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Multiescale computational modeling of heterogeneous gas-solid reactions of the direction reduction process of iron ores

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MULTIESCALE COMPUTATIONAL MODELING OF HETEROGENEOUS NON-CATALYTIC GAS-SOLID REACTIONS OF THE DIRECT REDUCTION PROCESS OF IRON ORE

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Agosto 2023

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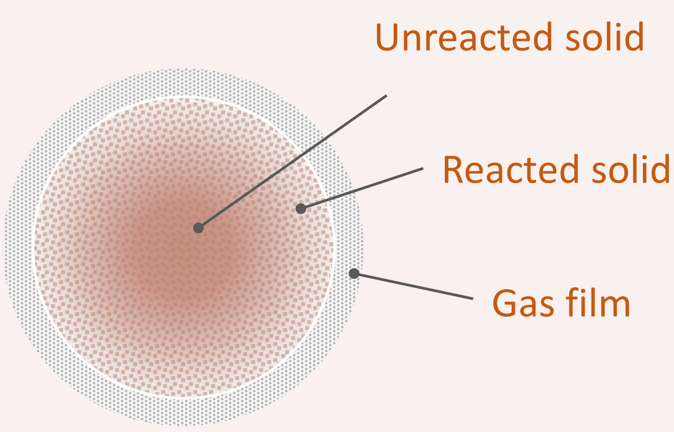
INTRODUCTION

Importance of multiscale modeling



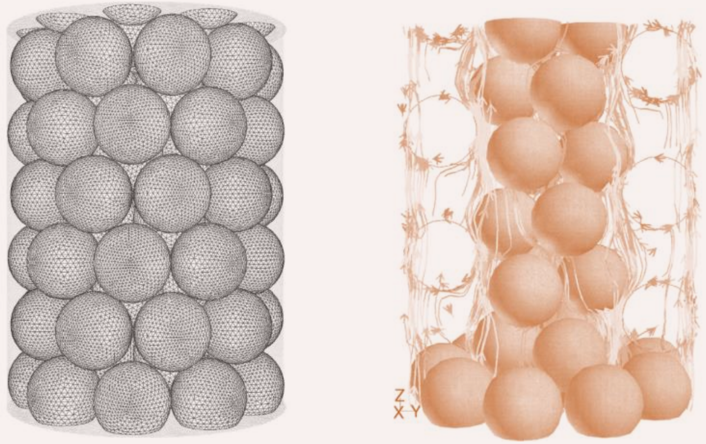
Particle (inside modeling)

- ✓ Mass and heat transport mechanisms
- ✓ Structural changes over time
- ✓ Physical properties of the systems changes

Non-catalytic gas-solid reactions

Coupling

Multi-scale approach



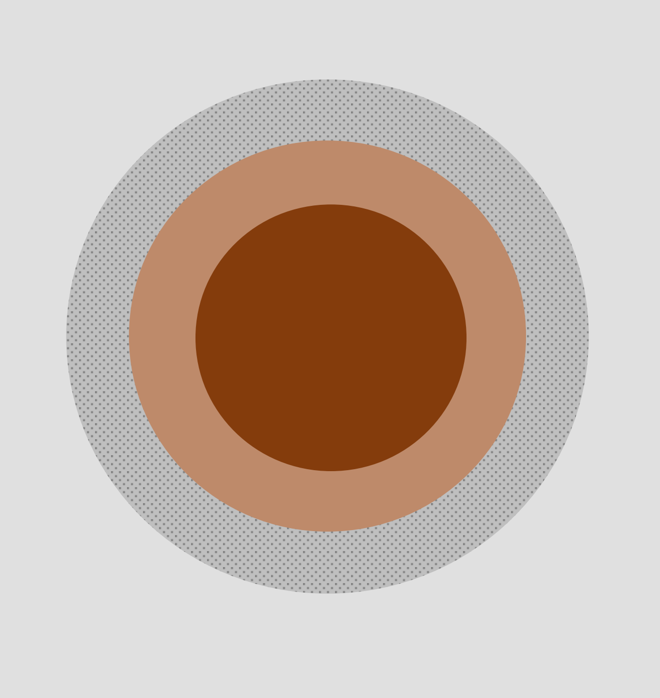
Moving - Bed

- ✓ Mass and heat transport mechanism
- ✓ Fluid flow between particles
- ✓ Random arrangement of particles

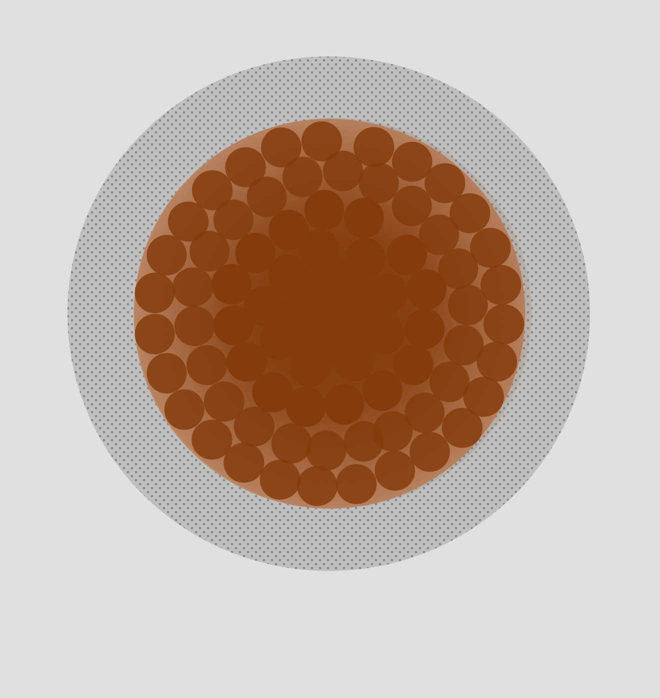
INTRODUCTION

Non-catalytic gas-solid reactions models

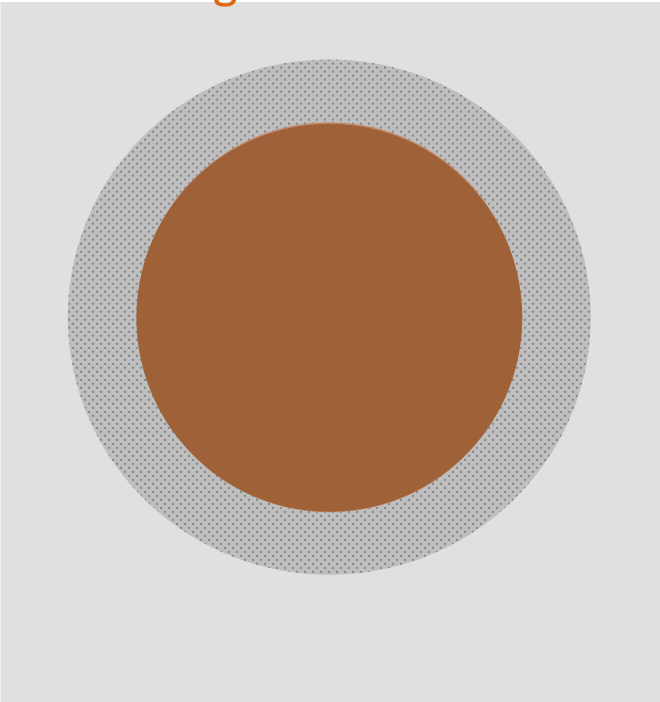
Shrinking Core Model (SCM)



Grain Model (GM)



Homogeneous Model



Heterogeneous ⟷ Homogeneous

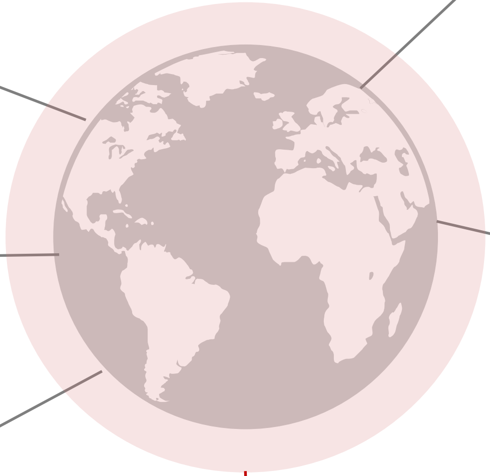
INTRODUCTION

Direct Reduction Of Iron Ore (DRI)

~110 million tons of iron
is the annual world production
(MIDREX, 2022)

High energy consumption
is decreased compared to blast furnace
(IEAGHG, 2018)

Smaller units are more flexible
(Béchara et al., 2018)



Reduction in CO_2 emissions
40 to 50% compared to blast furnace (IEAGHG, 2018)
Zero emission using only H_2

Substitution **for green H_2**
via electrolysis
(Patisson and Mirgaux, 2020)

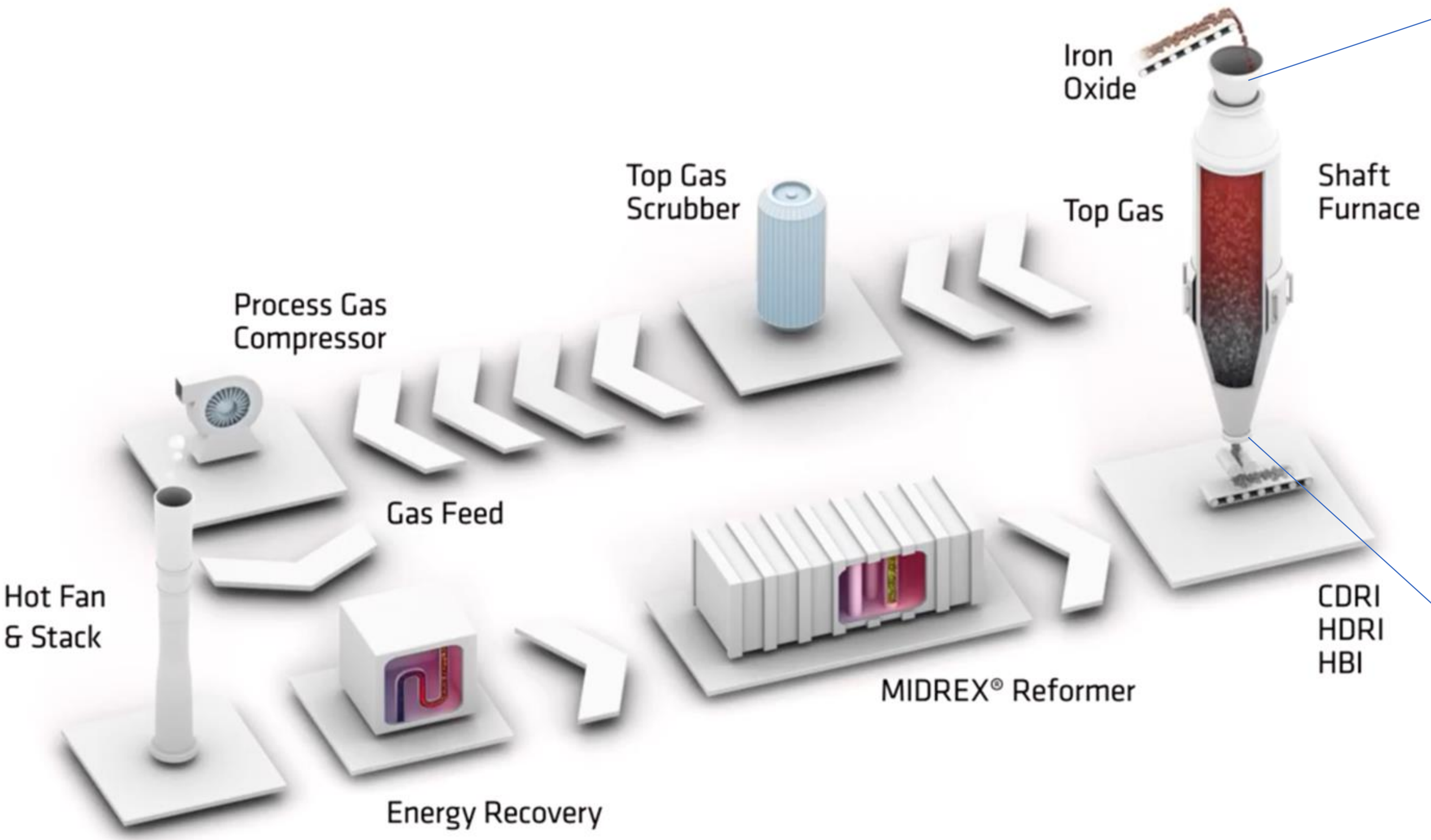
climate change

Steelmaking (1/3 of industrial CO_2 emissions)
(IPCC, 2014)

Paris Agreement
European Green Deal

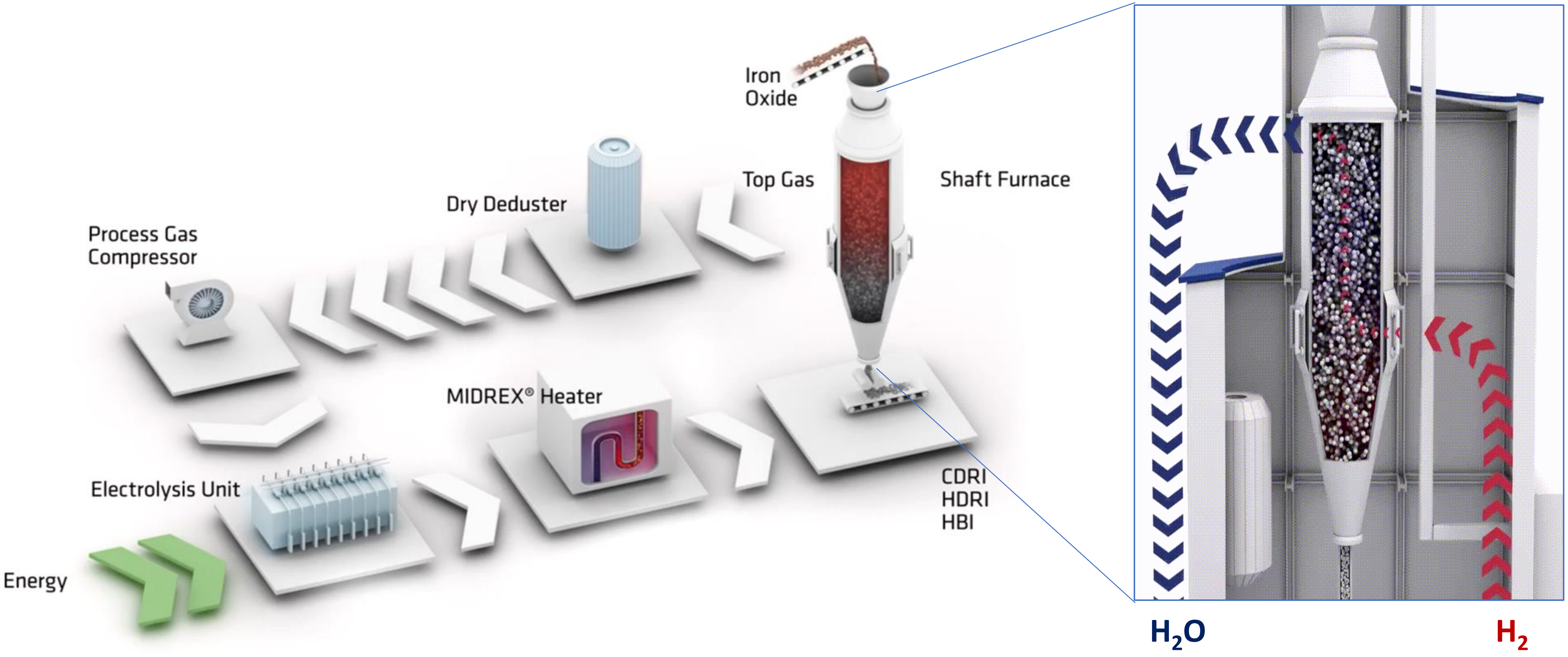
- Limit global warming to 1.5 °C by 2050
- 55% in CO_2 emission until 2030 and carbon neutrality by 2050

MIDREX Process: Direct Reduction of Iron Ore



MIDREX (2021)

H-DR Process: Hydrogen Direct Reduction of Iron Ore



MIDREX (2021)

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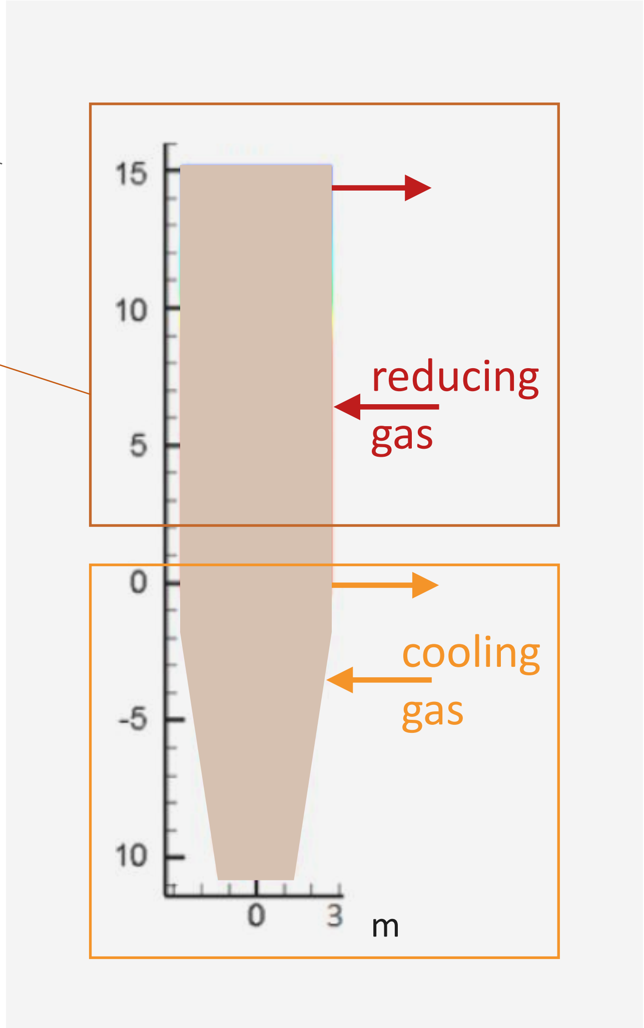
Main studies on reactor scale DR modeling

Study	Dimension	Features
Hamadeh et al. (2018)	2D	Complete reactor model
Ranzani da Costa et al. (2013)	2D	Reaction zone **(H_2–DR)**
Rahimi & Niksiar (2013)	1D	GM and SCM discrepancy
Valipour & Saboohi (2007)	1D	Finite Volume Method GM
Negri et al. (1991)	1D	3 reduction reactions + Shift reaction
Parisi & Laborde (2004)	1D	Mass and energy balance Global reactions SCM



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OBJECTIVES

Develop a multiscale mathematical model to represent non-catalytic gas-solid reactions applied to the direct reduction of iron ore process

1. Explore the influence of the structural parameters of the pellets such as size, porosity on process efficiency.
2. Validate the models with experimental data.
3. Predictions for the hydrogen direct reduction (HDR) process.

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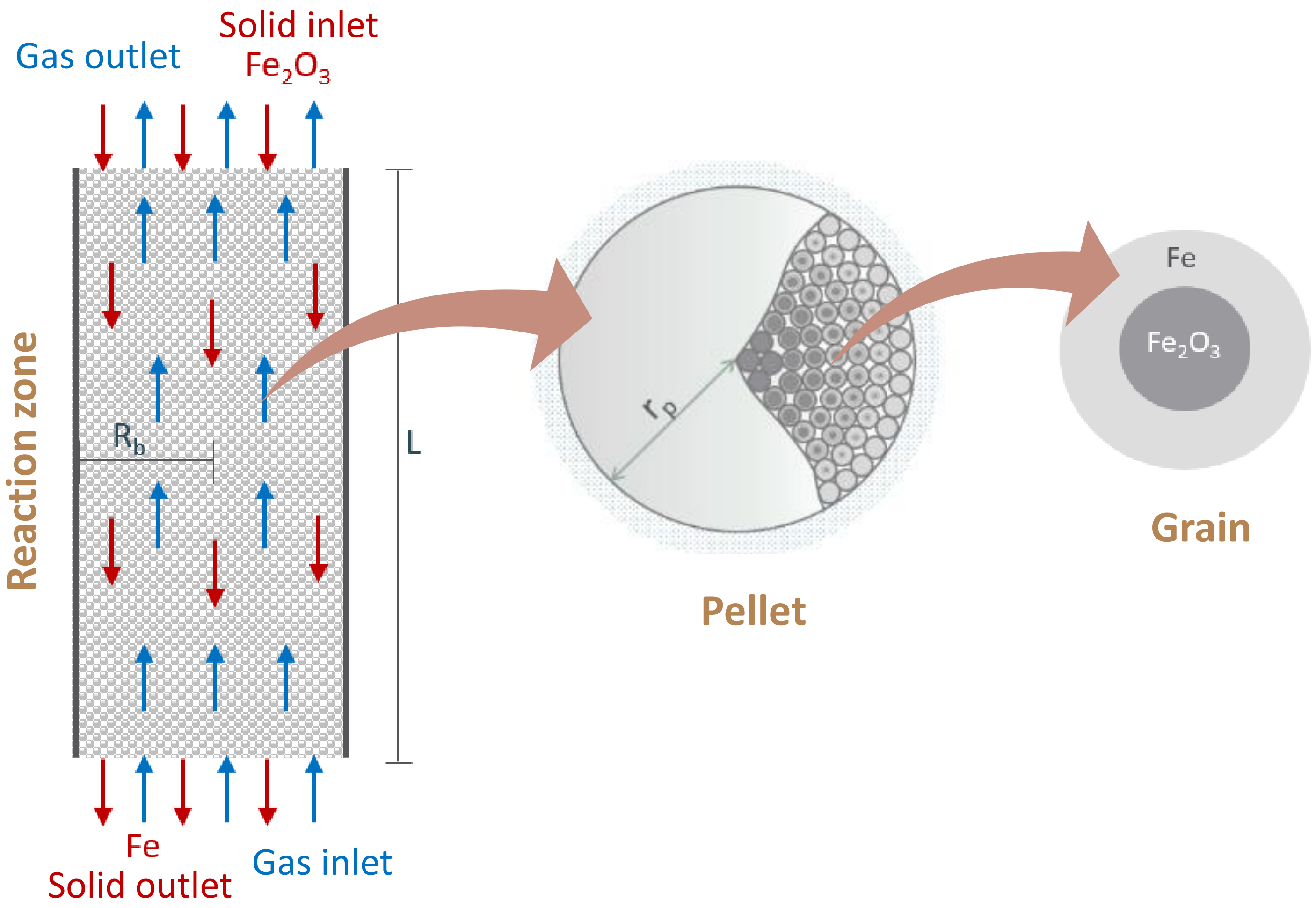
Multiscale Modeling

✓ **Assumptions:**

- Ideal gas mixture
- Plug-flow for both gas and solid
- Ergun equation
- Spherical pellet and grain
- Pellet and grain size constant
- Porosity change
- 2 global reduction reaction



Mathematical Modeling

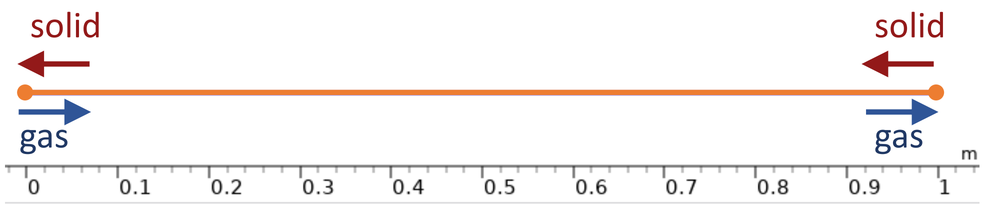
- ✓ **Finite element method**
  - Comsol Multiphysics 6.0

✓ **Reactor-pellet scale coupling**

General Extrusion

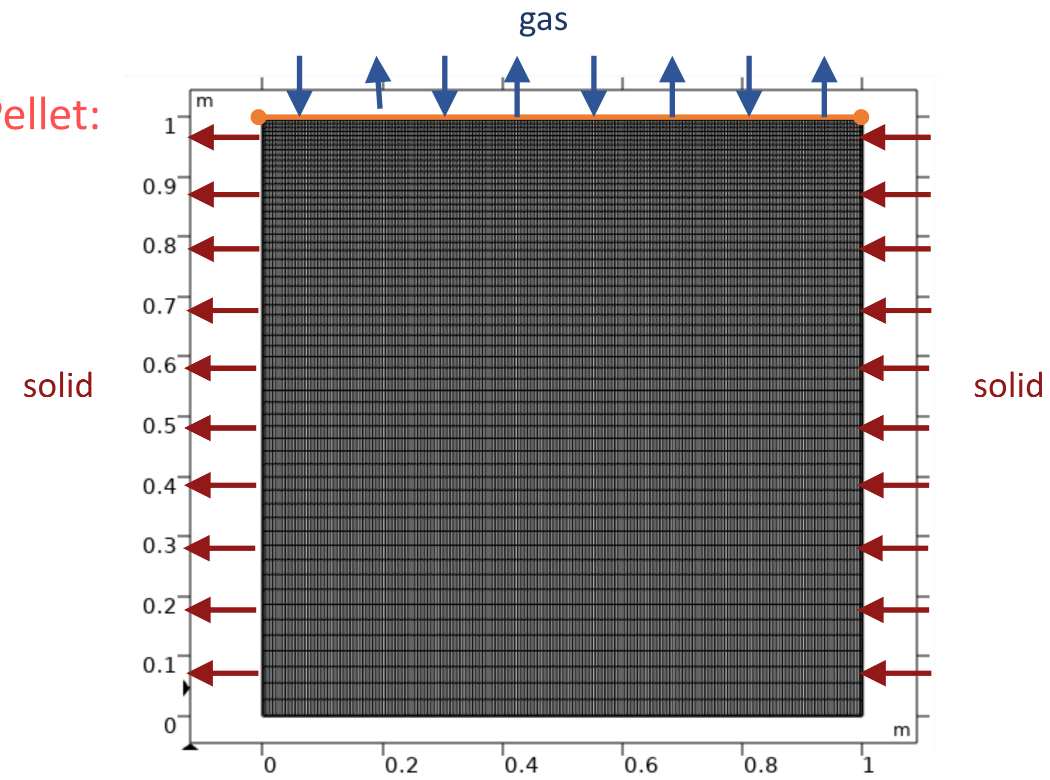
✓ 1D Reactor:

(x axis)



✓ 1D symmetric Pellet:

Extra dimension
(y axis)



Mathematical Modeling

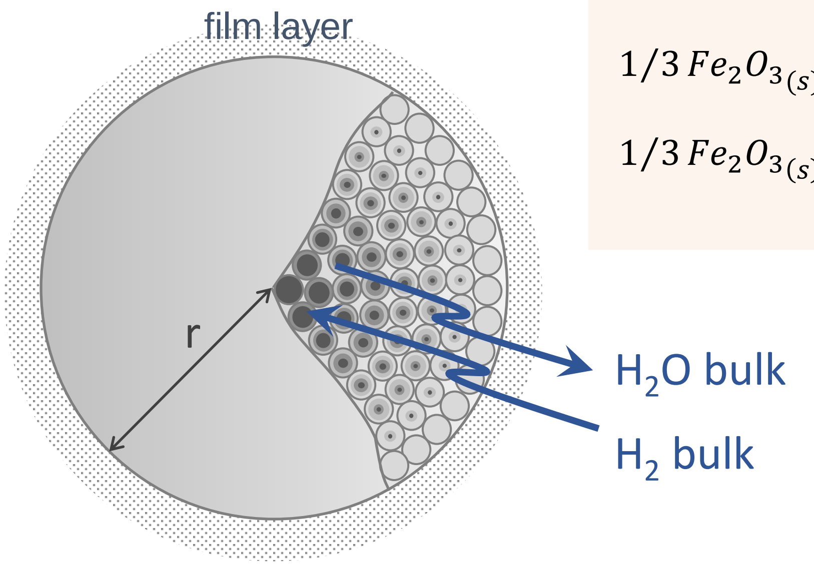
✓ **Pellet scale model**

▪ Mass balance for gas (i= H_2, H_2O, CO, CO_2, N_2)

$$-D_{i,eff}\frac{\partial^2 C_i}{\partial r} = \frac{2}{r}D_{i,eff}\frac{dC_{p,i}}{dr} + R_i(r,z)$$

▪ Mass balance for solid (j= Fe_2O_3, Fe)

$$u_s\frac{dC_j}{dr} = (1-\varepsilon_b)R_i(r,z)$$



Reactions

$$1/3\,Fe_2O_{3(s)} + H_{2(g)} \rightarrow 2/3\,Fe_{(s)} + CO_{2(g)}$$

$$1/3\,Fe_2O_{3(s)} + CO_{(g)} \rightarrow 2/3\,Fe_{(s)} + CO_{2(g)}$$

▪ Kinetic model (Grain model)

$$R_{\mathrm{Fe_2O_3}} = -\frac{1}{3}A_g\,k_1 f(x_1)C_{\mathrm{H_2}} - \frac{1}{3}A_g\,k_2 f(x_1)C_{\mathrm{CO}}$$

$$R_{\mathrm{Fe}} = \frac{2}{3}A_g\,k_1 f(x_1)C_{\mathrm{H_2}} + \frac{2}{3}A_g\,k_2 f(x_1)C_{\mathrm{CO}}$$

$$f(x_n) = \left[(1-x_n)^{-2/3} + \frac{k_n r_g}{D_{effg,i}}(1-x_n)^{-1/3} - \frac{k_n r_g}{D_{effg,i}}\right]^{-1}$$

Overall conversion of the pellet

$$X_n = \frac{3}{r_p^3}\int_0^{rp} x_n(r,t)r^2dr$$

Mathematical Modeling

✓ **Moving-bed reactor scale model**

- Mass balance for gas (i= H_2, H_2O, CO, CO_2, N_2)

$$\frac{d}{dz}\left(-D_i\frac{dC_i}{dz}\right)+u_g\frac{dC_i}{\partial z}+C_i\left(\frac{u_gP}{T_g}\right)=-(1-\varepsilon_b)A_pD_{i,eff}\frac{dC_{i,p}}{dr}|_{r=r_p}$$

- Mass balance for solid (j= Fe_2O_3, Fe)

$$\frac{dC_j}{dz}=\frac{3}{{r_p}^3}\int_0^{r_p}C_{j,p}\,r^2dr\,(1-\varepsilon_b)$$

- Heat balance for gas

$$-\frac{d}{dz}\left(k_{gt}\frac{dT_g}{dz}\right)+\rho_gCp_gu_g\frac{dT_g}{dz}=-(1-\varepsilon_b)\mathrm{A}_ph\left(T_g-T_s|_{r=r_p}\right)$$

- Heat balance for solid

$$-\frac{d}{dz}\left(k_s\frac{dT_s}{dz}\right)+\rho_sCp_{eff,p}u_s\frac{dT_s}{dz}=(1-\varepsilon_b)h\sum R_j(-\Delta H)_j+(1-\varepsilon_b)\mathrm{A}_ph(T_g-T_s)$$

- Ergun equation

$$-\frac{dP}{dz}=\frac{u_g}{d_p}\frac{(1-\varepsilon_b)}{{\varepsilon_b}^3}\left[\frac{150\mu(1-\varepsilon_b)}{d_p}+1.75\rho_gu_g\right]$$

where: $$\frac{u_g}{u_{feed}}=\frac{P_{feed}}{P}\frac{T_g}{T_{feed}}$$

Industrial Plant Data

Gilmore Plant (Parisi and Laborde, 2004)

Inlet solid

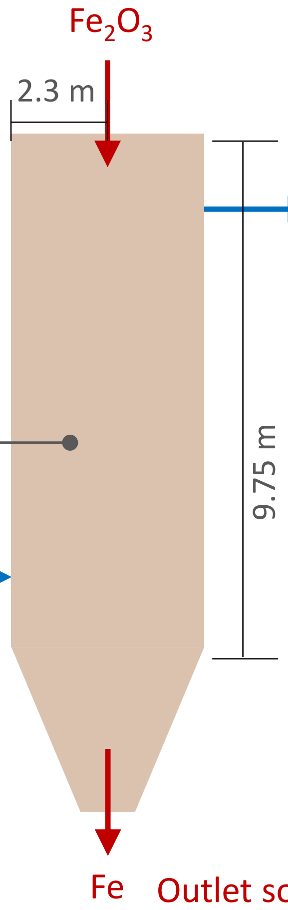
Impurity	4	%
Mineral pellet density	4.7	g/cm³
Pellet diameter	11	mm
Temperature	30	°C
Inlet velocity	3.490E-04	m/s
initial pellet porosity	0.14	

Bed properties

Pellets/volume	0.64	pellet/cm³
Bed density	2	g/cm³

Inlet gas

Flow rate	53863	Nm³/h
Pressure	1.4	atm
Temperature	930	°C
Inlet Gas Composition		
H2	52.58	%
CO	29.97	%
H2O	4.65	%
CO2	4.8	%
CH4	1.4	%
N2	6.6	%



Outlet gas

Pressure	131325	Pa
Temperature		°C
Oultlet Gas Composition (dry base)		
H2	37	%
CO	18.9	%
H2O	21.2	%
CO2	14.3	%
CH4+N2	8.6	%

Outlet solid

Metallization	93	%
Mineral pellet density	3.2	g/cm³
Production	26.4	t/h

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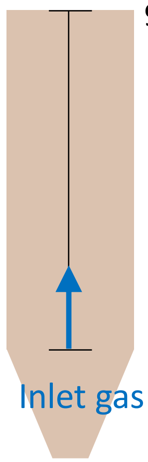
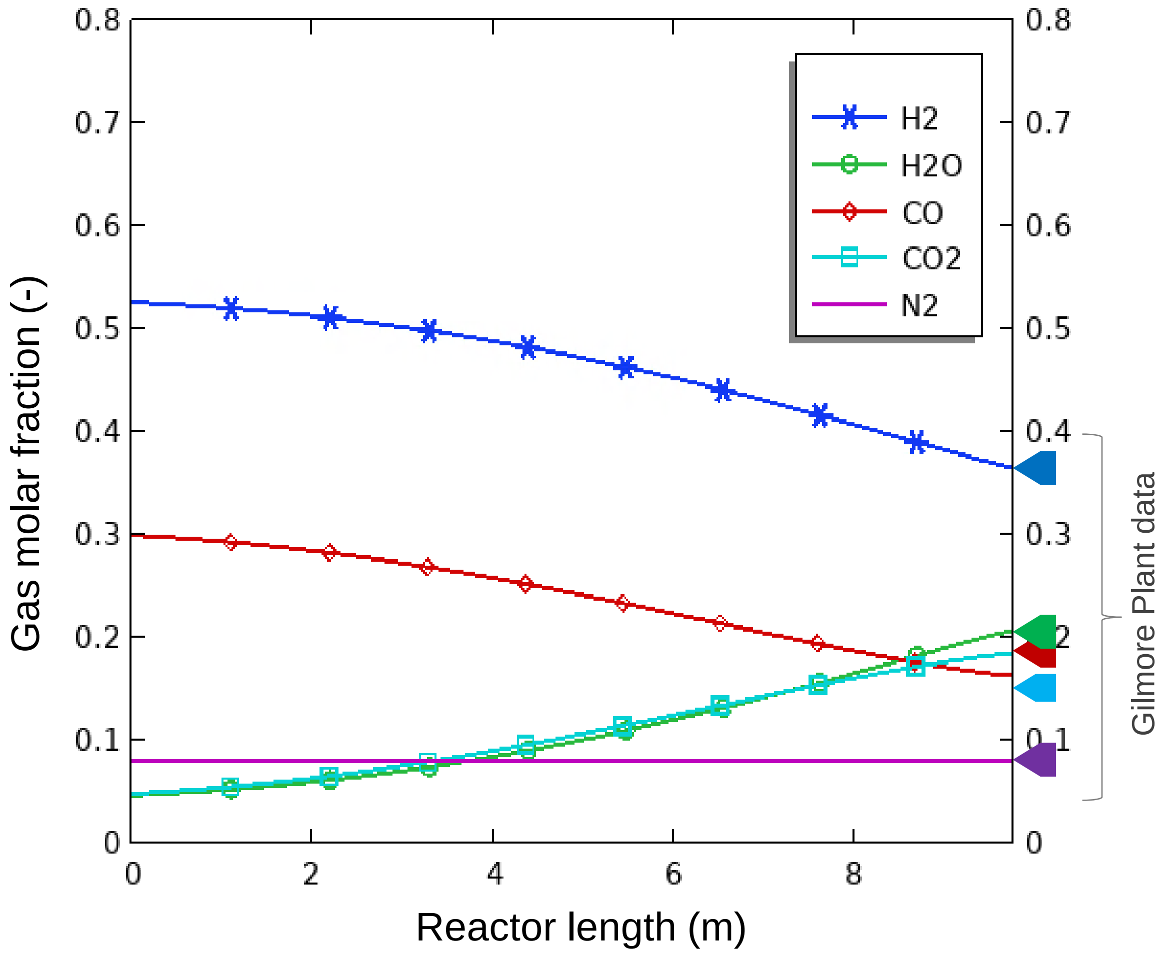
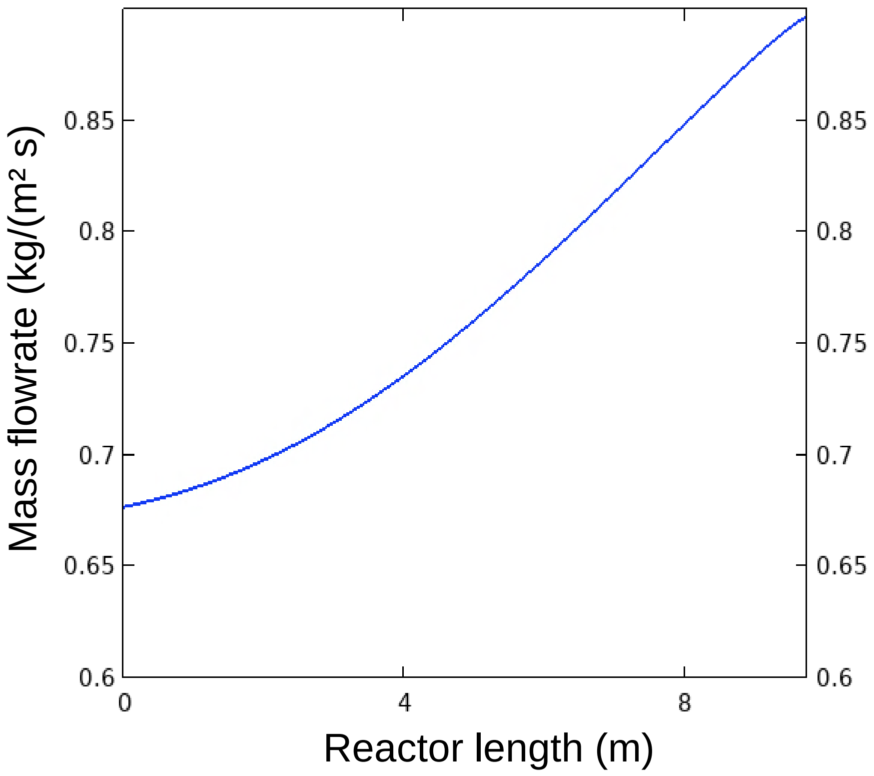
Reactor Scale



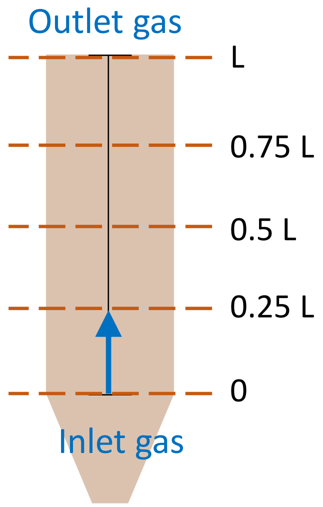
Gas Phase

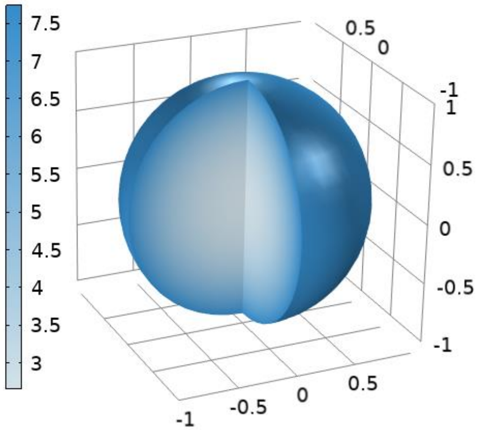


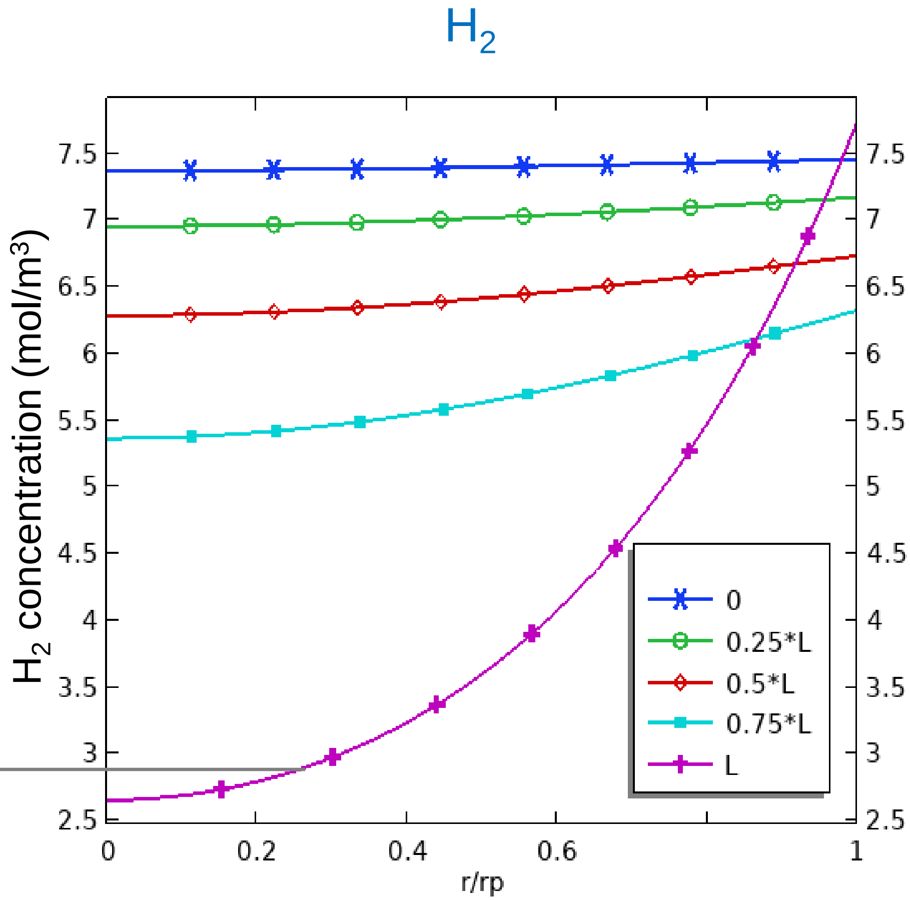


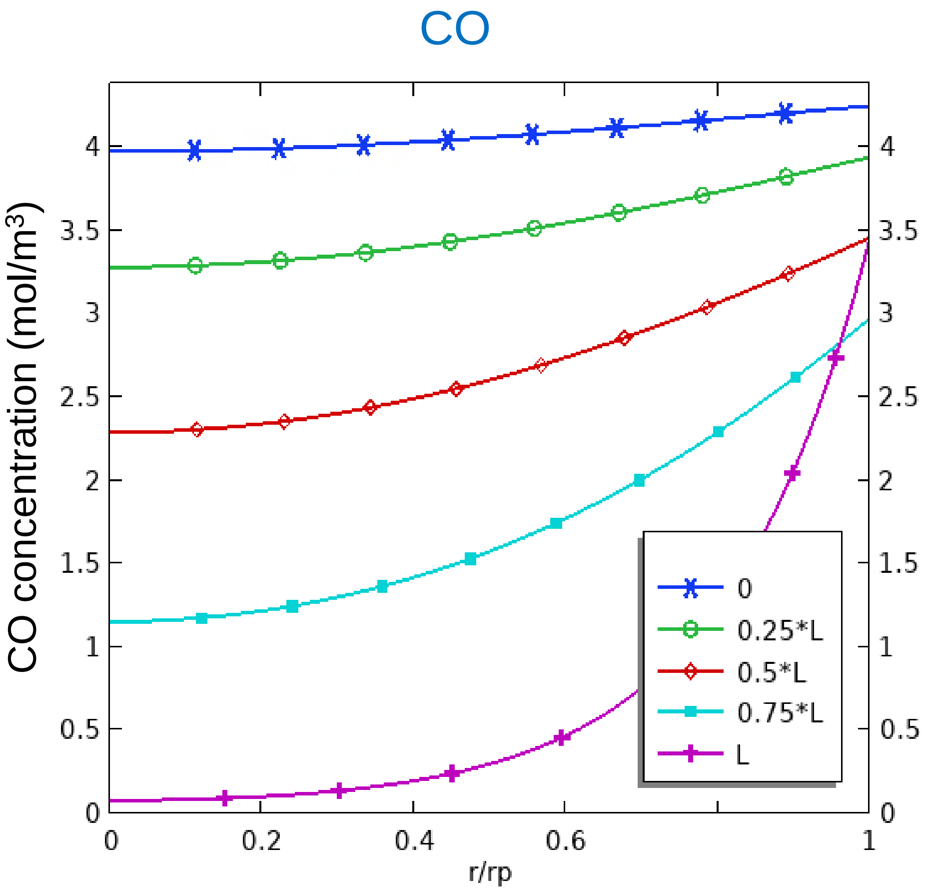
Pellet Scale

Gas Phase

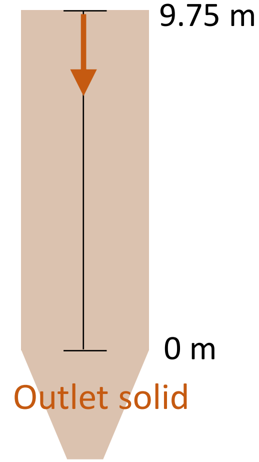




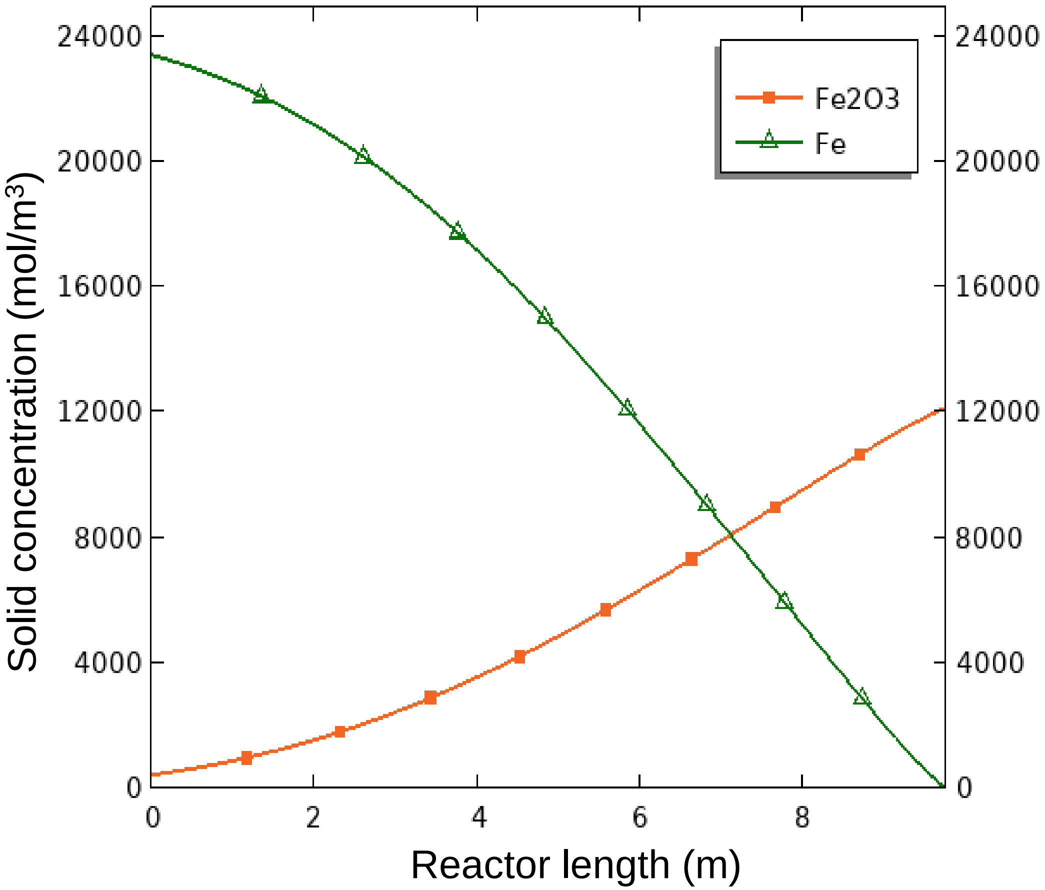




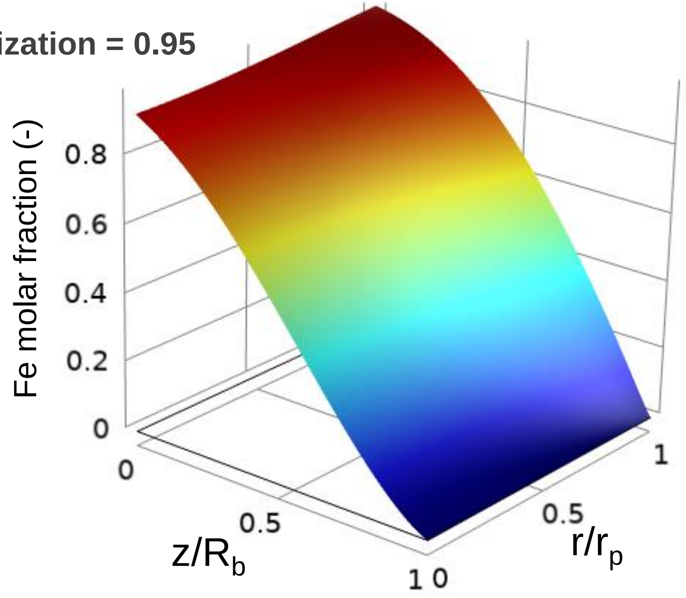
Reactor-Pellet Scale



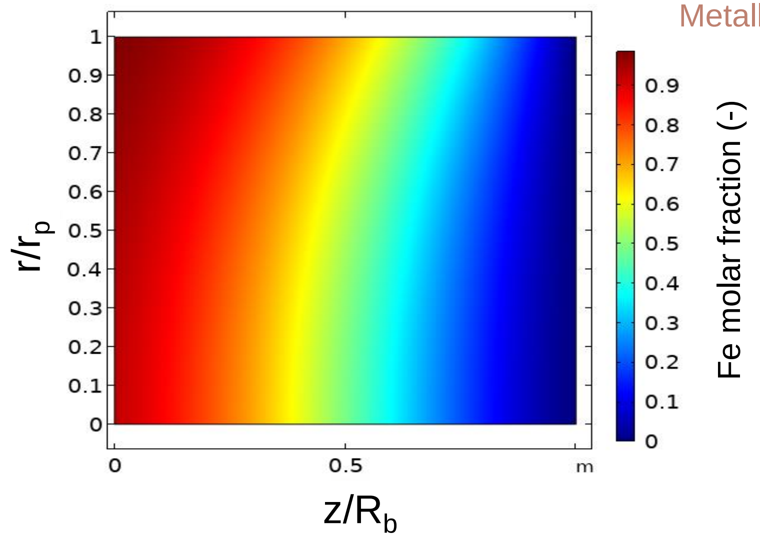
Solid Phase



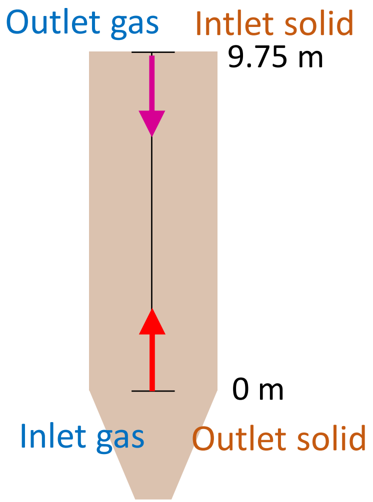
Metallization = 0.95



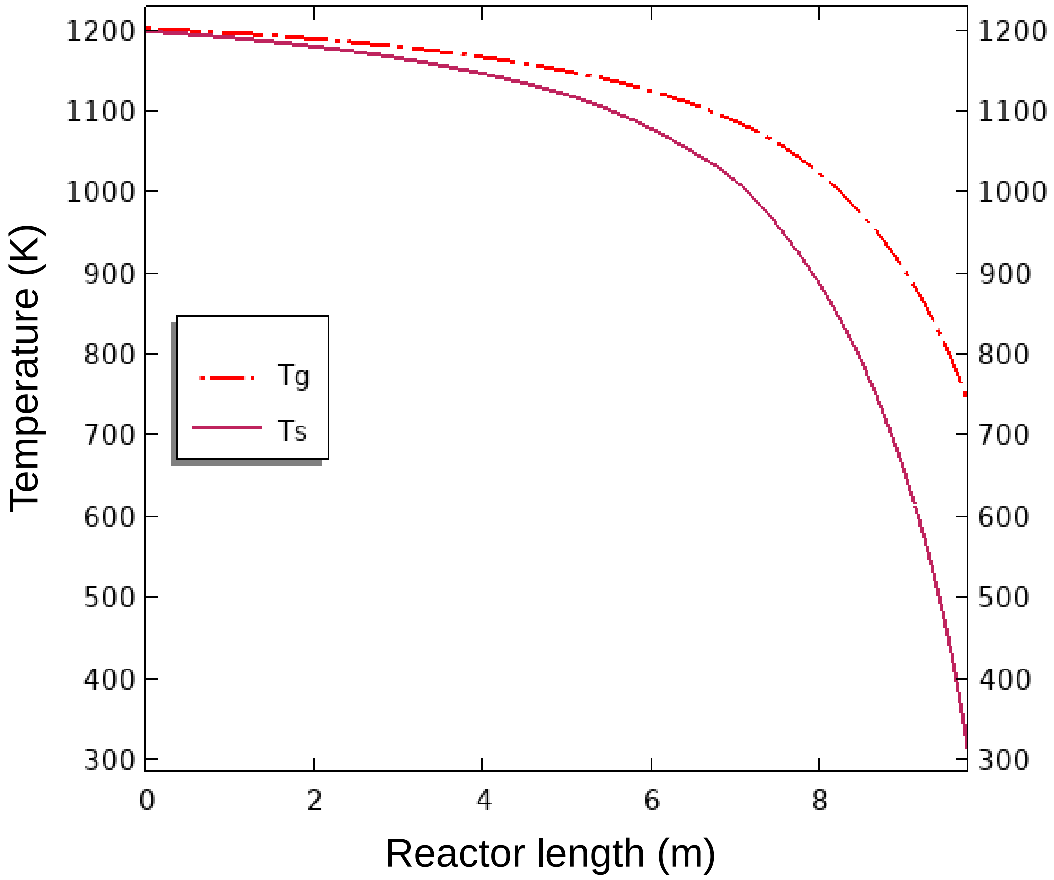
Gilmore Plant data
Metallization = 0.93



Reactor Scale



Temperature of the gas (Tg) and solid (Ts) along the reactor lenght



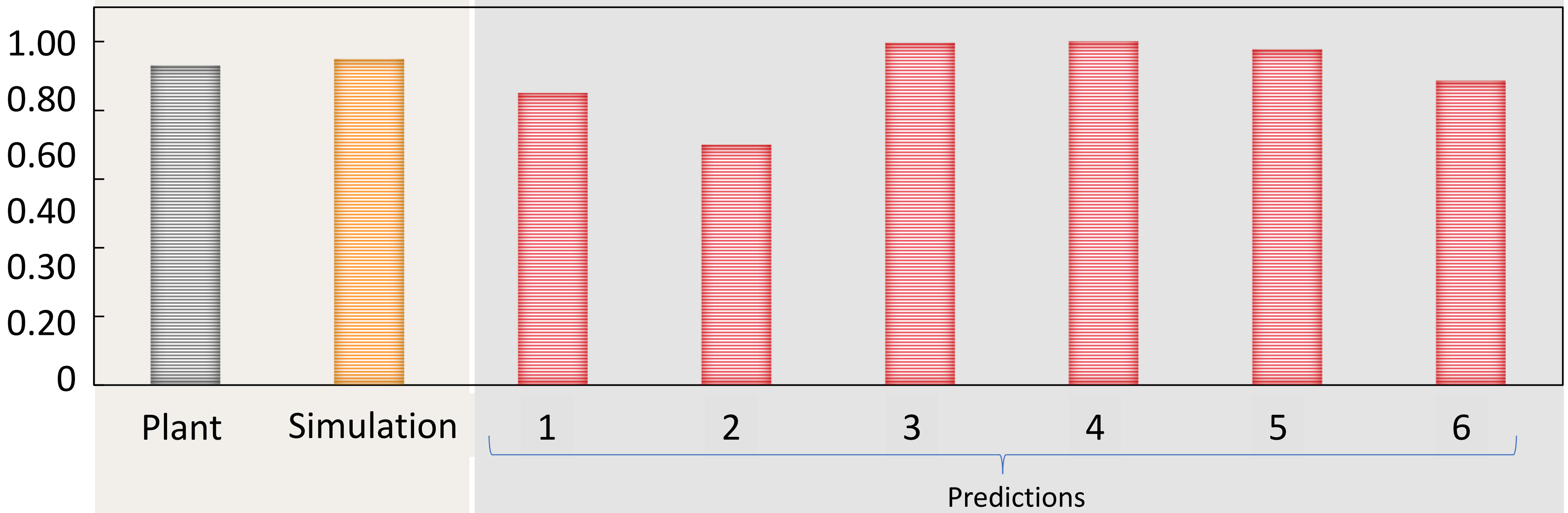
Pellet Scale

Isothermal pellet

Biot number < 0.1

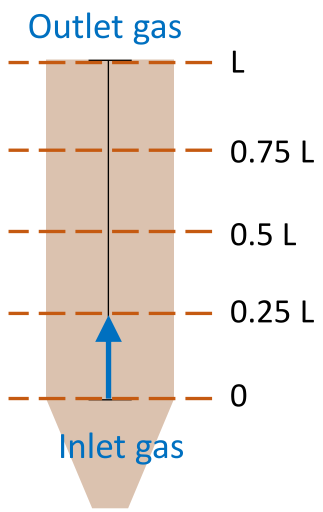
Reactor Scale

Sensitivity analysis of the structural parameters of the pellet

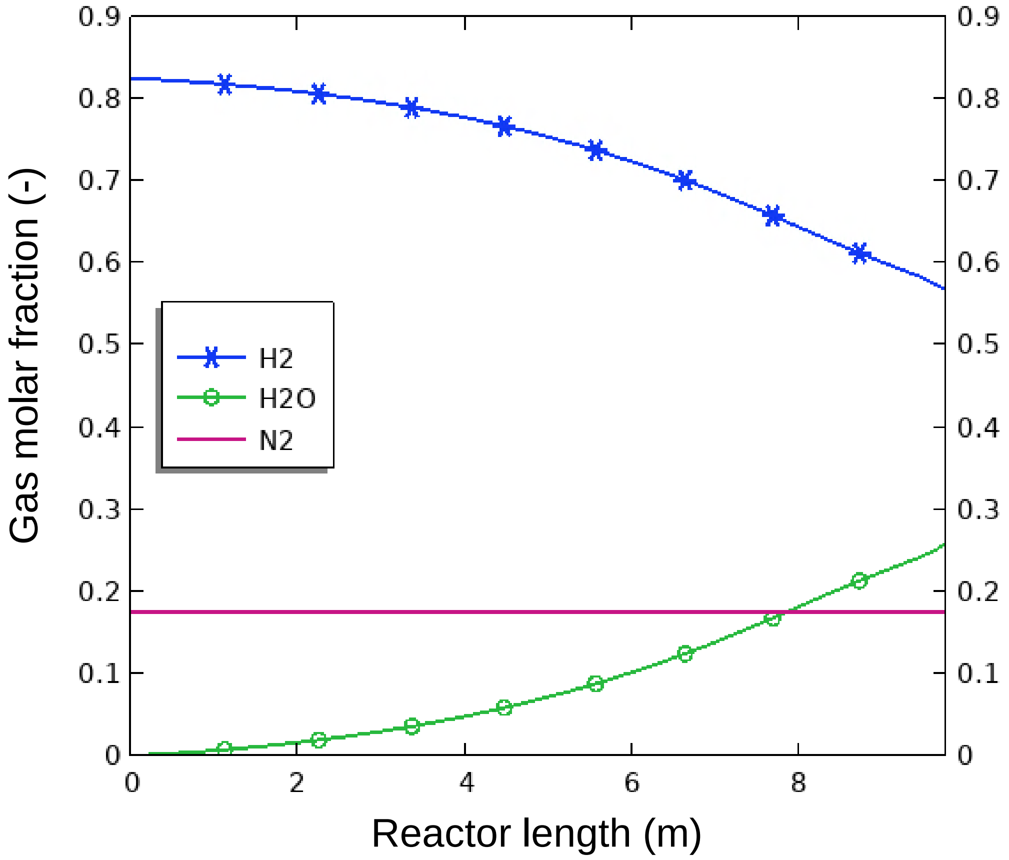


	Plant	Simulation	1	2	3	4	5	6
dp (mm)	11 mm	11 mm	↑ 15 mm	↑ 20 mm	11 mm	11 mm	↑ 15 mm	↑ 20 mm
ε_0 (-)	0.13	0.13	0.13	0.13	↑ 0.25	↑ 0.35	↑ 0.35	↑ 0.35

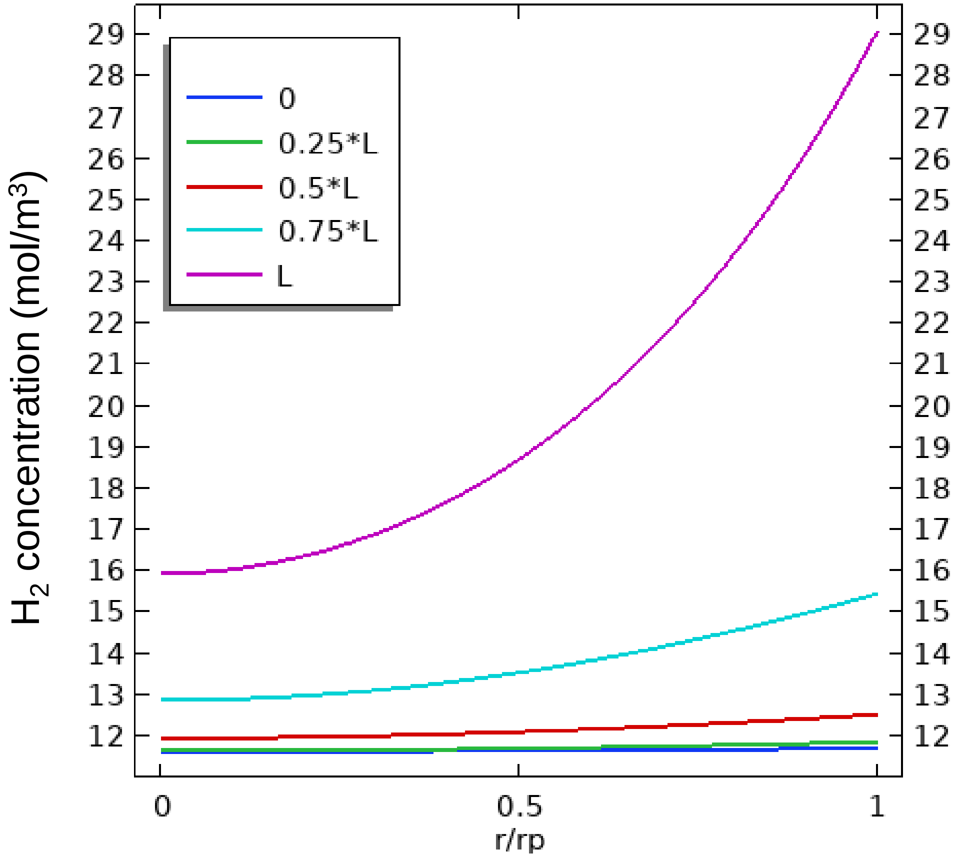
Reactor Scale for H-DR process



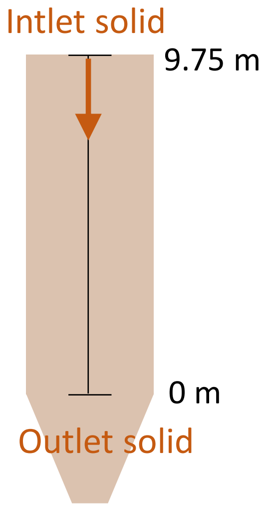
Gas phase – reactor scale



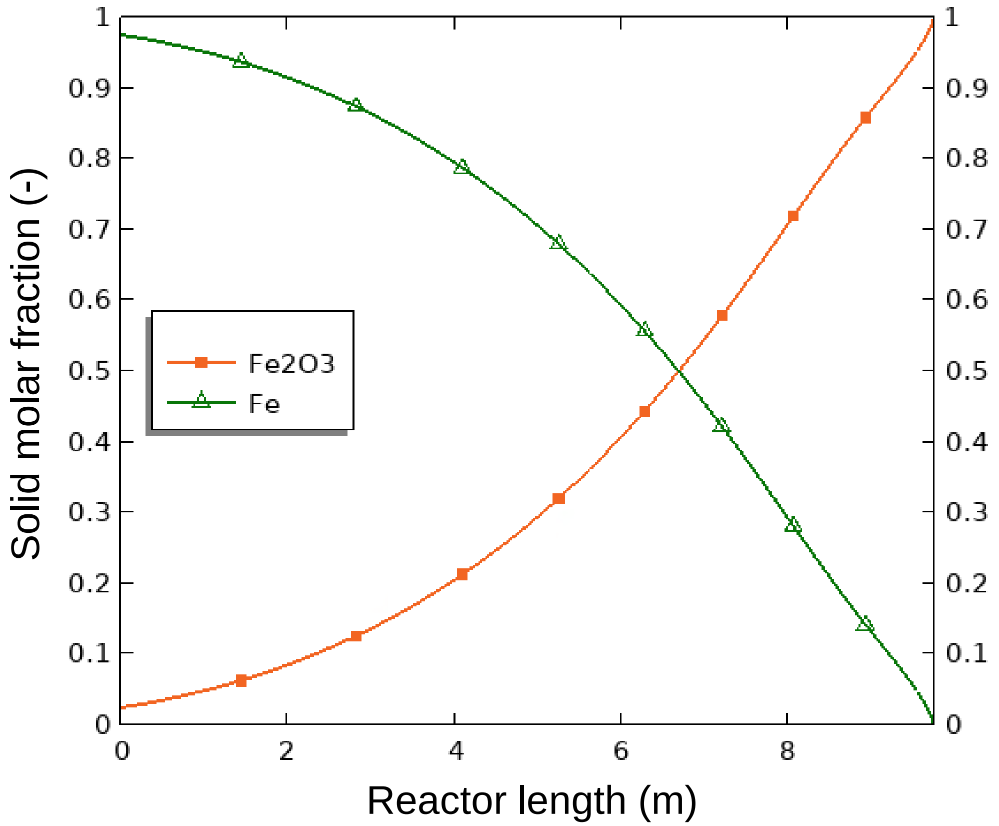
Gas phase – pellet scale



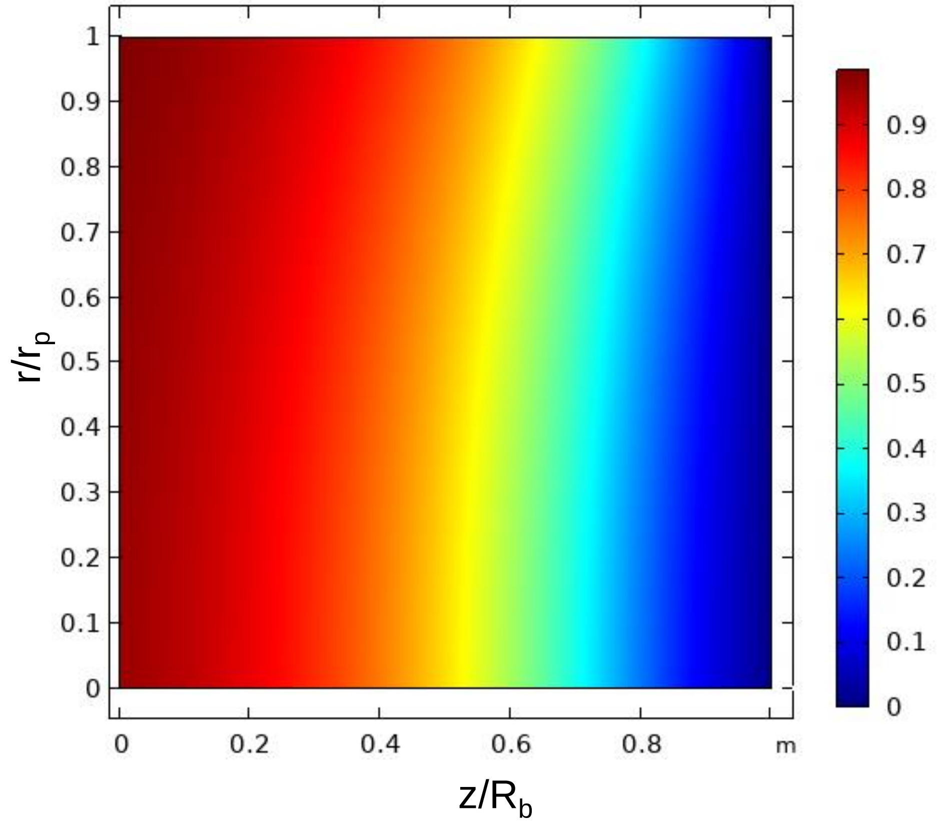
Reactor-Pellet Scale for H-DR process



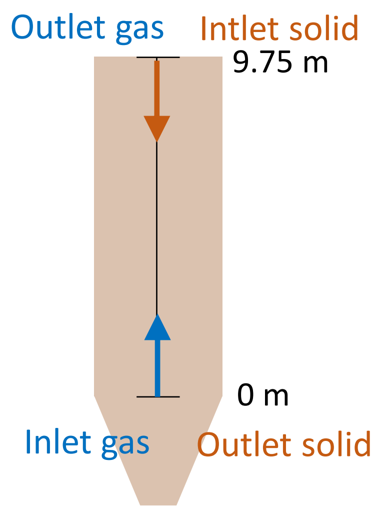
Solid phase – reactor scale



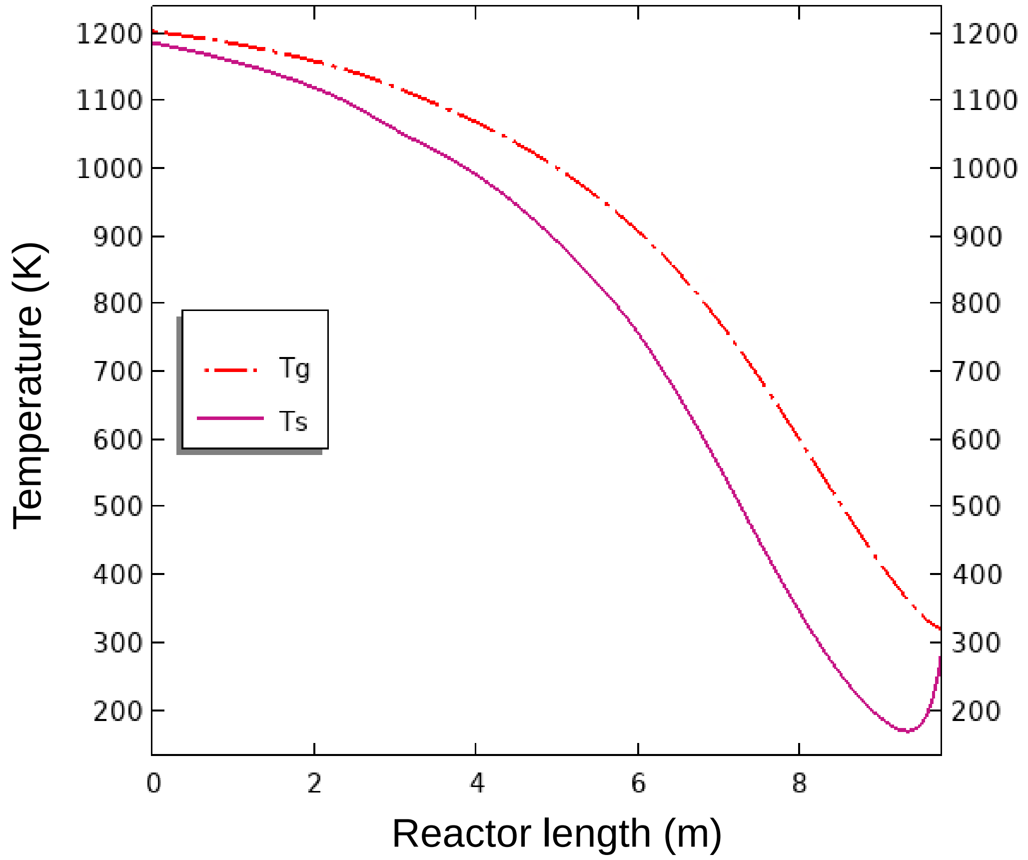
Solid phase – reactor-pellet scale



Reactor Scale for H-DR process



Temperature of the gas (Tg) and solid (Ts) along the reactor lenght



Pellet Scale

Isothermal pellet

Biot number < 0.1

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Conclusions

- ✓ Multiscale modelling shows good agreement with industrial plant data.
- ✓ Structural pellet parameters considerable influence the reduction rate.
- ✓ Smaller the pellet size, higher the reduction rate.
- ✓ Greater the pellet porosity, higher the reduction rate.
- ✓ Useful predictions for H-DR.

THANK YOU !

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