gas in fluidized gasification is not easy at all but it is possible. Control technologies of tar production can broadly be divided into two approaches; treatments inside the gasifier (primary methods) and hot gas cleaning after the gasifier (secondary methods). Although secondary methods are proven to be effective, treatments inside the gasifier are gaining much attention due to economic benefits.

In primary methods, the operating parameters such as temperature, gasifying agent, equivalence ratio, residence time, bed material and catalytic additives play important roles in the formation and decomposition of tar.

4.8. Kinetics

Kinetics is important for the modelling of biomass gasification especially those concerning pyrolysis since pyrolysis step is very important step in fluidized bed gasification. *Thus, kinetic studies on the specific raw material are needed.*

In that purpose we have studied and presented, in a previous study (Damartzis et al., 2007) the development of a mathematical model for the to description o the pyrolysis of a single solid olive kernel particle and the prediction of the fast pyrolysis products yields. Chemical kinetic model was coupled with heat transfer model. The analysis was focused on primary degradation for small particle. The numerical method applied is finite difference for the heat transfer model and Runge-Kutta 4th method for chemical kinetics model equations. The model has been validated against experiments carried out in a laboratory wire mesh reactor.

In the above study spherical particle size were modeled. Of course olive kernels can be prepared by cutting and crushing pieces to fractions of the desired particle size and thus they can be simulated as spherical because they are woody-like biomass. However, as mentioned before biomass issued from agricultural residues has not always uniform particle shape as it is the case of stalks from crops and energy crops. The most of the biomass remaining at the fields after harvesting cannot be considered as spherical-like particle biomass.

This fact requires the experimental study of each specific residue and the collection of operation data in a pilot fluidized bed reactor.

5. Recommendations for further experimental studies

In view of the above analysis made and in order to develop multiphase flow models, combining elements from experimental findings to guide design and operation of agricultural residues fluidised gasification processes, some recommendations can be made concerning future experimental work on the following issues:

- Measurements of the chemical, physical and thermal characteristics of agricultural residues to be used as raw material in the gasification process and their char characteristics produced during the gasification process and identification of their impacts.
- Identification of the mechanisms or parameters limiting the production of charcoal with high reactivity with respect to its heterogeneous oxidation during the gasification.
- Identification of the impacts of the bed properties (porosity, permeability, density, mass diffusivity, specific heat capacity and thermal conductivity), and its catalytic effect on tar destruction.
- Understanding of the influence of key particle properties shape and size (e.g. long thin stalks or flat chips) in order to improve improved performance.
- Study of the effect of temperature, air ratio on agro-biomass particles fluidisation.

6. Conclusion

Given the importance of agricultural residues gasification of nowadays, a study on fluidised gasification modelling approaches was performed. Agricultural residues are generated after crops harvesting or in the industrial processing of these products. Recently are recognized as valuable fossil fuel with great potential for sustainable energy conversion processes. The utilization of biomass in bubbling and circulating fluidized bed reactors is the most promising technology available till. This process can produce fuel gases with low or medium heating values from a variety of agricultural residues in an environmentally acceptable manner and are suitable for fertiliser manufacturing and Fisher–Tropsch chemical synthesis and biofuels production of varying scales.

Mathematical modelling is an alternative means to study fluidisation and fluidised bed biomass gasification. Modelling can not only account for the fundamental hydrodynamic behaviour of fluidisation and the coal gasification process, but also serve as a predictive tool to assist with the design, optimisation and scale-up of fluidised bed gasifiers. Therefore, in recent years mathematical modelling of fluidised beds has increasingly attracted more attention

In this study a prioritising of the key area of gasifier modelling was made and the weak spots needed for further understanding of gasifier hydrodynamics were pointed out. In view of the previous work summarized in this paper, it is clear that research is needed in the areas related to fluidization hydrodynamic characteristics for wide ranges of agricultural species and particles (e.g. long thin stalks or flat chips), so that to provide improved performance.

To evaluate fluidization quality and optimize gas–solid flow, among the topics requiring attention are mixing of binary (biomass and bed material) particles. Those bed materials can have a catalytic aspect on tar destruction. Tar destruction of course is another issue; further research is needed to provide a better understanding of interactions among heterogeneous reactions.

In our future work, the previously developed pre-mathematical model for bubbling fluidised bed gasifiers will be specifically applied for agricultural residues by incorporation of their specific characteristics. It will be used to simulate gasifiers of scale. Simulation results will be validated by using experimental data which will be produced in a bubbling fluidised bed bench scale reactor of 5 kW h.

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