

Appendix A. Fuel and inert material properties

Table 1. Properties of the fuel and inert material.

Property	Value
LHV (MJ/kg)	10.81 (wb), 21.72 (db)
Lignite particle density (kg/m ³)	1350
Fuel Sauter mean diameter (μm)	499.2
Inert sand Sauter diameter (μm)	240
Inert sand particle density (kg/m ³)	2650

Table 2. Ultimate and proximate analyses of the fuel.

Ultimate analysis		
Mass fraction (wt %)	wb	db
C	0.363	0.661
H	0.026	0.047
O	0.132	0.240
N	0.004	0.008
S	0.002	0.003
H ₂ O/moisture	0.450	0.000
Ash	0.023	0.041
Proximate analysis		
Mass fraction (wt %)	wb	db
H ₂ O/moisture	0.450	0.000
Ash	0.023	0.041
Fixed carbon	0.254	0.462
Volatile matter	0.273	0.497

Appendix B. Mathematical model

B.1 Balance equations

Dynamic conservation equations for mass, momentum and energy are solved one-dimensionally (i.e. properties are averaged over the cross section) simultaneously for the entire model network. Gas side is described by the 3-equation flow model [1], which is suitable for single-phase flow component, whereas the water/steam cycle is described by the 6-equation flow model [2], which is suitable when more than one phases are present [3-5]. The equations of the 3-equation flow model are:

- Mass balance: $\frac{\partial \varepsilon \rho}{\partial t} + \frac{\partial \varepsilon \rho v}{\partial z} = 0$ (1)

- Momentum balance: $\frac{\partial \varepsilon \rho v}{\partial t} + \frac{\partial \varepsilon \rho v^2}{\partial z} = \frac{\partial \varepsilon p}{\partial z} + S$ (2)

- Energy balance: $\frac{\partial \varepsilon \rho h}{\partial t} + \frac{\partial \varepsilon \rho v h}{\partial z} = S$ (3)

Note, h is total enthalpy including the kinetic energy:

$$h = h_{stat} + \frac{1}{2} v^2 \quad (4)$$

In the case of flue gas phase, a conservation equation for the mass fractions of the various gas components is also solved.

The 6-equation flow model, applied at the water/steam side, is presented in the equations below:

- Mass balance: $\frac{\partial(\varepsilon_k \rho_k)}{\partial t} + \frac{\partial \varepsilon_k \rho_k v_k}{\partial z} = \Gamma_k$ (5)

- Momentum balance: $\frac{\partial(\varepsilon_k \rho_k v_k)}{\partial t} + \frac{\partial(\varepsilon_k \rho_k v_k^2)}{\partial z} = \Gamma_k v_{ik} + \varepsilon_k \rho_k \vec{g} + F_{wk} + F_{ik} + F_{fl} + \Delta p$ (6)

- Energy balance: $\frac{\partial(\varepsilon_k \rho_k h_k)}{\partial t} + \frac{\partial(\varepsilon_k \rho_k v_k h_k)}{\partial z} = \varepsilon_k \frac{\partial p}{\partial t} + \Gamma_k h_{ik} + q_{ik} + q_{wk} + F_{wk} v_k + F_{ik} v_k$ (7)

Subscript k is the phase (liquid or gas), so the equations are six when written for both phases. The terms Γ , F and q are calculated from empirical correlations, taking into account the phases separately and the prevailing process conditions, such as flow regimes and wall temperature.

B.1.1 Modeling of the gas/solid side

B.1.1.1 Gas modeling

Apart from the flow equations, chemical reactions also take place in the gas side, as shown in Table 3 [6].

Table 3. Reactions in the riser.

Reaction	Type
$CR_1 \rightarrow \text{volatiles}(CH_4, S, H_2) + C$	CR ₁ is part of solid heat material
$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	Combustion of volatiles
$C + O_2 \rightarrow CO_2$	Char combustion
$2C + O_2 \rightarrow 2CO$	Char combustion
$2CO + O_2 \rightarrow 2CO_2$	Combustion of volatiles
$S + O_2 \rightarrow SO_2$	Combustion of volatiles
$2H_2 + O_2 \rightarrow 2H_2O$	Combustion of volatiles
$SO_2 + \frac{1}{2}O_2 \rightarrow SO_3$	Oxidation

The reaction rate model of the char particle (3rd and 4th reactions of the table) is based on the assumption that the boundary layer diffusion controls the burning. Then the following equation is applied [6]

$$r = 24 \Phi \frac{D(p_g - p_s)}{d_p RT_g} = k_d (p_g - p_s) \quad (8)$$

Where r is the reaction rate, Φ is a parameter with value of 1 for the 3rd reaction and value of 3 for the 4th reaction, D is a parameter proportional to $T^{1.75}$, p_g the average partial pressure of oxygen, p_s the oxygen partial pressure at the surface of a char particle, d_p the diameter of the char particle (m), and k_d a parameter (kg/m²/s/atm). k_d is given by the following equations for the 3rd and 4th reactions respectively [6]:

$$k_d = 2.53 \cdot 10^{-7} T_g^{0.75} / d_p \quad (9)$$

$$k_d = 5.06 \cdot 10^{-7} T_g^{0.75} / d_p \quad (10)$$

If it is assumed that the surface diffusion does not limit the burning rate, p_s can be set to zero and the quantity of the char burned per second through the surface area of fuel particles is [6]:

$$r = k_d p_g \quad (11)$$

For the concentration solutions, an equation similar to the discretized equation of enthalpy is used:

$$v_i \frac{(\rho_i C_i^k - \rho_i^{t-\Delta t} C_i^{t-\Delta t})}{\Delta t} - \sum_{in} \dot{m}_{ij}^k C_j^k + \sum_{out} \dot{m}_{ij}^k C_i^k = S_i \quad (12)$$

The concentration solution for the composition grid is done explicitly.

B.1.1.2 Solids modeling

Hydraulic head over a node

Hydraulic head over a node is calculated in APROS by the following equation of Lappalainen et al. [3], which has an easily computable solution compared to other equations found in the literature (Ergun equation [7, 8] and Yerushalmi equation [9]).

$$\Delta p = \frac{g m_s (\rho_s - \rho_g)}{\rho_s a} \quad (13)$$

This simplistic correlation neglects the induced pressure drop due to particle acceleration, as it only encounters for the pressure drop that cancels out gravitational forces. Indirect calculation of solid particulate (inert + fuel) mass can be computed by the same equation when the pressure drop is known.

If the gas velocity is larger than the minimum fluidization velocity (eq. (22)) then the pressure loss coefficient k is set such that the pressure loss is the same as a hydraulic head, i.e.

$$k = \frac{2\Delta p}{\rho_g v_g^2} \quad (14)$$

If the gas velocity is less than the minimum fluidization velocity, the pressure loss coefficient is interpolated between the minimum value of 0.01 and k .

Finally, the pressure loss due to the form losses, i.e. friction due to geometrical changes and pipe roughness, is calculated with the formula:

$$Dp_K = K\rho \frac{v^2}{2} \quad (15)$$

Bed material distribution

Two solid materials are present in the bed: fuel and sand; ash is assumed to have the same properties as the sand, since it is present in much less quantities.

The bed material distribution in the vertical direction z is based on the equation by [10]:

$$\bar{\varepsilon}_s = \varepsilon_{s,\infty} + (\varepsilon_{s,d} - \varepsilon_{s,\infty})e^{-a_c z} \quad (16)$$

The coefficient a_c has a major role in the solid distribution in the furnace, as also in the solid mass flow that can be extracted for recirculation. It is estimated using the particle diameter and superficial gas velocity [11]:

$$a_c = \frac{200d_p^{0.572}}{v_0} \quad (17)$$

The dense bed solid volume fraction and the gas volume fraction at minimum fluidization are calculated according to the following formula [12]:

$$\varepsilon_{s,d} = \varepsilon_{s,mf}(1 - \varepsilon_b) \quad (18)$$

$$\varepsilon_{g,mf} = 0.586\varphi^{-0.72} Ar^{-0.029} \left(\frac{\rho_g}{\rho_s}\right)^{0.028} \quad (19)$$

The bubble fraction is calculated based on [13] as:

$$\varepsilon_b = \frac{1}{1 + \frac{1.3}{f_2} (v_0 - v_{mf})^{-0.8}} \quad (20)$$

where $f_2 = 0.24(1.1 + 2.9e^{-330d_p})(0.15 + (v_0 - v_{mf}))^{-0.33}$. The minimum fluidization velocity typically is calculated via semi-empirical correlations [7] but in this work, following APROS approach it is calculated based on the Ergun's equation [14]:

$$Ar = 150 \frac{1 - \varepsilon_{mf}}{\varepsilon_{mf}^3} \frac{Re_{mf}}{\varphi^2} + 1.75 \frac{Re_{mf}^2}{\varphi \varepsilon_{mf}^3} \quad (21)$$

, with the corresponding Re number given by eq. (22) [7]:

$$v_{mf} = \frac{\mu_g Re_{mf}}{d_s \rho_g} \quad (22)$$

Bed voidage is calculated at minimum fluidization velocity. The Archimides number is calculated as [15]:

$$Ar = \rho_g (\rho_p - \rho_g) g \frac{d_p^3}{\mu_g^2} \quad (23)$$

The solid material distribution calculated by equation (16) is considered as the target material distribution. For calculating the particle mass flow between adjacent nodes, the difference between the actual simulated and the target mass distribution is calculated in (24); the energy balance due to particle mass flows should also be satisfied as well.

$$\Delta m = V \rho_s (\varepsilon_{sim} - \varepsilon_{tar}) \quad (24)$$

If $\Delta m > 0$ then flow is upwards and the particle mass flow is calculated as:

$$\dot{m}_p = \Delta m / \tau \quad (25)$$

, where τ is the time constant equal to 1 sec.

Entrainment

The mass flow of solid particles that exits the bed and is recirculated through the cyclone, is calculated as:

$$\dot{m}_{rec} = \frac{(m_{exit,sim} - m_{exit,tar})}{\tau} \quad (26)$$

Where $m_{exit,sim}$ is actual solid mass of the last node (at maximum height) and $m_{exit,tar}$ is the solid mass of highest calculation node according to the target profile.

Thermal and fuel diffusion in bed

Thermal equalization in bed between two adjacent nodes i and $i+1$ or $i-1$ due to back and forth movement of particles, is calculated by using the diffusion equation:

$$q = C_p D_{th} \text{MIN}(m_i, m_{i+1})(T_i - T_{i+1}) \quad (27)$$

The thermal diffusion coefficient (D_{th}) of particle flow is used to calculate the thermal smoothing of bed and has the default value of 0.1.

The same principle is used to adjust fuel movement in the bed:

$$\dot{m} = D_{fuel}(m_{i,fuel} - m_{i+1,fuel}) \quad (28)$$

Convective heat transfer from the furnace to the water pipes

The convective heat flux from the gas/particle suspension to the cooling water tubes is calculated as (radiation is not considered):

$$q_{conv} = \eta_{HT} h_{s,g}(T_w - T_g) \quad (29)$$

In the equation above, the terms T_w and T_g stand for the tube wall and fluid temperatures, respectively, while the term η_{HT} is the efficiency of heat transfer and has been selected such to match the extracted heat from the experimental data.

For the computation of the convective heat transfer coefficient $h_{s,g}$, various correlations can be used. In the current model, the equation of [16] is utilized:

$$Nu_{s,g} = \frac{h_{s,g} d_p}{\lambda_g} = 2.85 \left(\frac{\Delta p}{(\rho_s - \rho_g)(1 - \varepsilon_{mf})g\Delta L} \right)^{0.5} + 3.28 \cdot 10^{-3} RePr \quad (30)$$

The second term represents the gas convection. When particles are not present in a node, the hydraulic head ΔP becomes zero, and only heat transfer from the gas is present.

B.1.2 Modeling of the water/steam side

The heterogeneous 6-equation model was used for the computations in the water side, although no phase change is observed within the water lances in the experiment. The basic equations for the thermal hydraulic solution are shown in section B.1. The heat transfer (convection) from the fluidized bed gas and particles to the water circulation pipes is calculated in the CFB module (eq. (29)) and the heat flow is then taken into account in the water circulating system.

Friction between wall and phases

Constitutive equations for wall friction, interfacial friction and interfacial heat transfer are used to couple the conservation equations. The friction F_{wk} between one phase and the wall is computed as follows [5]:

$$F_{wk} = -\frac{1}{2} \frac{f_k \rho_k u_k |u_k|}{D_H} \quad (31)$$

The variables D_H and f_k represent the hydraulic diameter and the friction pressure loss coefficient (or friction factor) for phase k , respectively. Correlations depending on the pipe roughness and a two-phase multiplier are used for the friction factor calculation. The interfacial friction F_{ik} is strongly depended on the flow regime that is prevailing in the flow and different interfacial friction correlations are used depending on the flow regime. The modelled flow regimes in the current work are stratified flow and non-stratified one, consisting of bubbly, annular and droplet flow.

Interfacial friction is calculated from three different correlations, which describe three types of flows: bubbly flow (low void fractions), annular flow (high void fractions) and droplet flow (high void fractions, liquid is in the form of droplets). The final value of interfacial friction is obtained as a weighted average of the correlations:

$$F_i = (1 - E)[(1 - \varepsilon)F_{ib} + \varepsilon F_{ia}] + E F_{id} \quad (32)$$

The variables $F_i, F_{ib}, F_{ia}, F_{id}$ represent the per volume interfacial friction in stratified, bubbly, annular and droplet flow respectively, which are computed with special correlations., while E is the rate of entrainment, i.e. the fraction of the liquid phase existing in droplets.

Enthalpy modelling

When the void fractions have been solved and the phase velocities have been calculated, the enthalpy solution for both phase enthalpies is obtained directly from the discretized energy equation of the 6-equation model. For the liquid and gas phases the equation can be written in the form:

$$\varepsilon_{l,i} h_{l,i}^n = \varepsilon_{l,i+1} h_{l,i+1}^n + \varepsilon_{l,i-1} h_{l,i-1}^n + b_{l,i} \quad (33)$$

$$\varepsilon_{g,i} h_{g,i}^n = \varepsilon_{g,i+1} h_{g,i+1}^n + \varepsilon_{g,i-1} h_{g,i-1}^n + b_{g,i} \quad (34)$$

Calculation of evaporating and condensing mass flow

The calculation of interfacial mass transfer is based on the requirement that the energy production of the interface is zero. Therefore, the following correlation is obtained:

$$\Gamma_i = -\frac{q_{il,i} + q_{ig,i} - q_{wi,i}}{h_{g,sat} - h_{l,sat}} \quad (35)$$

Interfacial heat transfer rates are calculated as follows:

$$q_{il,i} = -K_{il,i}(h_{i,stat} - h_{l,sat})_i \quad (36)$$

$$q_{ig,i} = -K_{ig,i}(h_{g,stat} - h_{g,sat})_i \quad (37)$$

Separate heat transfer correlations are used for the evaporation ($h_k > h_{k,sat}$) and condensation ($h_k < h_{k,sat}$) cases, in order to calculate the interfacial heat transfer coefficients K_{il} and K_{ig} .

Interfacial heat transfer

The interfacial heat transfer in the two-fluid model has to be calculated separately for the liquid and gas. For the gas, when the vapour is subcooled, the interfacial heat transfer coefficient is calculated by the Lee-Ryley correlation [17]:

$$K_{ig} = \frac{6(1-\varepsilon)\lambda_g(2+0.74Re_d^{0.5}Pr_g^{1/3})}{\delta^2 c_{pg}} \text{ (if } h_{g,stat} < h_{g,sat} \text{)} \quad (38)$$

The interfacial heat transfer coefficient of the liquid phase in vaporization is calculated as follows [18]:

$$K_{il} = \frac{1.2 \cdot 10^{-8} \exp(4.5a)\rho_l^2 v_l^2}{\mu_l Pr_l} \text{ (if } h_{g,stat} > h_{g,sat} \text{)} \quad (39)$$

B.2 Calculation procedure and numerical details

Discretization of modules for the solution of the equations is done upwind with nodes, junctions and branches in respect to space and time. First order upwind discretization is used for the case of enthalpy. It involves the calculation of the fluid state variables (i.e. pressure, enthalpy etc.) in the centre of the control volumes, assuming that their values are averaged over the whole control volume. On the contrary, the flow related variables (i.e. velocities) are calculated at the junction of two control volumes, called a branch. The simulation time step is equal to 0.2 sec. The set of equations is completed by correlations for interfacial and wall friction and finally heat transfer. The calculation of wall friction F_w , interfacial friction F_i , interfacial heat transfer q_i and wall heat transfer q_w from empirical correlations has a strong effect on the solution. The linearization of these terms depends on the form of each correlation. Given that many fluid properties, such as density, and constitutive relations, such as heat flows, depend on the fluid state variables, an iteration procedure is adopted. During this procedure, heat flows, pressures, velocities and enthalpies are solved first and then the fluid properties (i.e. density) are updated as a function of the solved pressure and enthalpy. Thermal equalization in

bed between two adjacent nodes due to back and forth movement of particles, is calculated in both ways as shown in the “Thermal and fuel diffusion in bed” section in B.1.1. With regards to the fluid movement, no back mixing is modelled. This iteration cycle is repeated several times during one time-step until solution is converged. As an overall convergence criterion, the mass error is applied, whereas flow and heat transfer tests are used to check the convergence of the pressure and enthalpy solutions in the intermediate cycle steps.

Appendix C. Tuned design parameters in the simulations

Table 4. Tuned design parameters.

Design parameter	Values tested	Value selected	Reason
Reaction speed coefficient	0.1-5	3.8	Temperature and reactions calibration
Diffusion coefficient in bed	0.1-1	0.9	Temperature profile calibration
Heat transfer efficiency of the cooling lances	0.08-1	0.14	Calibration of actual heat extracted by the lances
Wall heat losses	70-180 kW	107 kW (~12.6 kW/m) same for all loads	Energy balance and Temperature profile
Min. number of particles allowed in one node	10e4–50e9	5e6	Solids profile
Profile coefficient	0.1–2	1.67	Recirculation mass flow

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