5-25-2016

Modelling of a chemical looping combustion system equipped with a two- stage fuel reactor

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MODELLING OF A CHEMICAL LOOPING COMBUSTION SYSTEM EQUIPPED WITH A TWO-STAGE FUEL REACTOR

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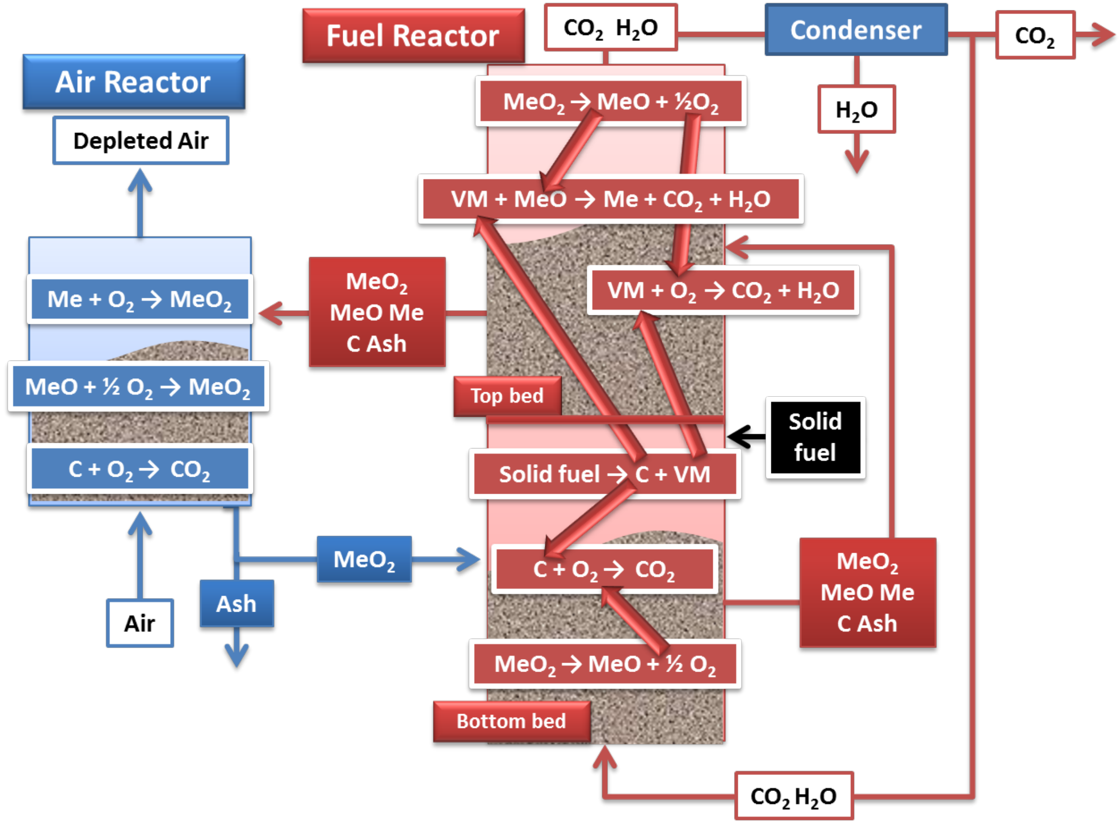
Introduction

Exploiting of CLOU effect for combustion of the most difficult part of the fuel: Char

Two-stage Fuel Reactor: better utilization of the oxygen carrier

Conversion of VM using the residual oxidative potential of the OC

RTD is closer to a plug flow than a single-stage FR



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Aim of the work

Literature

Most of numerical simulations of CLC in DIFB are focused only on kinetic scheme

What you need?

An appropriate hydrodynamic model of the whole system in order to point out "stable" operating conditions.

Aim of the work

To develop a simple mathematical tool coupling a CLC reactive scheme and a simple hydrodynamic model of a DIFB system.

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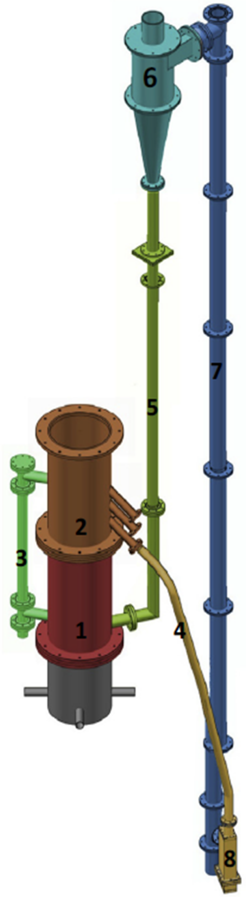
Mathematical Model: hypothesis

1. FR split in two zones: dense zone below diluted zone/FreeBoard (FB)
2. Dense zone is modelled as a CSTR, while FB is modelled as a PFR
3. Instantaneous devolatilization
4. AR is modelled as CSTR (dense regime) or PFR (diluted regime)
5. The rate of heterogeneous reactions is ruled by chemical kinetics
6. Conversion is uniform throughout solid particles
7. Conversion of oxygen carrier and char in the air reactor is complete.

Mathematical Model: hydrodynamic model (I)



$$m_{inv} = m_{BFB} + m_{LS} + m_R + m_{D/LV}$$

$$m_{BFB} = (A_{BFB}/g) \cdot \Delta P_{BFB}$$

$$m_{LS} = (1-\varepsilon_m) \cdot \rho_P \cdot A_{SP} \cdot (L_s - I_{sc}) + (1-\varepsilon_m) \cdot \rho_P \cdot A_{SC} \cdot I_{SC} + (1-\varepsilon_R) \cdot \rho_P \cdot A_{RC} \cdot h_{RC}$$

$$m_R = (A_R/g) \cdot \Delta P_R$$

$$m_{D/LV} = (1-\varepsilon_H) \cdot \rho_P \cdot A_H \cdot L_H + (1-\varepsilon_V) \cdot \rho_P \cdot A_D \cdot [H \cdot \eta(L_V - H) + L_V \cdot \eta^*(H - L_V)]$$

$$\frac{dm_{D/LV}}{dt} = W_R - W_s$$

$$\frac{dm_R}{dt} = W_{LS} - W_R$$

$$\frac{dm_{LS}}{dt} = W_B - W_{Ls}$$

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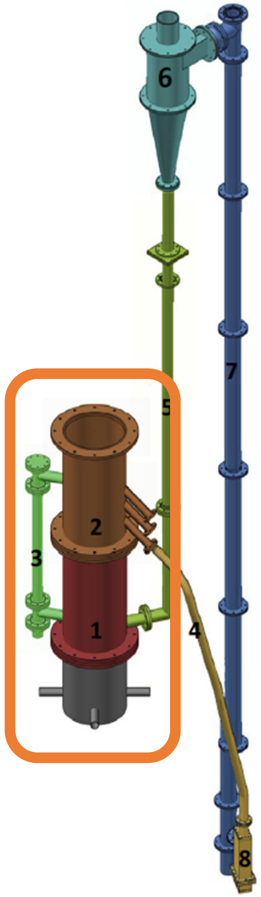
Mathematical Model: hydrodynamic model (II)



Bubbling Fluidized Beds (BFBs)

hp: elutriation is negligible

- Mass flow rate to the riser

$$W_B = \begin{cases} 0 & \rightarrow h_{D,B} < h_B \\ W_s & \rightarrow h_{D,B} \geq h_B \end{cases}$$

- Pressure drop

$$\Delta P_{BFB} = \rho_P \cdot (1 - \varepsilon_D) \cdot g \cdot h_{D,B}$$

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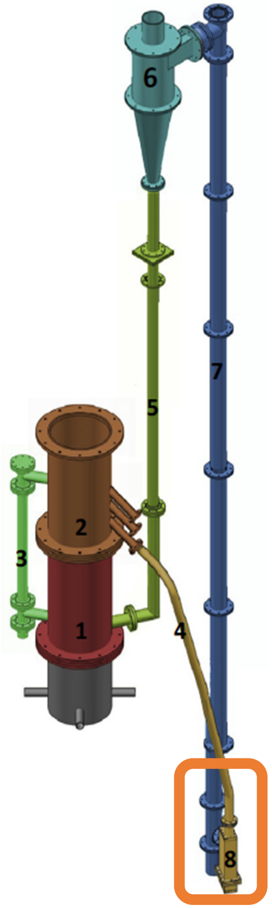
Mathematical Model: hydrodynamic model (III)



Loop Seal

Loop Seal works in complete fluidization condition between Supply Chamber (SC) and Recycle Chamber (RC).

- Mass flow rate

$$W_{LS} = W_s$$

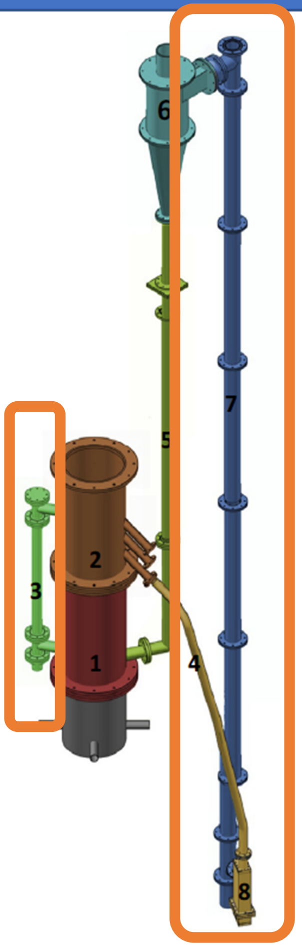
- Aeration gas flow rate

$$Q_{LS} = Q_{SC} + Q_{RC}$$

- Gas "leakage" between SC and RC

$$U_{Ls} \geq U_{mf} - \frac{W_R \cdot \varepsilon_{mf}}{A_{SC} \cdot \rho_P \cdot (1 - \varepsilon_{mf})}$$

Mathematical Model: hydrodynamic model (IV)



Risers

hp: transition between dense and dilute phase takes place when mass flow rate approaches the value corresponding to saturation carrying capacity.

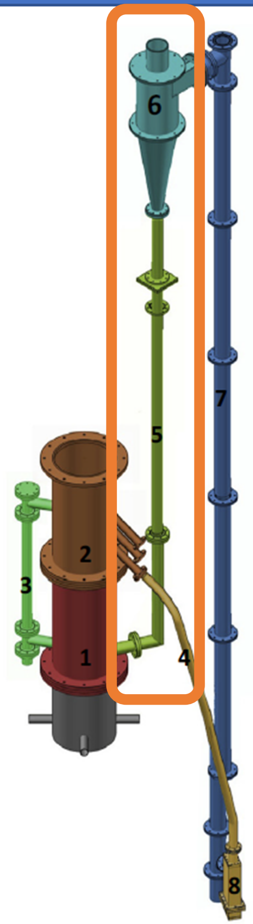
- Mass flow rate

$$G_s = \begin{cases} G_W = \beta \cdot \rho_P \cdot (1 - \varepsilon_{mf}) \cdot U_R \rightarrow G_s \geq G_W \\ G_d = (U_S / h_R) \cdot (m_R / A_R) \quad \rightarrow G_s < G_W \end{cases}$$

- Pressure drop

$$\Delta P_R = \rho_P \cdot (1 - \varepsilon_D) \cdot g \cdot h_D + \frac{g \cdot W_R}{A_R \cdot U_S} \cdot (h_R - h_D)$$

Mathematical Model: hydrodynamic model (V)



Cyclone

hp: Collection efficiency was assumed to be 1

- Pressure drop

$$\Delta P_{CYC} = \rho_f \cdot K_C \cdot U_C$$

Downcomer/L-Valve

- Pressure drop

$$\frac{\Delta P_{DOW}}{H - L_E} = K_V \cdot (u_{fy} - u_{sy})$$

$$\frac{\Delta P_{LV}}{L_H} = K_H \cdot (u_{fx} - u_{sx})$$

$$\Delta P_{LV} = \frac{0.0649 \cdot \rho_P{}^{0.996} \cdot L_H}{D_{LV}{}^{0.574} \cdot d_P{}^{0.237}} \left(\frac{W_S}{A_R}\right)^{0.178}$$

- Aeration gas flow rate

$$Q_{LV} = Q_H + Q_V$$

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Mathematical Model: kinetic scheme

Oxygen carrier: CuO (50% in mass) on ZrO_2

Fuel: bituminous South-African coal
(VM: CO CO_2 H_2 H_2O CH_4)

Oxygen carrier reactions

$CuO + ½CO \rightarrow ½Cu_2O + ½CO_2$

$CuO + ½H_2 \rightarrow ½Cu_2O + ½H_2O$

$Cu_2O + CO \rightarrow 2Cu + CO_2$

$Cu_2O + H_2 \rightarrow 2Cu + H_2O$

$CuO \rightarrow ½Cu_2O + ¼O_2$

$CuO + ¼CH_4 \rightarrow Cu + ¼CO_2 + ½H_2O$

Oxygen carrier re-oxidation (air reactor)

$Cu + ½O_2 \rightarrow CuO$

$Cu_2O + ½O_2 \rightarrow 2CuO$

Gas phase combustion

$CO + ½O_2 \rightarrow CO_2$

$H_2 + ½O_2 \rightarrow H_2O$

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Char reactions

$C + CO_2 \rightarrow 2CO$

$C + O_2 \rightarrow CO_2$

$C + H_2O \rightarrow CO + H_2$

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Mathematical Model: mass and energy balances

Mass Balances

Dense regime/phase

$$Q_{k,in} \cdot C_{j,in} - Q_{k,out} \cdot C_{j,k} + m_{sc,k} \cdot \sum_i r_i \cdot \alpha_j = 0$$

$$W_{k,in} \cdot C_{sc,in} - W_{k,out} \cdot C_{sc,k} + M_{sc} \cdot m_{sc,k} \cdot \sum_i r_i \cdot \alpha_j = 0$$

Dilute regime/Free Board

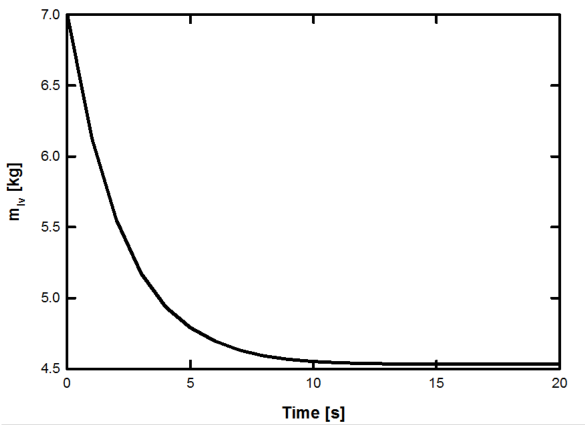
$$\left(\frac{1}{A_k}\right)\frac{dn_{j,k}}{dh_k} = \sum_i (r_i \cdot \alpha_j)$$

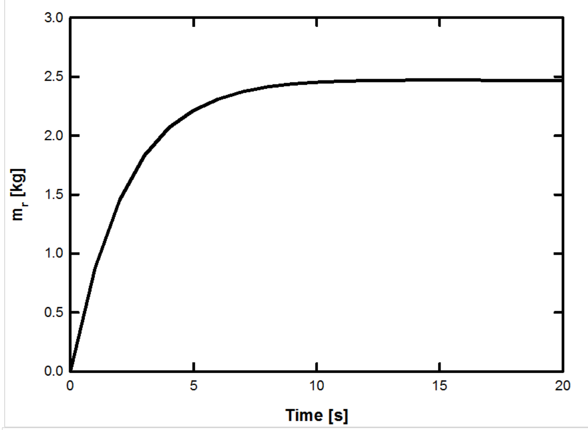
Energy balances

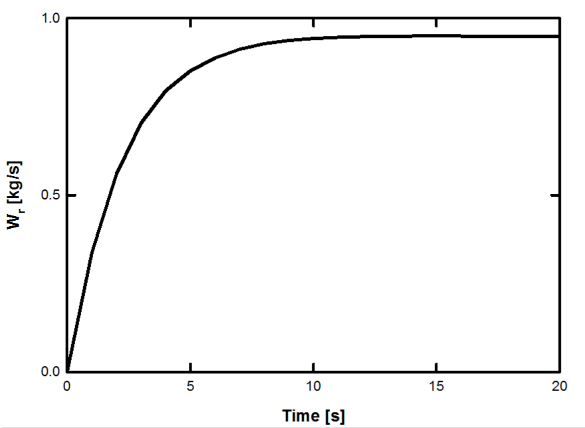
$$\sum \dot{n}_i^{in} \cdot c_{p,i} \cdot (T^0 - T_i^{in}) + \sum \dot{n}_i^{out} \cdot c_{p,i} \cdot (T_i^{out} - T^0) + \sum \left(-\Delta H_{r_j}^0\right) \cdot r_j + \dot{Q} = 0$$

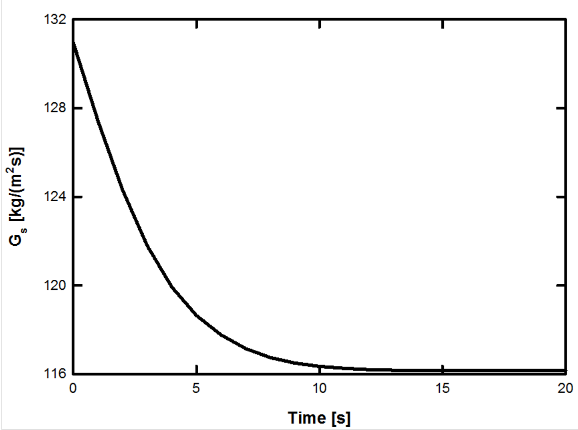
Operating conditions		Properties of bed materials	
T_{fuel} [K]	300	ρ_p [kg·m^{-3}]	2540
P [Pa]	10^5	d_p [m]	$2.55 \cdot 10^{-4}$
m_{inv} [kg]	56.7	ε_{mf} [-]	0.445
U_B [m·s^{-1}]	0.5	ε_D [-]	0.445
U_R [m·s^{-1}]	12	ε_B [-]	0.445
Q_{LV} [m^3·s^{-1}]	$2.2 \cdot 10^{-4}$	ε_V [-]	0.423
U_{LS} [m·s^{-1}]	$2U_{mf}$	ε_H [-]	0.488
GEOMETRICAL CHARACTERISTICS			
Riser		L-Valve	
D_R [m]	0.102	D_{LV} [m]	0.04
h_R [m]	5.6	L_H [m]	0.4
Air reactor		L_E [m]	0.4
D_B [m]	0.38	Cyclone	
h_{BFB} [m]	(2x)1	K_c [-]	78
Downcomer		Loop-Seal	
D_D [m]	0.04	A_{sc} [m^2]	0.0025
L_V [m]	3.6	h_{rc} [m]	0.2

Mathematical Model: results (I)









Time evolution up to the steady-state conditions of:

A)Solids inventory in the return leg m_{lv}

B)Solids inventory in the riser m_r

C) Riser mass flow rate W_r

D)Solids mass flux G_S

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Mathematical Model: results (II)

Steady-state conditions	
Fuel mass flow rate	*1 kg s^{-1}*
Recirculated OC mass flux	*116 kg m^{-2}s^{-1}*
Air Reactor temperature	*1223 K*
Fluidizing gas temperature Fuel Reactor	*623 K*
Fuel inlet temperature	*300 K*
Fluidizing gas temperature Air Reactor	*300 K*
Bottom bed inventory	*15 kg*
Top bed inventory	*15 kg*
Fuel Reactor pressure	*10^5 Pa*
Fuel reactor temperature	*10^3 K*
Riser pressure drop	*2966 Pa*
Carbon conversion degree	*0.58*
CO_2 Capture Capacity	*0.62*

Carbon conversion degree

$$\eta_{CO_2} = \frac{total\ CO_2\ at\ the\ outlet\ of\ the\ FR\ (produced\ by\ fuel\ combustion)}{total\ carbonaceous\ fuel\ fed\ to\ the\ FR}$$

CO_2 capture capacity

$$\eta_{CC} = \frac{total\ C\ at\ the\ outlet\ of\ the\ FR\ (in\ the\ gas\ stream)}{total\ C\ fed\ to\ the\ FR}$$

Conclusions

A simple tool to evaluate the performances of a novel two-stage CLOU process carried out in a MIFB was developed.

The model is able to predict both main hydrodynamic variables and kinetic performances of the proposed system.

Further work is needed in order to determine the range of operability of the system and to highlight the effects of different operating conditions on process performances.

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Thank you for your kind attention