CFB SIM: A QUASI-1D MODEL OF BIOMASS CO-FIRING IN CIRCULATING FLUIDIZED BED

Michal Beneš, Pavel Strachota, Radek Máca,
Vladimír Havlena, Jan Mach

Product sheet

Outline

Mathematical Model

Numerical Solution and Results

Outline

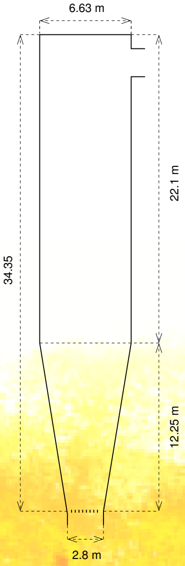
Mathematical Model

Numerical Solution and Results

Model properties

Simulated phenomena

- **quasi-1D nozzle multi-phase flow**
- primary, secondary & tertiary **air inflow**
- fuel and bed material **injection**
- fuel and bed material **recirculation**
- fuel **devolatilization** and **burnout**
- particle **attrition**
- **heat** production and transfer



Expected results

- **local**: vertical solids distribution, temperature
- **global**: bed inventory, heat production
- **general**: response to control

Mass balance

$$\frac{\partial(\rho_i\varepsilon_i)}{\partial t} + \frac{1}{A}\frac{\partial(A\rho_i\varepsilon_i u_i)}{\partial x} = \mathcal{M}_i(t,x) + \mu_i,$$

$$\frac{\partial\left(\rho_g\varepsilon_g Y_{\mathrm{X}}\right)}{\partial t} + \frac{1}{A}\frac{\partial\left(A\rho_g\varepsilon_g u_g Y_{\mathrm{X}}\right)}{\partial x} = \mathcal{M}_{\mathrm{X}}(t,x) + \mu_{\mathrm{X}}$$

for $i \in \{$gas, solid (bed material), coal, biomass$\}$ and $\mathrm{X} \in \{O_2, \mathrm{VM}_c, \mathrm{VM}_b\}$

$\varepsilon_i, \rho_i, u_i$ .... volume fraction, velocity, and density of phase i

Y_{X} .... mass fraction of species X in the flue gas

$\mathcal{M}_g, \mathcal{M}_i$ ... injection of the secondary air, bed material, and fuels

$\mathcal{M}_{\mathrm{VM}_c}, \mathcal{M}_{\mathrm{VM}_b}$ .... inflow of VM as part of the fuel inflow

$-\mu_c, -\mu_b$ .... mass loss rate due to char particle burnout

μ_g ... production rate of flue gas due to combustion of char

$-\mu_{O_2}$ .... rate of oxygen consumption by combustion

$\mu_{\mathrm{VM}_c}, \mu_{\mathrm{VM}_b}$ .... burnout rate of coal and biomass VM

Passive particle transport

$$\frac{\partial n_i}{\partial t} + \frac{1}{A}\frac{\partial \left(A n_i u_i\right)}{\partial x} = \mathcal{M}_{n_i}\left(t, x\right) + \mu_{n_i}$$

n_i .... number of particles per unit volume

$\mathcal{M}_{n_i}$ .... rate of particle number change due to inflow

μ_{n_i} .... rate of particle number change due to attrition

- for spherical particles, particle diameter is $d_{p,i} = \sqrt[3]{6\varepsilon_i / \left(\pi n_i\right)}$.

Momentum balance

$$\frac{\partial\left(\rho_i\varepsilon_i u_i\right)}{\partial t}+\frac{1}{A}\frac{\partial\left(A\rho_i\varepsilon_i u_i^2\right)}{\partial x}=-\frac{\partial P_i}{\partial x}+\sum_{k\in\{g,s,c,b\}}\beta_{ki}\left(u_k-u_i\right)-\frac{2f_i\varepsilon_i\rho_i u_i^2}{D}$$
$$+R_i\varepsilon_i g+\mathcal{P}_i\left(t,x\right)+\pi_i$$

for $i\in\{g,s,c,b\}$

P_g .... pressure of gas and for $i\in\{s,c,b\}$, we put $\frac{\partial P_i}{\partial x}=G\frac{\partial\varepsilon_i}{\partial x}$

$G\left(\varepsilon_g\right)$ .... *solids stress modulus*

f_i,β_{ki} .... wall friction and inter-phase friction forces

$R_i\varepsilon_i g$ .... gravity / buoyancy term with $R_g=\rho_g$ and $R_i=\rho_i-\rho_g$ for $i\in\{s,c,b\}$

π_i .... inter-phase momentum transfer

$\mathcal{P}_i$ .... momentum source term

Energy balance

- local inter-phase thermal equilibrium assumed
  $\implies$ single (summed) equation for internal energy in terms of temperature T

$$\sum_{i\in\{g,s,c,b\}} \rho_i \varepsilon_i c_{p,i} \left(\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x} \right) = \frac{1}{A} \sum_{i\in\{g,s,c,b\}} \left(-P_i \frac{\partial \left(A u_i \right)}{\partial x} + \varepsilon_i \frac{\partial}{\partial x} \left(A \lambda_i \frac{\partial T}{\partial x} \right) \right)$$
$$+ \sum_{i\in\{g,s,c,b\}} \left(\mathcal{E}_i - u_i \left(\mathcal{P}_i + \pi_i \right) + \left(\mathcal{M}_i + \mu_i \right) \left(\frac{u_i^2}{2} - \int_0^T c_{p,i} \left(\tau \right) \mathrm{d}\tau \right) \right) + \dot{Q}$$

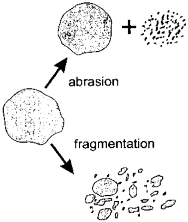
where $\dot{Q}, \mathcal{E}_i$ are the total heat and internal energy source terms, respectively

Momentum transfer

- friction between the gas phase and the solid phases β_{gi} , $i \in \{s, c, b\}$ *(Gidaspow)*
- friction between two solid phases β_{ik}, $i, k \in \{s, c, b\}$ *(Syamlal)*
- wall friction f_i *(Gidaspow)*

Attrition 1

Bed material (long term) attrition *(Tomeczek, Mocek)*



Particle **mass decrease rate**

$$\frac{\mathrm{d}m_s}{\mathrm{d}t} = -k_\mathrm{a} f(\phi_s) \frac{H_\mathrm{e}}{d_\mathrm{h}} \left(u_g - u_{g,\mathrm{mf}}\right) m_s$$

where

$m_s = \rho_s \varepsilon_s$ ....mass per unit volume of the bed material particles
k_a .... attrition rate constant, $k_a = (1.5 \pm 0.4) \times 10^{-4}$ m^{-1}
H_e ....effective bed height
d_h ....effective bed diameter
$u_{g,\mathrm{mf}}$ ....minimum superficial fluidization velocity of gas

and the *sphericity-dependent factor*

$$f(\phi_s) = \phi_s^{-2} \exp\left(\frac{\left(\phi_s^{0.75} - 1\right)^{1.75}}{\phi_s^2}\right)$$

Attrition 2

Combustion assisted attrition of fuel particles by bed material particles *(Syamlal)*

Particle **mass decrease rate**

$$\frac{\mathrm{d}m_i}{\mathrm{d}t} = K_a' \left| u_s - u_i \right| A_i = \frac{K_{a,i}}{d_{p,i}} \left| u_s - u_i \right| m_i$$

for $i \in \{c, b\}$ where

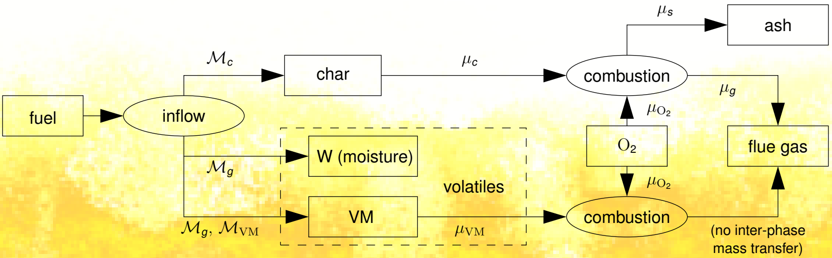
$K_{a,i} = \frac{6K_a'}{\rho_i}$ ....attrition rate constant (for spherical particles)

K_a' .. modified attrition rate constant, $K_a' \approx 7.87 \times 10^{-5}\ \mathrm{kg} \cdot \mathrm{m}^{-3}$

A_i ....surface area of particles with total mass m_i

Fuel conversion

- **devolatilization**: volatiles treated as already released into the flue gas
- **volatiles burnout**: $\mu_{\mathrm{VM},c}, \mu_{\mathrm{VM},b} \ldots$ Arrhenian kinetic theory, depneds on T , Y_{O_2}
- **char burnout**: $\mu_c, \mu_b \ldots$ governed by oxygen diffusion to particle surface and by carbon oxidization rate *(Basu, Halder)*



Proximate and ultimate fuel analysis

<table>
<tr><th colspan="8">as received basis</th></tr>
<tr><td>A</td><td colspan="2">C</td><td>H</td><td>O</td><td>N</td><td>S</td><td>W</td></tr>
<tr><td>ash (A)</td><td>fixed carbon (FC)</td><td colspan="5">volatile matter (VM)</td><td>moisture (W)</td></tr>
<tr><td colspan="2">char (coke)</td><td colspan="6">volatiles</td></tr>
</table>

Oxygen consumption rate

$$\mu_{O_2} = \mu_c \cdot \nu_{\text{char}} + \mu_b \cdot \nu_{\text{char},b} + \mu_{\text{VM},c} \cdot \nu_{\text{VM},c} + \mu_{\text{VM},b} \cdot \nu_{\text{VM},b}$$

where $\nu_{\text{char}}, \nu_{\text{VM},c}, \nu_{\text{VM},b}$ are the amounts of oxygen per unit mass of char, coal VM, and biomass VM

$$\nu_i = 32 \cdot \left(\frac{C_i}{12.01} + \frac{H_i}{4.032} + \frac{S_i}{32.06} \right) - O_i,$$

$$\nu_C = 32 \cdot \frac{1}{12.01},$$

$$\nu_{\text{char},i} = \frac{FC_i}{FC_i + A_i} \cdot \nu_C,$$

$$\nu_{\text{VM},i} = \frac{\nu_i - FC_i \cdot \nu_C}{VM}.$$

according to ultimate analysis C_i, H_i, O_i, N_i, S_i *in as received basis* and idealized combustion

$$C + O_2 \rightarrow CO_2,$$

$$4H + O_2 \rightarrow 2H_2O,$$

$$S + O_2 \rightarrow SO_2,$$

Heat production

- heating value of char from fuel $i \in \{c, b\}$

$$Q_{\mathrm{i}} = \frac{\mathrm{FC}_i}{\mathrm{FC}_i + \mathrm{A}_i} Q_{\mathrm{FC}} = \frac{\mathrm{FC}_i}{\mathrm{FC}_i + \mathrm{A}_i} \cdot 32.790 \times 10^6 \ \mathrm{J} \cdot \mathrm{kg}^{-1}$$

  according to the reaction

$$\mathrm{C} + \mathrm{O}_2 \rightarrow \mathrm{CO}_2 + 32.790 \times 10^6 \ \mathrm{J} \cdot \mathrm{kg}\,(\mathrm{C})^{-1}$$

- LHV of VM released from fuel $i \in \{c, b\}$ is therefore

$$Q_{\mathrm{LHV,VM},i} = \frac{Q_{\mathrm{LHV},i} - \mathrm{FC}_i \cdot Q_{\mathrm{FC}}}{\mathrm{VM}}$$

- **heat production** is given by the terms $\dot{Q}_c$ and $\dot{Q}_b$ which read

$$\dot{Q}_c\,(\mu_c, \mu_{\mathrm{VM},c}) = Q_c \cdot \mu_c + Q_{\mathrm{LHV,VM},c} \cdot \mu_{\mathrm{VM},c},$$
$$\dot{Q}_b\,(\mu_b, \mu_{\mathrm{VM},b}) = Q_b \cdot \mu_b + Q_{\mathrm{LHV,VM},b} \cdot \mu_{\mathrm{VM},b}.$$

Heat transfer

- **radiative** heat transfer:

$$\dot{Q}_R = \sigma \left(\epsilon (T) T^4 - \epsilon (T_{\text{wall}}) T_{\text{wall}}^4 \right)$$

  where ϵ is the flue gas emissivity

- **convective** heat transfer:

$$\dot{Q}_C = \frac{4}{D} \alpha (T - T_{\text{wall}})$$

  where D is the combustor diameter and α the heat transfer coefficient

$$\alpha = \frac{\text{Nu} \cdot \lambda (T)}{L}$$

Outline

Mathematical Model

Numerical Solution and Results

Finite volume scheme

- aggregate vector form:

$$\frac{\partial \boldsymbol{W}}{\partial t} + \frac{\partial}{\partial x}\left(\boldsymbol{F}_c - \boldsymbol{F}_v\right) = \boldsymbol{Q}$$

$\boldsymbol{W}$ .... vector of state variables

$\boldsymbol{F}_c$, $\boldsymbol{F}_v$ .... convective and viscous fluxes

- semidiscrete scheme

$$\frac{\mathrm{d}\boldsymbol{W}_K}{\mathrm{d}t} = -\frac{1}{|K|}\left[\left(\boldsymbol{F}_{c,R} - \boldsymbol{F}_{v,R} + \boldsymbol{F}_{\nu,R}\right) - \left(\boldsymbol{F}_{c,L} - \boldsymbol{F}_{v,L} + \boldsymbol{F}_{\nu,L}\right)\right] + \boldsymbol{Q}_K$$

R, L .. values at the left and right boundary of the cell K

- adjustable artificial diffusion $\boldsymbol{F}_\nu$ used for stabilization
- explicit adaptive time integration (Runge-Kutta-Merson)
- parallel implementation written using C/C++ and the MPI library

Initial and boundary conditions

Boundary conditions

- **implementation**: auxiliary (ghost) cells beyond the computational domain
- **default**: zero Neumann b.c. (extrapolation) is imposed on all *physical* quantities
- **overriden at inlet**: Dirichlet b.c. for ε_i, $d_{p,i}$, T, and gas mass inflow $\rho_g \varepsilon_g u_g$
- **overriden at outlet**: Dirichlet b.c. for atmospheric pressure

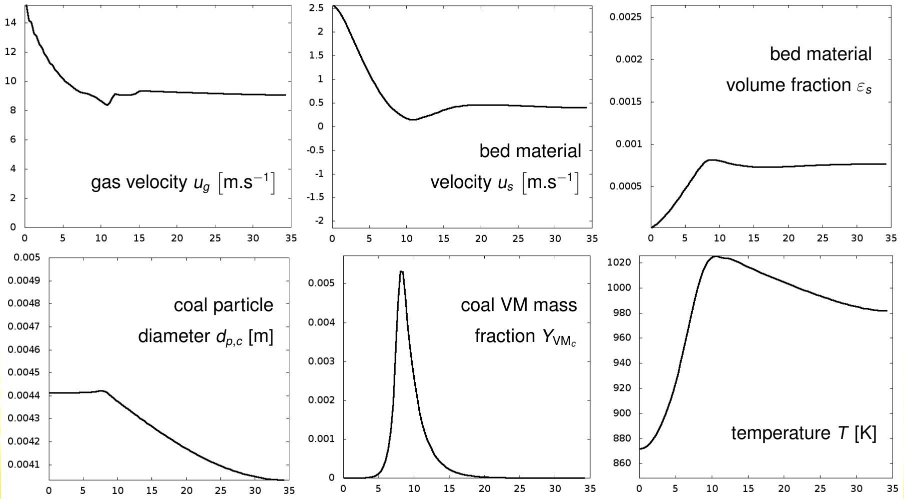
Initial conditions

- set up to quickly reach the stationary state
- zero flow velocities, atmospheric pressure, zero fuel inventory, and gas pre-heating

Solids recirculation

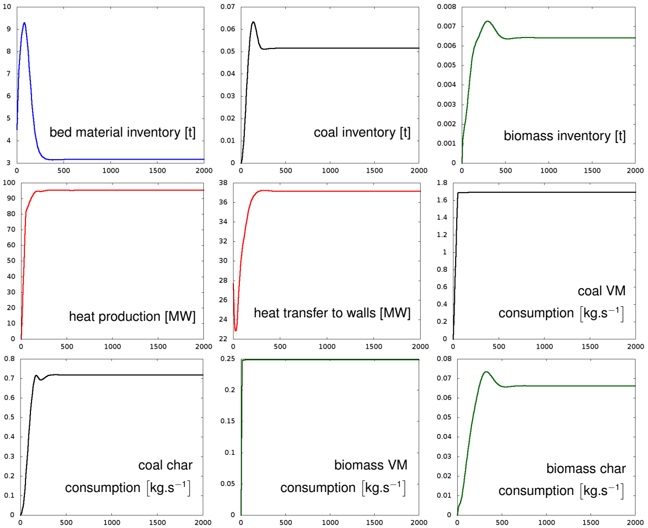
- a mixture of **bed material** (limestone and ash), **unburnt coal char**, and **unburnt biomass char**
- current **composition** of this mixture at the outlet used to calculate the composition of the injected material
- **rate of material injection** specified independently (large enough recirculation reservoir assumed)

Results



Vertical profiles of selected quantities at $t = 2000$ s

Results



Cumulative quantities $t \in \{0\ \text{s},\ 2000\ \text{s}\}$