



BABEȘ-BOLYAI UNIVERSITY
Faculty of Chemistry and Chemical Engineering



Dynamic simulation of a fluidized bed chemical looping combustion process with iron based oxygen carrier

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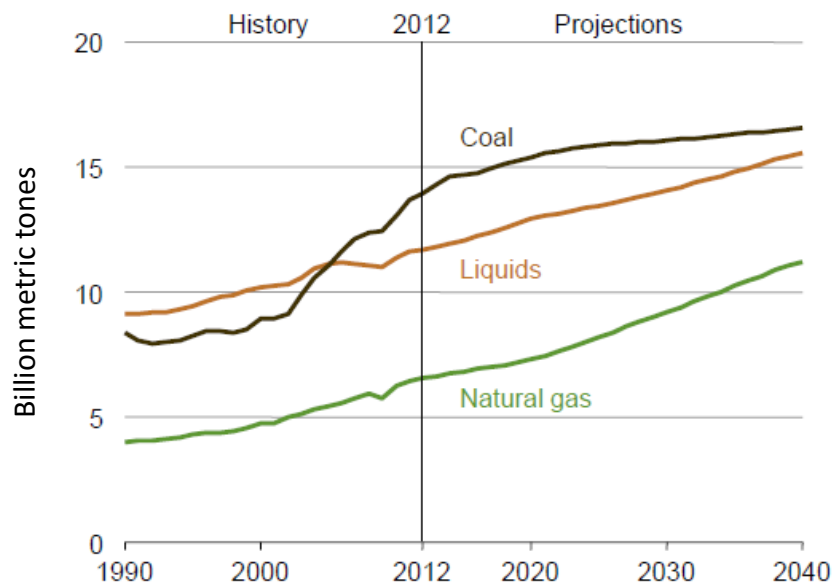
Assoc. Prof. Dr. Ana-Maria Cormoș

Presentation outline

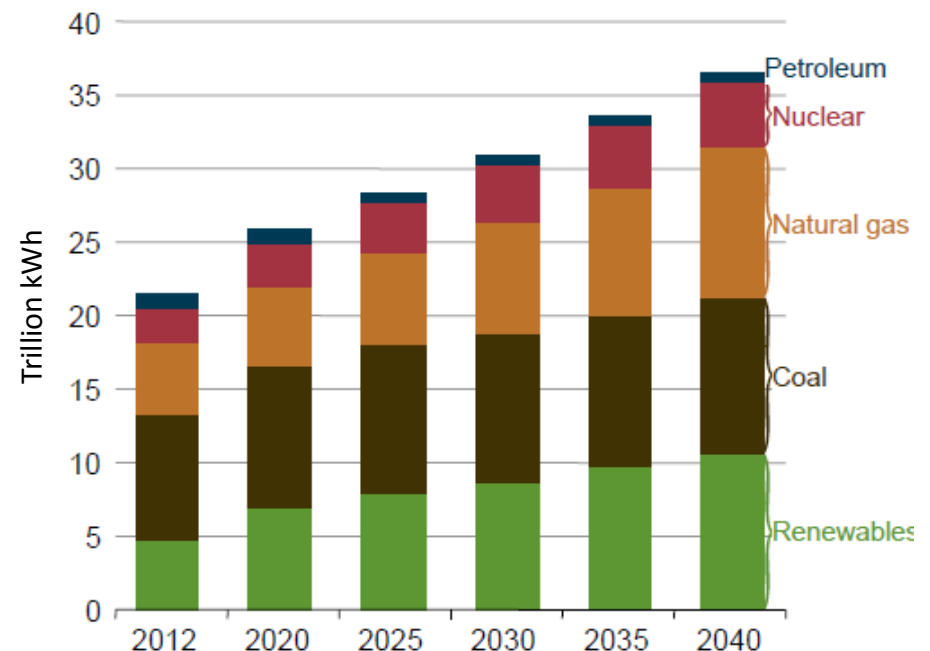
1. Introduction
2. Model development
 - 2.1. Mass and energy balance equations
 - 2.2. Kinetic and thermodynamic aspects
 - 2.3. Hydrodynamics
 - 2.4. Heat transfer
3. Results and discussion
4. Conclusions

1. Introduction

World energy-related carbon dioxide emissions by fuel type

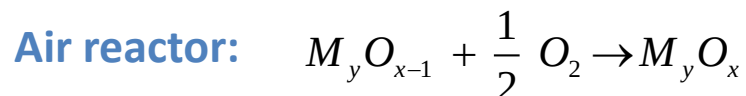
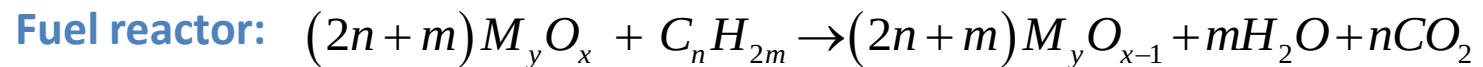
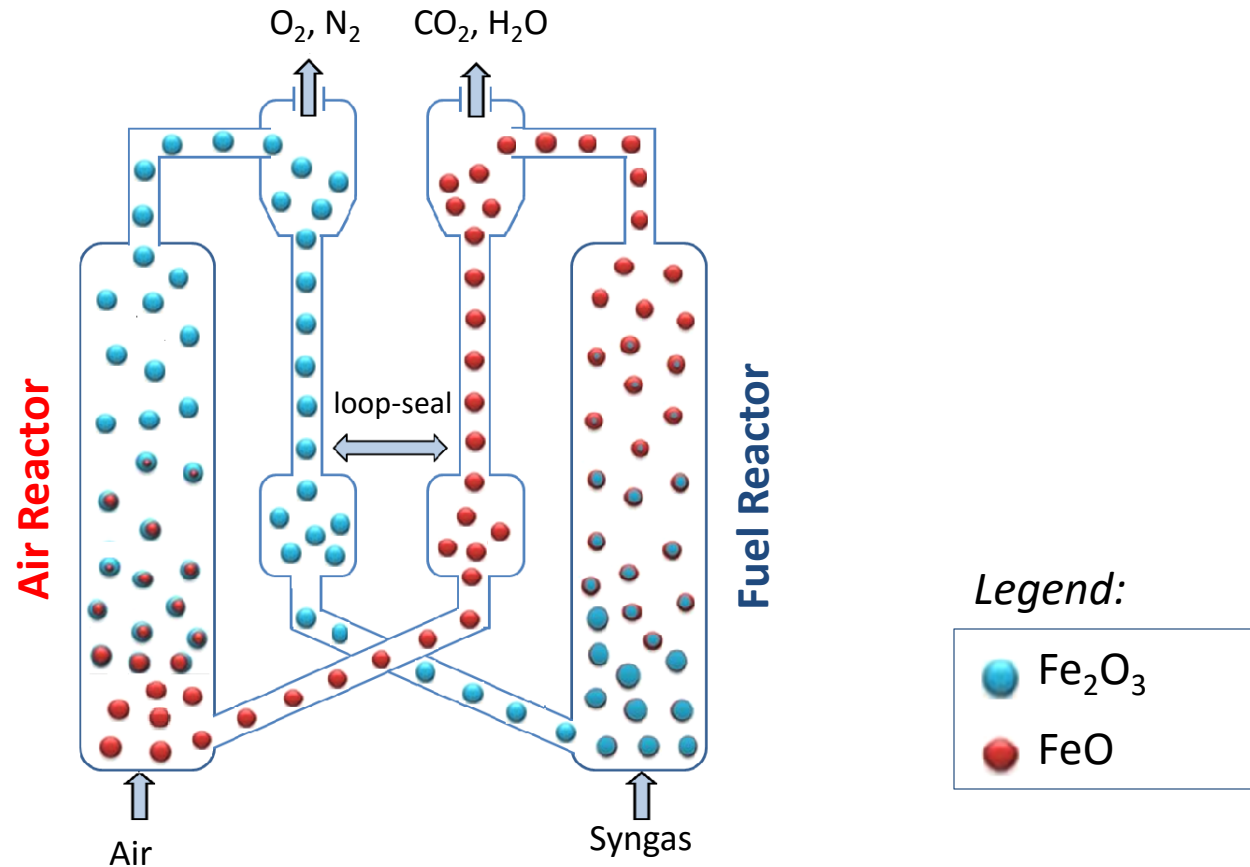


World net electricity generation by fuel type



(EIA, 2016, International Energy Outlook)

1. Introduction



2. Model development

2.1. Mass and energy balance equations

Assumptions:

- Perfectly spherical solid particles with constant diameter and macroscopic properties;
- Plug-flow of gases and solids in both reactors;
- Pseudo-homogeneous system within the elementary segment dz .

Total mass balance

$$\frac{1}{w_j} \cdot \frac{\partial(F_j)}{\partial t} = -\frac{\partial(F_j)}{\partial z} \pm S \cdot \frac{a \cdot M_i}{b \cdot M_{\text{FeO/Fe}_2\text{O}_3}}$$

Component mass balance

$$\frac{1}{w_j} \cdot \frac{\partial(F_j \cdot x_i)}{\partial t} = -\frac{\partial(F_j \cdot x_i)}{\partial z} \pm \sum \left(S \cdot \frac{a \cdot M_i}{b \cdot M_{\text{FeO/Fe}_2\text{O}_3}} \right)$$

Energy balance

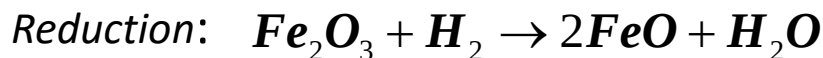
$$Cp_j \cdot \rho_j \cdot \frac{\partial T_j}{\partial t} = -Cp_j \cdot \rho_j \cdot U_j \cdot \frac{\partial T_j}{\partial z} \pm H_{pg} - H_{pw} - H_r$$

2. Model development

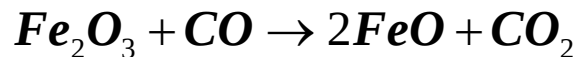
2.2. Kinetics and thermodynamic aspects



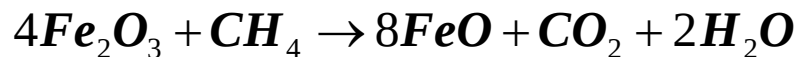
$$\Delta H_r = -517,85 \text{ [kJ / mol]}$$



$$\Delta H_r = 25,83 \text{ [kJ / mol]}$$



$$\Delta H_r = -7,86 \text{ [kJ / mol]}$$



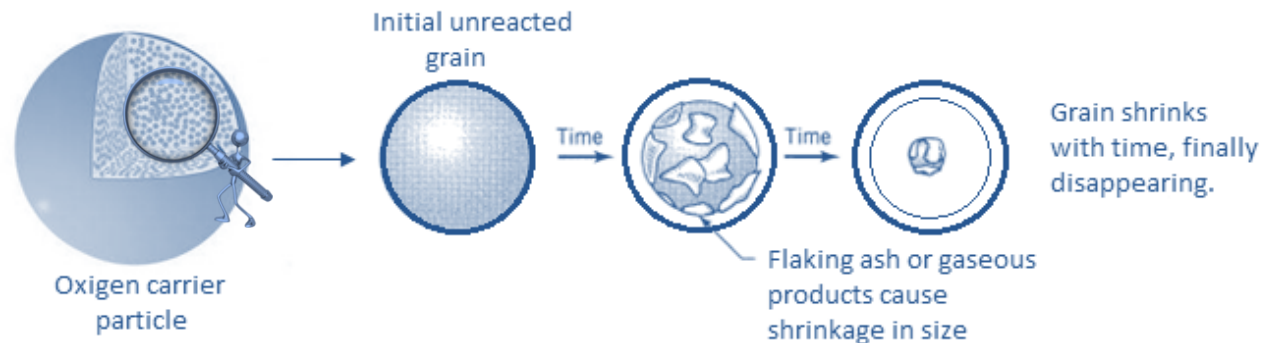
$$\Delta H_r = 307,2 \text{ [kJ / mol]}$$

Shrinking-core model

$$\frac{dX_{OC}}{dt} = \left[\frac{3}{\tau} \cdot (1 - X_{OC})^{\frac{2}{3}} \right]$$

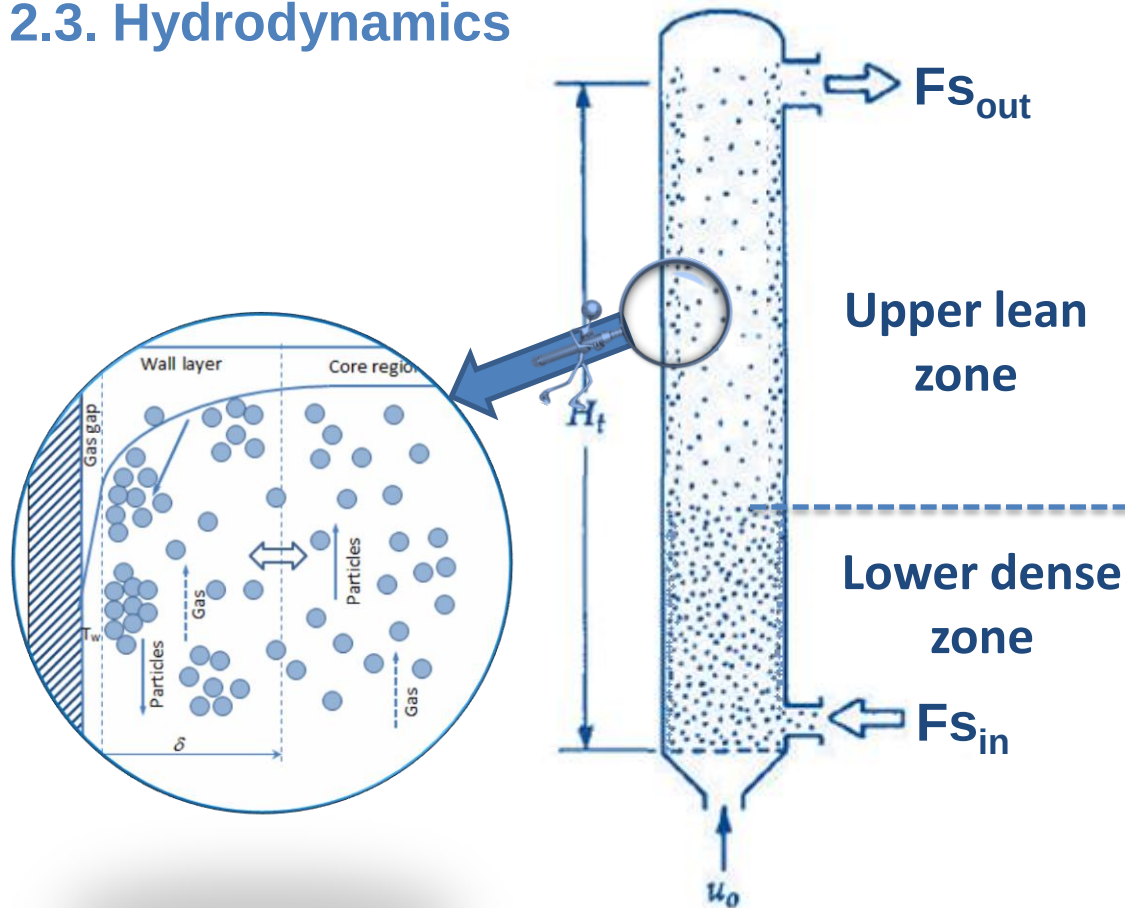
$$\tau = \frac{\rho_m \cdot r_g}{b \cdot k_s \cdot C_g^n}$$

$$k_s = k_{s0} \cdot e^{-E_a/RT}$$



2. Model development

2.3. Hydrodynamics



$$\frac{\varepsilon_s - \varepsilon_s^*}{\varepsilon_{s,dz} - \varepsilon_s^*} = e^{-a_d \cdot (H_{AR} - H_{dz})}$$

$$\Delta P_{tz} = \int_{H_{dz}}^H \rho_p \cdot \varepsilon_s \cdot g \cdot dh$$

$$\varepsilon_{s,dz} = 1 - \delta_b + (1 - \delta_b) \cdot \varepsilon_e$$

$$\Delta P_{dz} = \int_0^{H_{dz}} \rho_p \cdot \varepsilon_{s,dz} \cdot g \cdot dh$$

$$\Delta P = \Delta P_{dz} + \Delta P_{tz} \Rightarrow H_{dz}$$

(Johnsson F. et al, 1991, Powder Technology, vol. 68, pp. 117-123.)

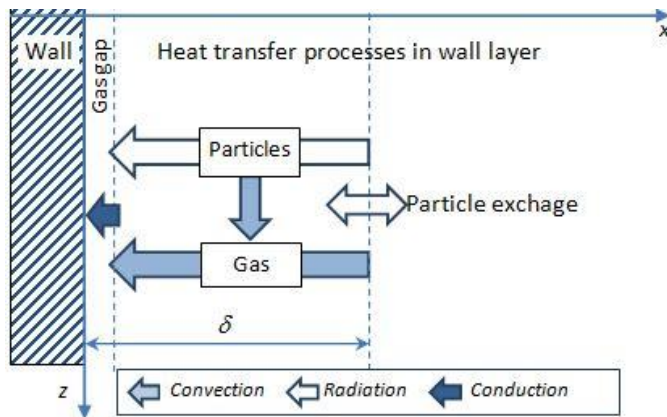
(Shrestha S. et al, 2016, Chemical Engineering Research and Design, vol. 109, pp. 791-805.)

2. Model development

2.4. Heat transfer

Mechanisms considered:

- Convection between oxygen carrier particles and gas phase inside the bed
- Conduction/conduction between particles, gas and wall
- Radiation



$$\Rightarrow h_{pg} = 8.4 \cdot Re_p^{0.871} \cdot \left[\frac{(1-\varepsilon) \cdot z}{d_p} \right]^{0.924}$$

$$\Rightarrow h_{pw} = f_c \cdot (h_c + h_{rc}) + (1 - f_c) \cdot (h_l + h_{rl})$$

$$h_c = \frac{1}{\left(\frac{k_c \cdot \rho_c \cdot c_c}{\pi \cdot t_c} \right)^{0.5} + h_w}$$

$$h_l = \frac{k_g \cdot Cp_p}{d_p \cdot Cp_g} \cdot \left(\frac{\rho_l}{\rho_p} \right)^{0.3} \cdot \left(\frac{Ut^2}{g \cdot d_p} \right)^{0.21} \cdot Pr$$

$$h_r = \frac{q_r}{T_b - T_w} = \frac{\sigma (T_b^4 - T_w^4)}{(T_b - T_w) \cdot \left[1 + \frac{1 - e_{c/l}}{e_{c/l}} + \frac{1 - e_b}{e_b} \right]}$$

(Makkawi Y., 2013, 10th International Conference on Circulating Fluidized Beds and Fluidization Technology)

(Scala F., 2015, Fluidized Bed Technologies for Near-Zero Emission Combustion and Gasification, Cambridge, UK, Woodhead Publishing, pp. 177-253)

2. Model development

Design and operational parameters

Parameter	Unit	Air Reactor	Fuel Reactor
Height, H	m	8.7	11.4
Diameter, D	m	0.59	0.4
Fluidizing gas	-	Air	Syngas
Superficial gas velocity, U_0	m/s	3-3.5	3-3.5
Solid circulation rate, F_{OC}	kg/s	0.55-2.5	0.55-2.5
Temperature, T	K	1300	1300
Pressure drop, ΔP	kPa	20	20
Oxygen carrier	-	ilmenite	
Particle diameter, d_p	μm	250	
Apparent density, ρ_p	kg/m^3	3710	

(Ströhle J. et al.,2014, Applied Energy, vol. 113, pp. 1490-1495.)

(Abad A. et al, 2013, Chemical Engineering Science, vol. 87, pp. 277-293.)

3. Results

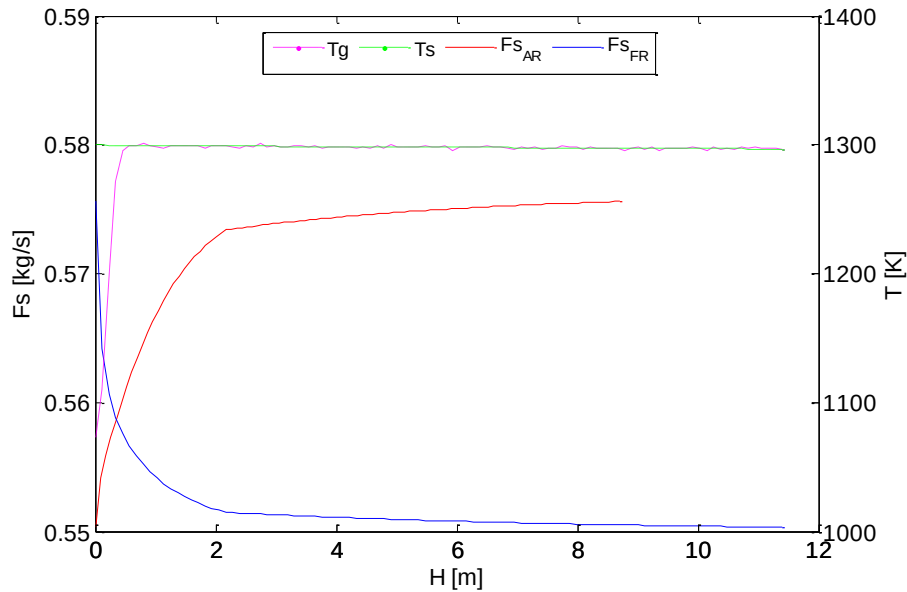


Figure 1. Oxygen carrier and temperature distribution

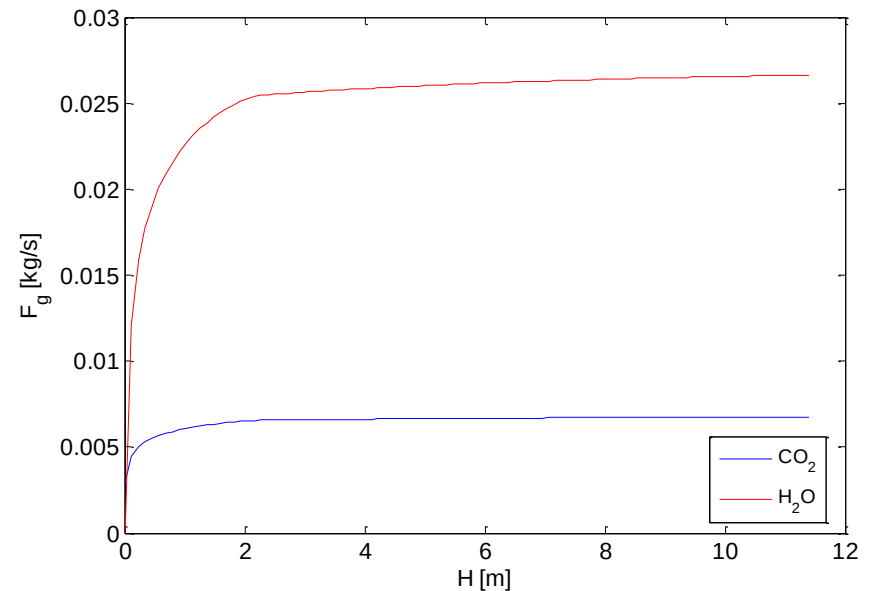


Figure 2. Gas products in FR

3. Results

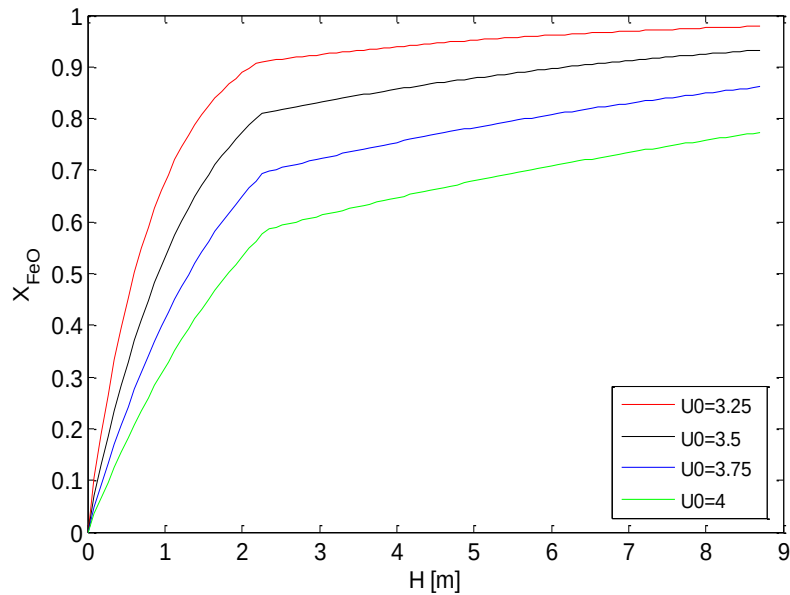


Figure 3. Conversion variation with velocity in AR

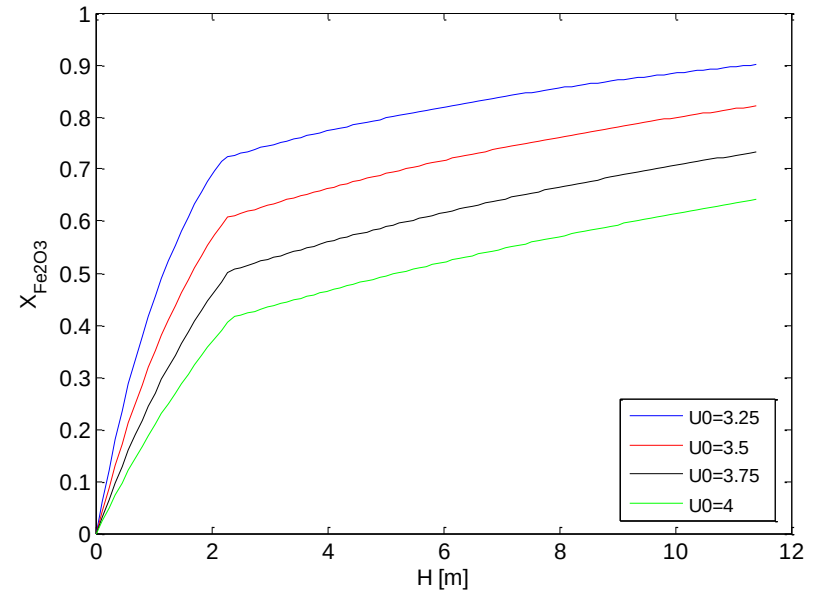


Figure 4. Conversion variation with velocity in FR

3. Results

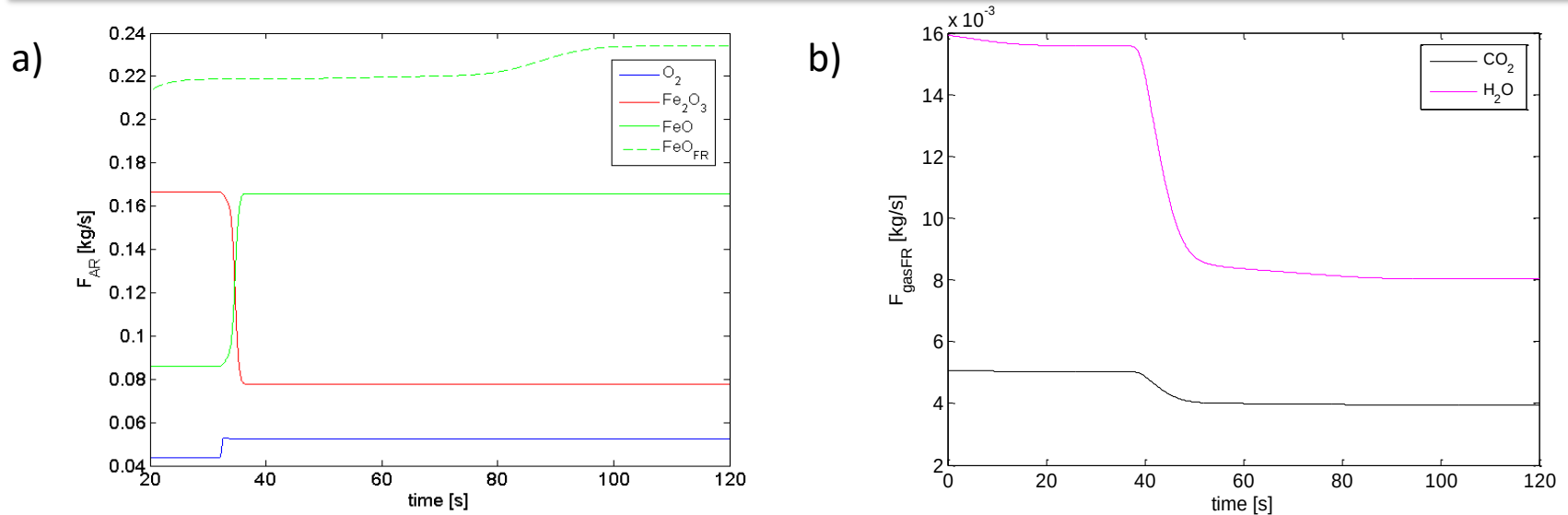


Figure 5. Dynamic response to a step signal of +20% F_g

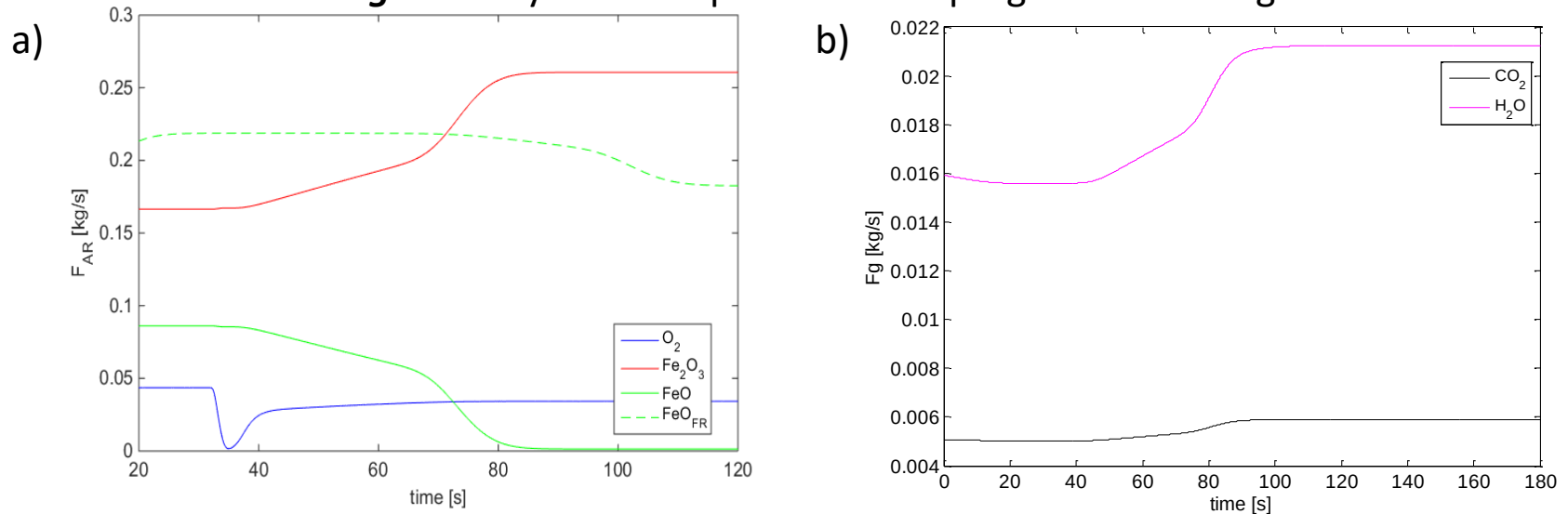


Figure 6. Dynamic response to a step signal of -20% F_g

3. Results

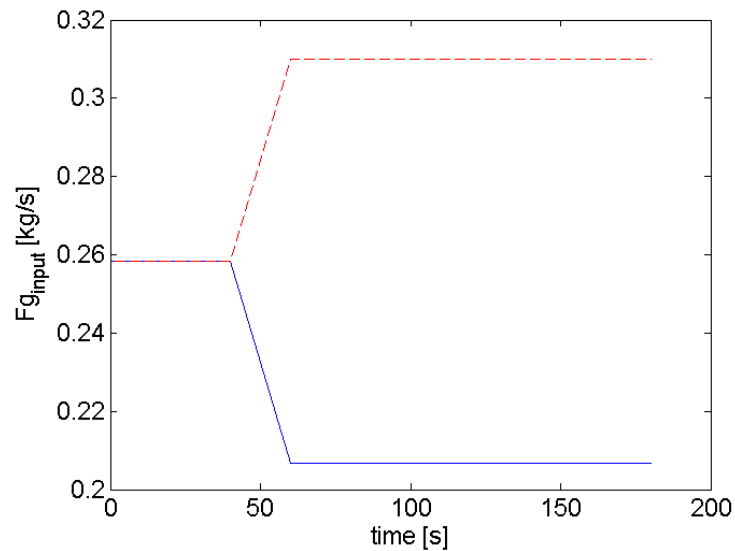


Figure 7. Ramp signal of $\pm 20\%$ F_g

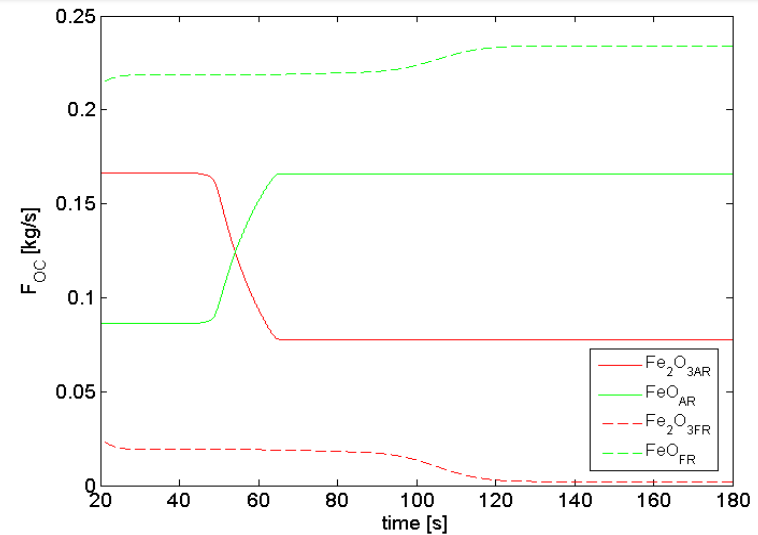


Figure 9. Oxygen carriers in AR and FR

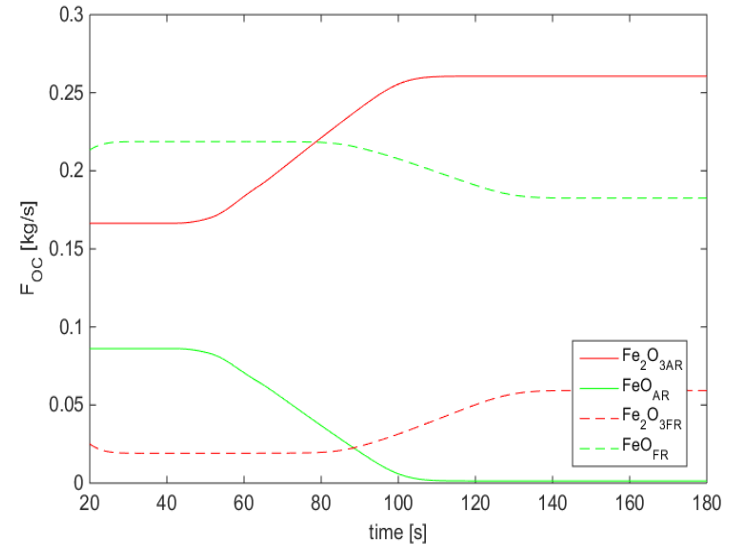


Figure 8. Flows in the AR

4. Conclusions

- ✓ Simulation results show that the oxidation and reduction of the oxygen carrier take place predominantly in the dense region of the fluidized bed reactor.
- ✓ The fluidizing gas velocity was shown to have a significant influence over the performance of the process.
- ✓ The dynamic behaviour of the syngas-based chemical looping combustion process was studied by step and ramp input changes of the gas flow rate in the air reactor.
- ✓ The dynamic behaviour of the here presented system is fast, with a slight delay propagated to the second reactor.
- ✓ A perturbation of the input gas flow with 20% triggers a 2 times variation of the oxygen carrier circulation rate.
- ✓ At a decrease signal, in both step and ramp situations, the response of the system is considerably slower than when the opposite sign perturbation appears.

Acknowledgements

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