Simulation of a Direct Reduction of Iron furnace using Cape Open

by

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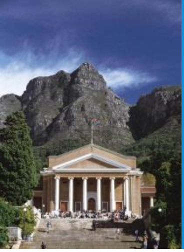


Decarbonising the steel industry

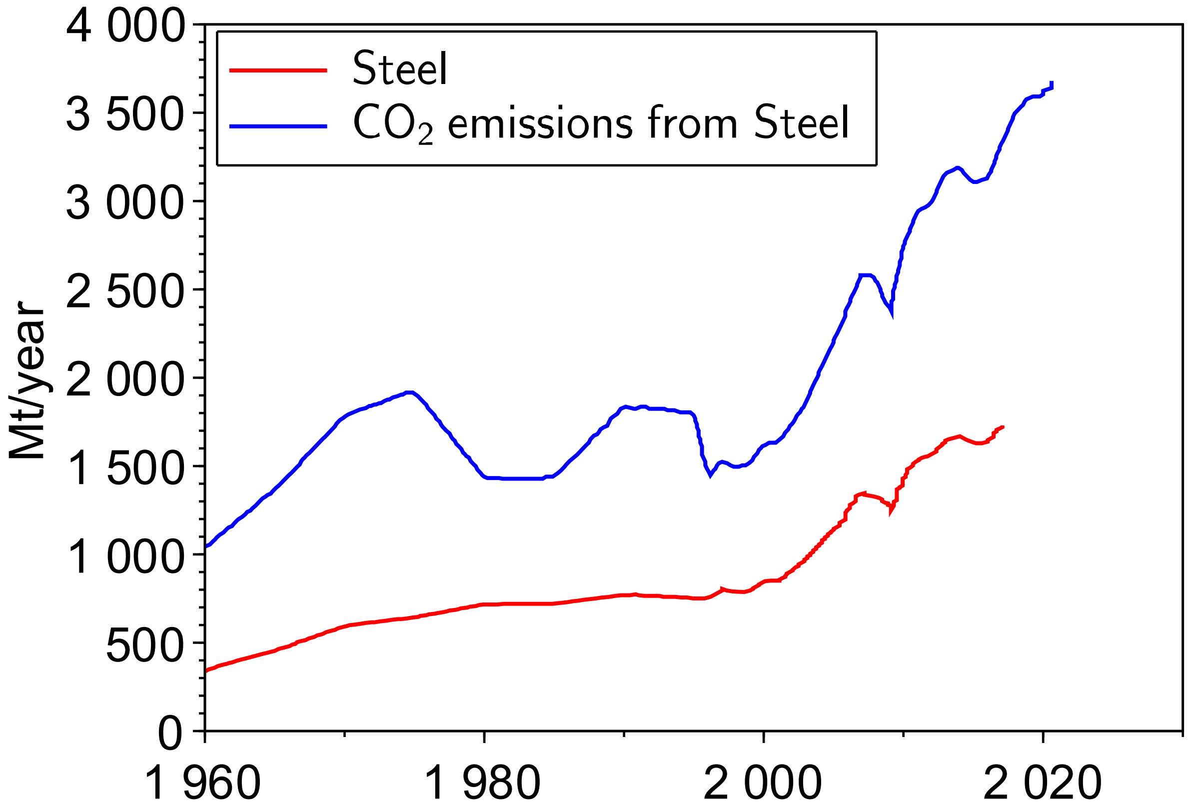
To meet global energy and climate goals, emissions from the steel industry must fall by at least 50% by 2050

25%

of industrial CO_2 emissions

7%

of global energy-related CO_2 emissions



2.1 kg CO_2 / kg Steel

Material efficiency measures will reduce steel demand by 40% by 2050

But global economic advancement and population growth counteract this trend

Deep CO_2 reduction requires new technology to make Fe

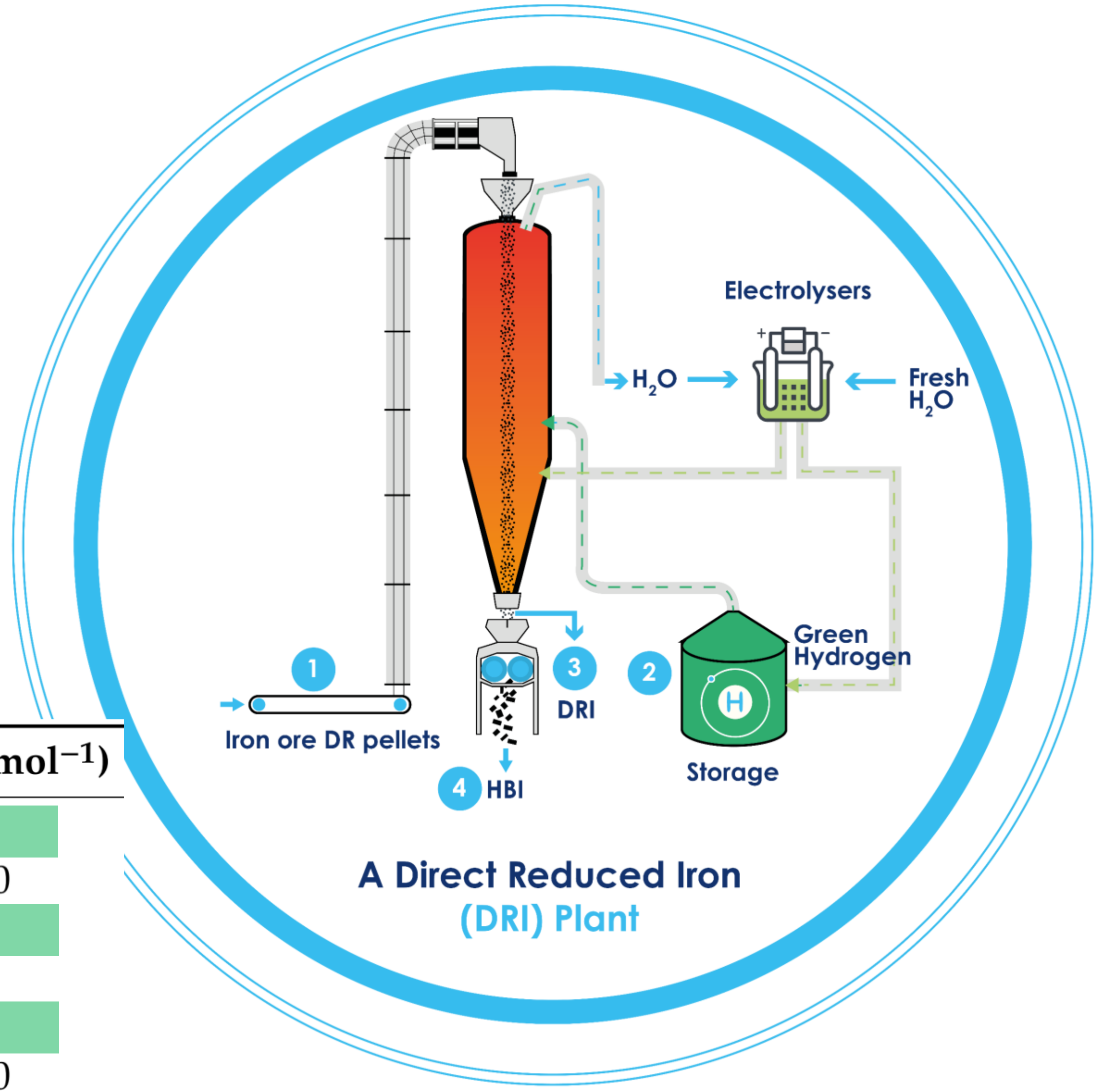
H_2-DRI Reactor concept

84% CO_2 Reduction

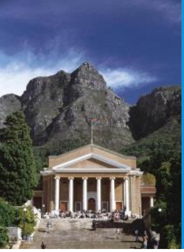
H_2-DRI
Overall reaction

$$Fe_2O_3 + 3H_2 \rightarrow Fe + 3H_2O$$

endothermic



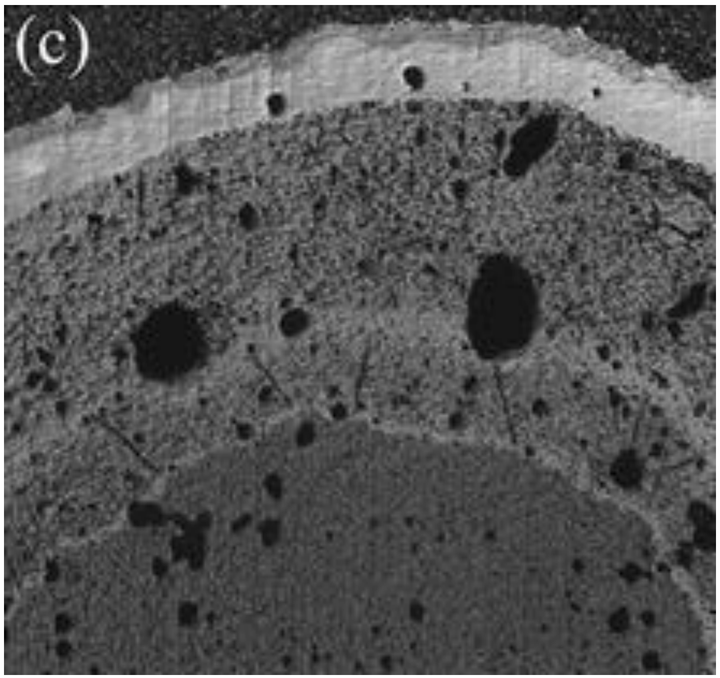
Reaction	$\Delta_r H_{800\,^\circ C}$ (J mol^{-1})
$3\,Fe_2O_3 + H_2 = 2\,Fe_3O_4 + H_2O$	−6020
$3\,Fe_2O_3 + CO = 2\,Fe_3O_4 + CO_2$	−40,040
$Fe_3O_4 + H_2 = 3\,FeO + H_2O$	46,640
$Fe_3O_4 + CO = 3\,FeO + CO_2$	18,000
$FeO + H_2 = Fe + H_2O$	16,410
$FeO + CO = Fe + CO_2$	−17,610



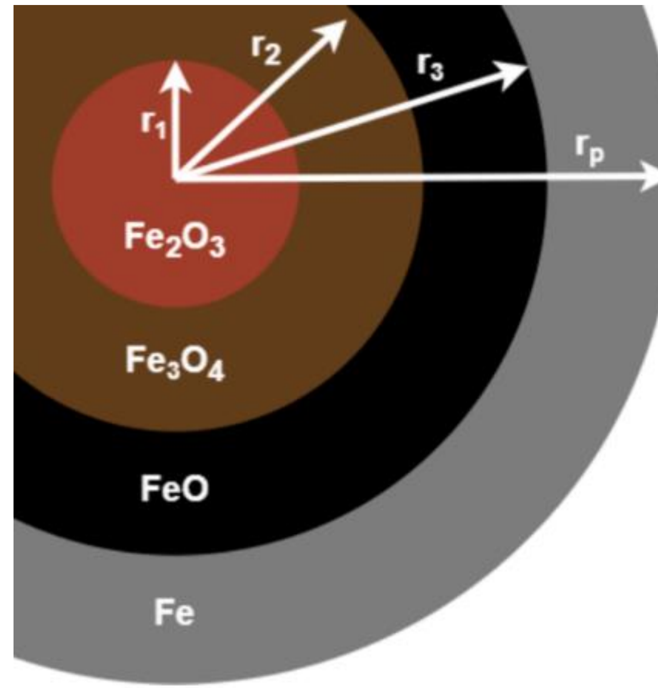
Modelling: Pellet scale

Reduced Dense Pellet[1]

$$Fe$$
$$\uparrow$$
$$Fe_xO$$
$$\uparrow$$
$$Fe_3O_4$$
$$\uparrow$$
$$Fe_2O_3$$



Shrinking Core Model[2]



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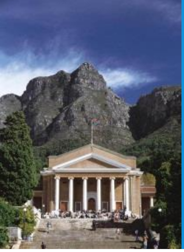
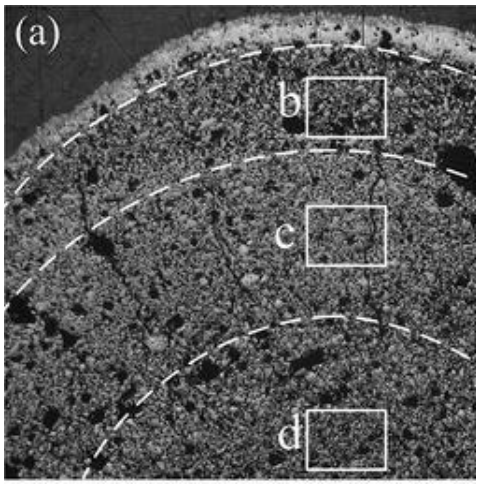
2. M. Kazemi, M. S. Pour, and D. Sichen, “Experimental and Modeling Study on Reduction of Hematite Pellets by Hydrogen Gas,” *Metallurgical and Materials Transactions B*, vol. 48, no. 2, pp. 1114–1122, Apr. 2017, doi: 10.1007/s11663-016-0895-3.



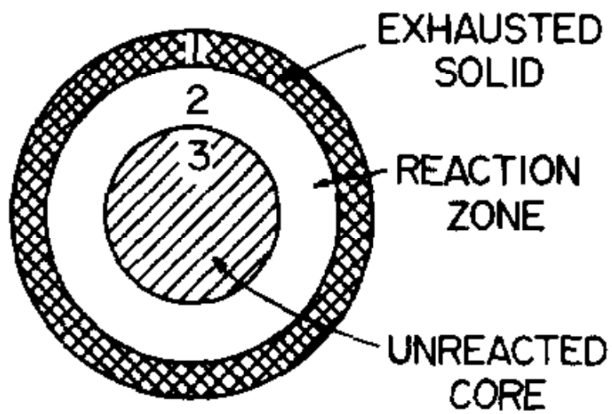
Modelling: Pellet scale

$$Fe$$
$$\uparrow$$
$$Fe_xO$$
$$\uparrow$$
$$Oxide\ mix$$
$$\uparrow$$
$$Fe_2O_3$$

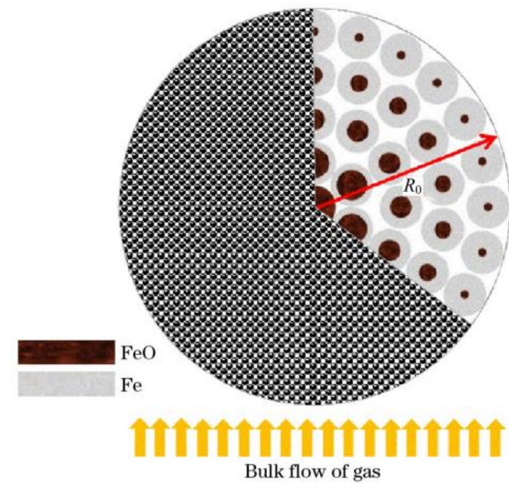
Industrial Pellet[4]



Reaction Zone Model[5]



Grain Model[6]



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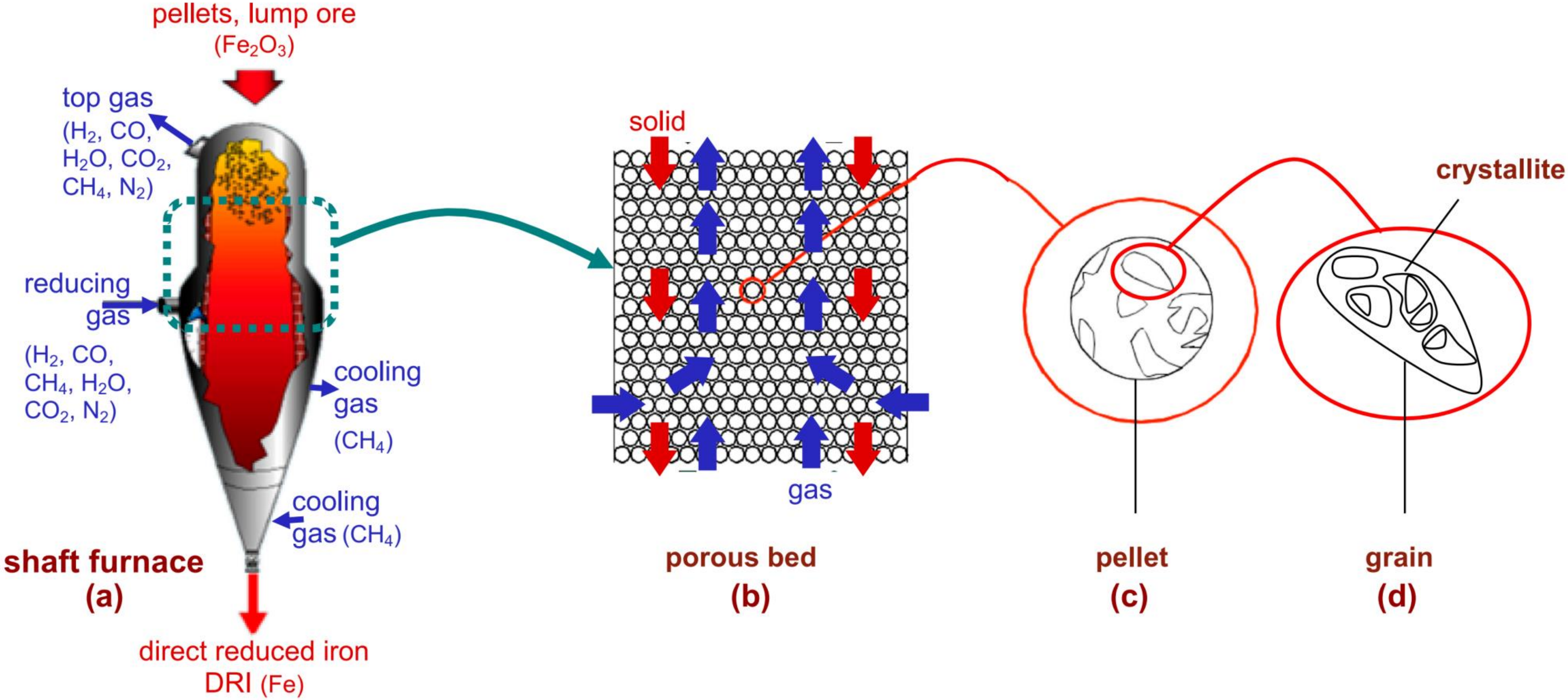
2. S. Arabi and H. Hashemipour, "Modeling and Simulation of Noncatalytic Gas-Solid Reaction in a Moving Bed Reactor," *Chemical Product and Process Modeling*, vol. 3, Jan. 2008, doi: 10.2202/1934-2659.1230.

3. A. Z. Ghadi, M. S. Valipour, and M. Biglari, "Numerical Analysis of Complicated Heat and Mass Transfer inside a Wustite Pellet during Reducing to Sponge Iron by H2 and CO Gaseous Mixture," *Journal of Iron and Steel Research, International*, vol. 23, no. 11, pp. 1142–1150, Nov. 2016, doi: 10.1016/S1006-706X(16)30169-8.

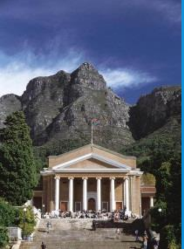
Modelling: furnace scale

The reductor model, most comprehensive model in literature

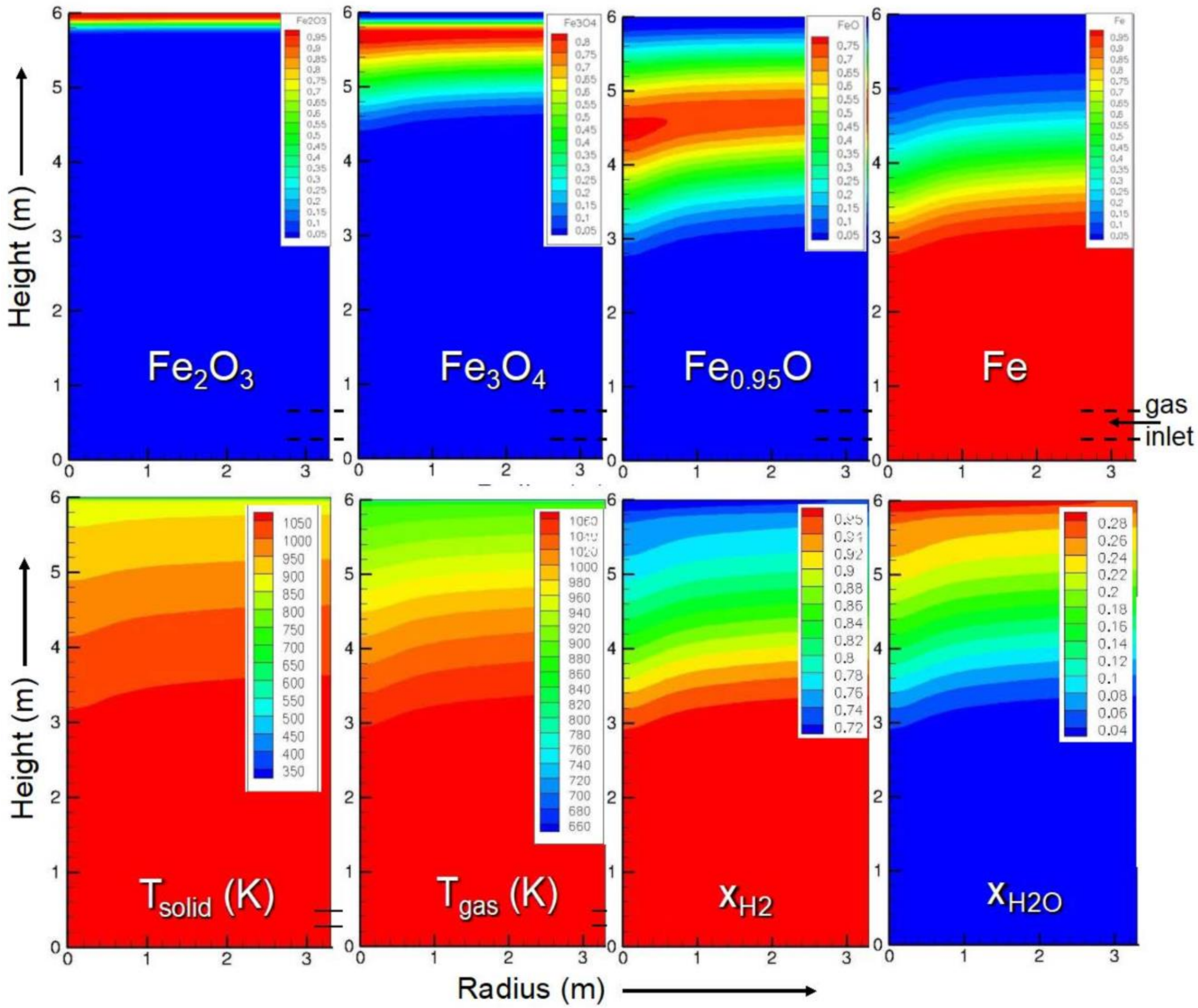
- **2D CFD flow model**
- **Two zone, grain pellet model**
- **Many approximations**



Fabrice Patisson and Olivier Mirgaux, Hydrogen Ironmaking: How It Works, Metals 2020, 10, 922



Modelling: furnace scale



Observations from CFD

- Fe conversion is key
- H2 is about 3 times excess
- Gas heats the solids quite rapidly
- Profiles are reasonably sharp approximately parabolic profile
- Temperature of the gas exceeds the temperature of the solids
- No experimental verification of these results
- Profile data scarce and unreliable

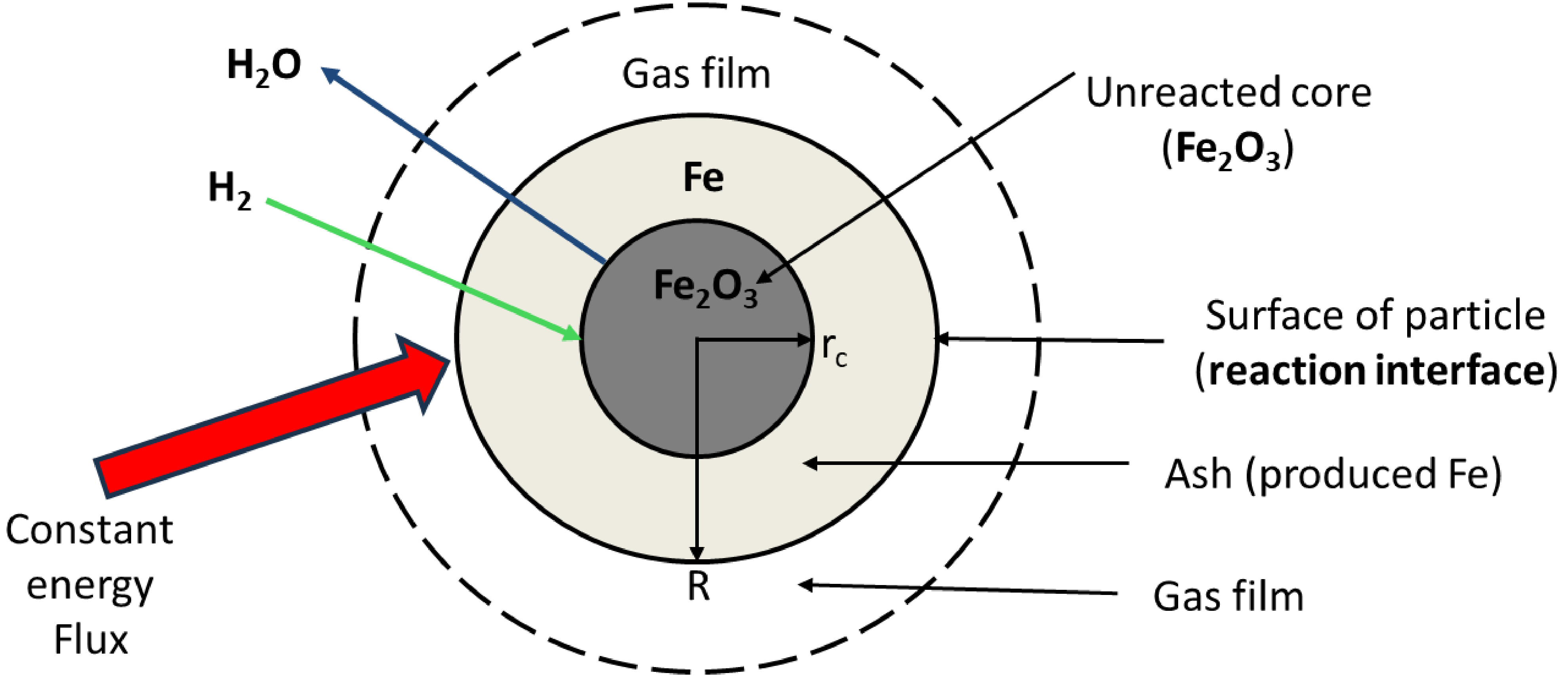
Fabrice Patisson and Olivier Mirgaux, Hydrogen Ironmaking: How It Works, Metals 2020, 10, 922

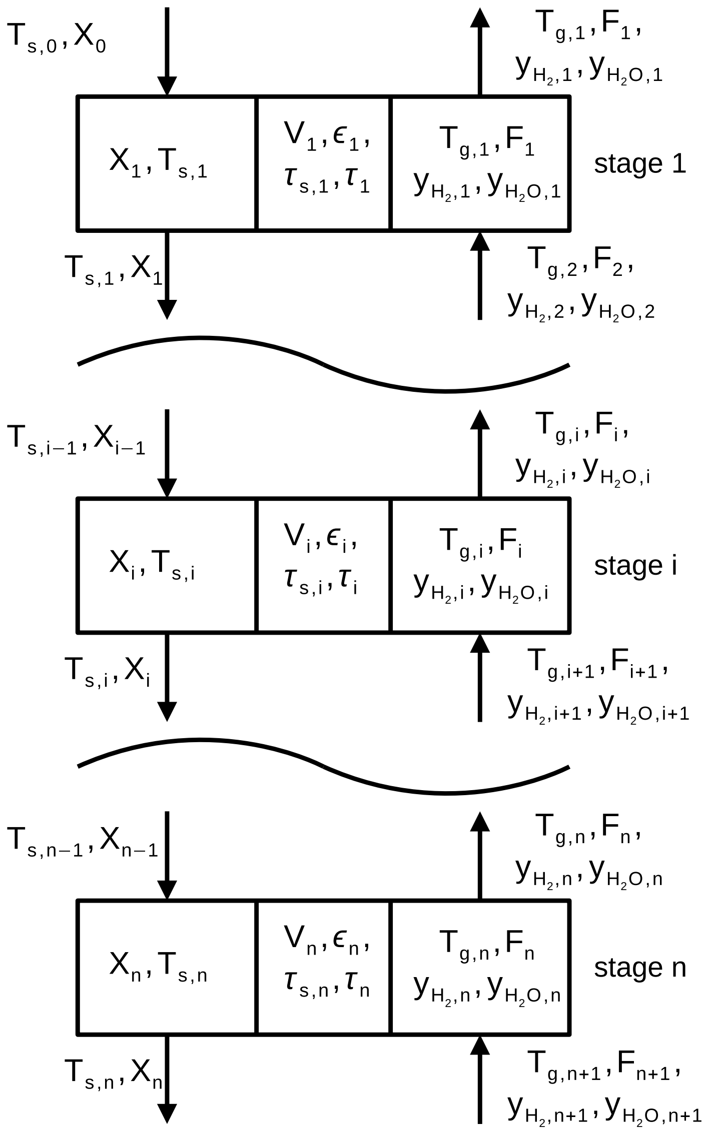
Tanks in Series approximation

Pellet model

$$3H_{2(g)} + Fe_2O_{3\,(s)} \rightarrow 2Fe_{(s)} + 3H_2O_{(g)}$$

$$\mathrm{a}A + bB \rightarrow cC + dD$$





Solid conversion

$$\frac{t}{\tau} = \frac{\left(\frac{1}{3k_g} - \frac{R}{3D_e}\right)X + \frac{R}{2D_e}\left(1-(1-X)^{\frac{2}{3}}\right) + \frac{1}{k}\left(1-(1-X)^{\frac{1}{3}}\right)}{\frac{1}{3k_g} + \frac{R}{6D_e} + \frac{1}{k}}$$

This equation is converted to a cubic in X(i) and solved stage to stage with residence time t for stage i which changes the conversion from X(i-1) to X(i) at the time for complete conversion tau(i) at conditions in stage i

Solid phase mole balance

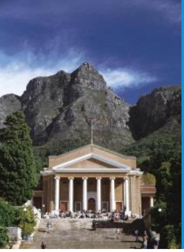
$$S_0(X_i - X_{i-1}) + \nu_j R_{j,i} V_i = 0$$

$$N_{j,i} = \nu_j S_0(X_i - X_{i-1}) = \nu_j R_i V_i$$

Gas phase mole balance

$$F_{t,i+1} y_{j,i+1} - F_{t,i} y_{j,i} + \nu_j R_{j,i} V_i = 0$$

$$F_{t,i+1} y_{j,i+1} - F_{t,i} y_{j,i} + \nu_j S_0(X_i - X_{i-1}) = 0$$



Tanks in Series approximation stage energy balance

Solid phase energy balance

$$\nu_j S_0(1-X_{i-1})H_{S,j,i-1} + \nu_j S_0 X_{i-1} H_{S,j,i-1} - \nu_j S_0(1-X_i)H_{S,j,i} - \nu_j S_0 X_i H_{S,j,i}$$
$$+ hA\left(T_{g,i} - T_{s,i}\right) - \sum_{j=gas}\left(\nu_j S_0(X_i - X_{i-1})H_{f,j,i}\right) = 0$$

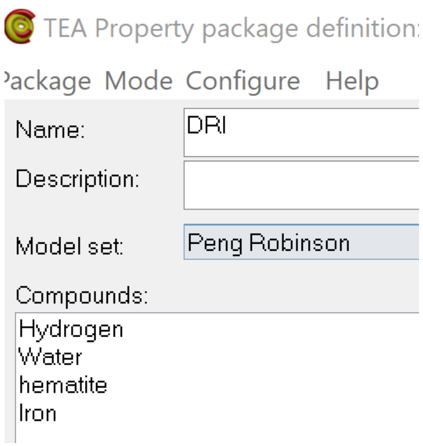
Gas phase energy balance

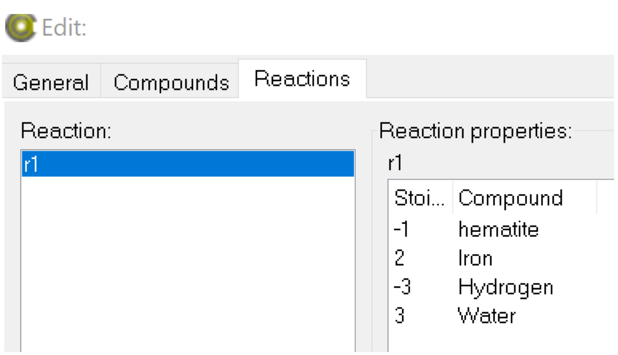
$$\sum_j F_{t,i+1} y_{j,i+1} H_{fj_{i+1}} - \sum_j F_{t,i} y_{j,i} H_{fj_i} + hA\left(T_{g_{i+1}} - T_{s_{i-1}}\right) + \sum_j \nu_j\, S_0 X_i H_{fj_{Tf,i}}$$

Unknowns per stage: mole fraction H2, H2O, total flow rate, temperature of the gas and solid (5 variables)
X(i) can be found implicitly given an initial guess of the above variables
System of 5*n equations for n tanks in series in counter current operations
Must be solved simultaneously
These equations written in matrix-vector format

Tanks in series model
Cape open

Thermo data base





Enthalpy and property calls

```
ThermoLibraries=capeOpenPackages("TEA (CAPE-OPEN 1.1)")
//capeOpenShowMessages(0)
tea=capeOpenGetPackage("TEA (CAPE-OPEN 1.1)","DRI")
```

Gas phase and film properties

```
[Hfg1,viscosityC rhogC ktherm C]=capeOpen1PhaseProp(tea,"enthalpyF viscosity density thermalConductivity","vapor",Tg',p,Yi)
```

Solid phase properties

```
Hfs1=capeOpen1PhaseProp(tea,"enthalpyF","solid",Ts'(1:n+1),p,Xis)
```

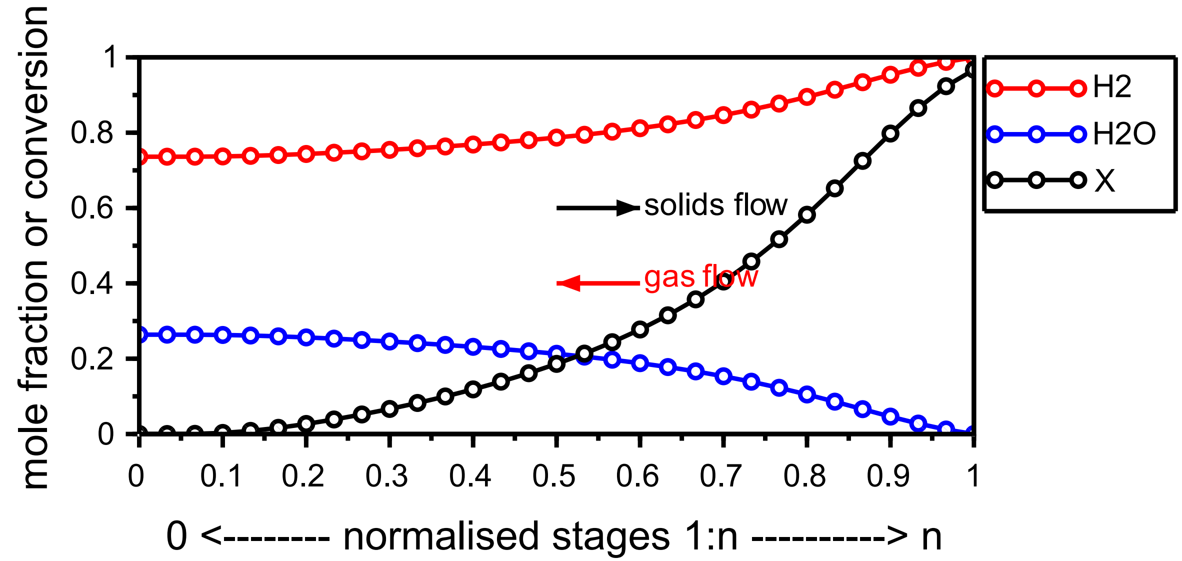
Tanks in series
Cape Open

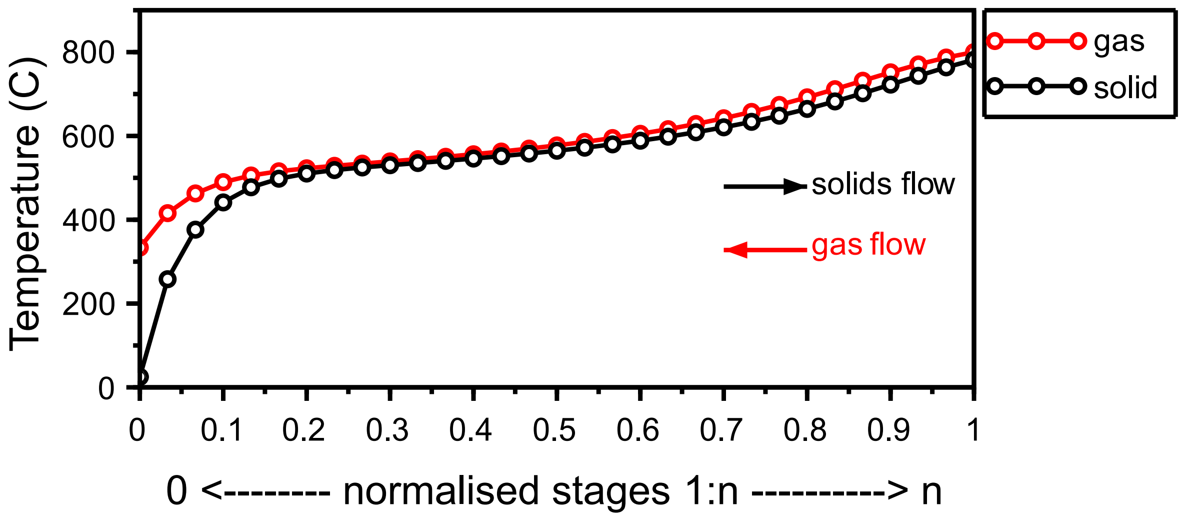
Sample simulation

- 30 stages, equally sized
- 10/1 H2/Solids molar ratio
- 2m x 10m furnace

Features

- Excess gas needed to heat the solids and start the reaction
- Endothermic reaction, Tsolids<Tgas





COCO simulator

Two objectives

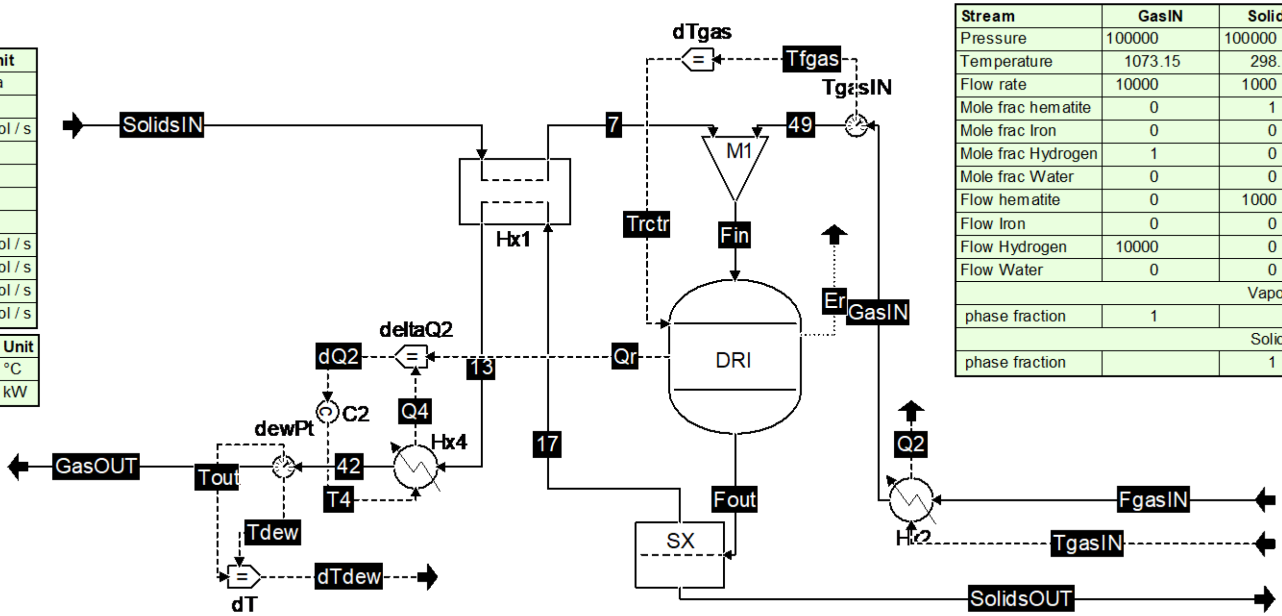
- **Energy and mass balance surrogate model**
- **Embedded tanks in series model**

DRI fixed conversion reactor with gas heat exchange
* this will give some indication of the gas and solid thermal demands some notes of operation:
1. The gas comes in hot (800C) and leaves cold (ca. >100C) BUT must be above its dew point
2. The solids come in cold (ca. 25C) and leave hot (ca. 800C) and are then cooled by the cooling gas
3. In the reactor most of the reaction happens at the high temperature (ca. 800C)
4. The dew point of the exit gas depends on the feed gas flow rate and temperature at fixed solids flow rate
so to get the right unit energy demands, the elements of the flow sheet must reproduce this overall operation

To ensure correct counter current operation adiabatic heat exchange:
1. The temperature the solids is the same as the reactor
2. The reactor temperature is <= the feed gas temperature
3. The solids exchange 100% heat with the gas leaving the reactor
4. The heat duty of the furnace and the cooling duty of the second cooling exchanger must be the same

Stream	Fin	Fout	Unit
Pressure	100000	100000	Pa
Temperature	1072.83	1072.15	K
Flow rate	11000	11753.8	mol / s
Mole frac hematite	0.0909091	0.0209442	
Mole frac Iron	0	0.128269	
Mole frac Hydrogen	0.909091	0.658383	
Mole frac Water	0	0.192403	
Flow hematite	1000	246.174	mol / s
Flow Iron	0	1507.65	mol / s
Flow Hydrogen	10000	7738.52	mol / s
Flow Water	0	2261.48	mol / s

Stream	Q2	Q4	Qr	dTdew	Unit
DT				254.427	°C
Heat duty	229081	-47839.1	47839.1		kW



Stream	GasIN	SolidsIN	SolidsOUT	GasOUT	Unit
Pressure	100000	100000	100000	100000	Pa
Temperature	1073.15	298.15	1072.15	592.295	K
Flow rate	10000	1000	1753.83	10000	mol / s
Mole frac hematite	0	1	0.140364	0	
Mole frac Iron	0	0	0.859636	0	
Mole frac Hydrogen	1	0	0	0.773852	
Mole frac Water	0	0	0	0.226148	
Flow hematite	0	1000	246.174	0	mol / s
Flow Iron	0	0	1507.65	0	mol / s
Flow Hydrogen	10000	0	0	7738.52	mol / s
Flow Water	0	0	0	2261.48	mol / s
Vapor phase					
phase fraction	1			1	
Solid phase					
phase fraction		1	1		

How the controller works to ensure 100% heat exchange of the reactor heat:
C2: receives the resultant heat duty of DRI and Hx4, and adjusts T4 of Hx4 such that Qr+Q4=0

COCO simulator

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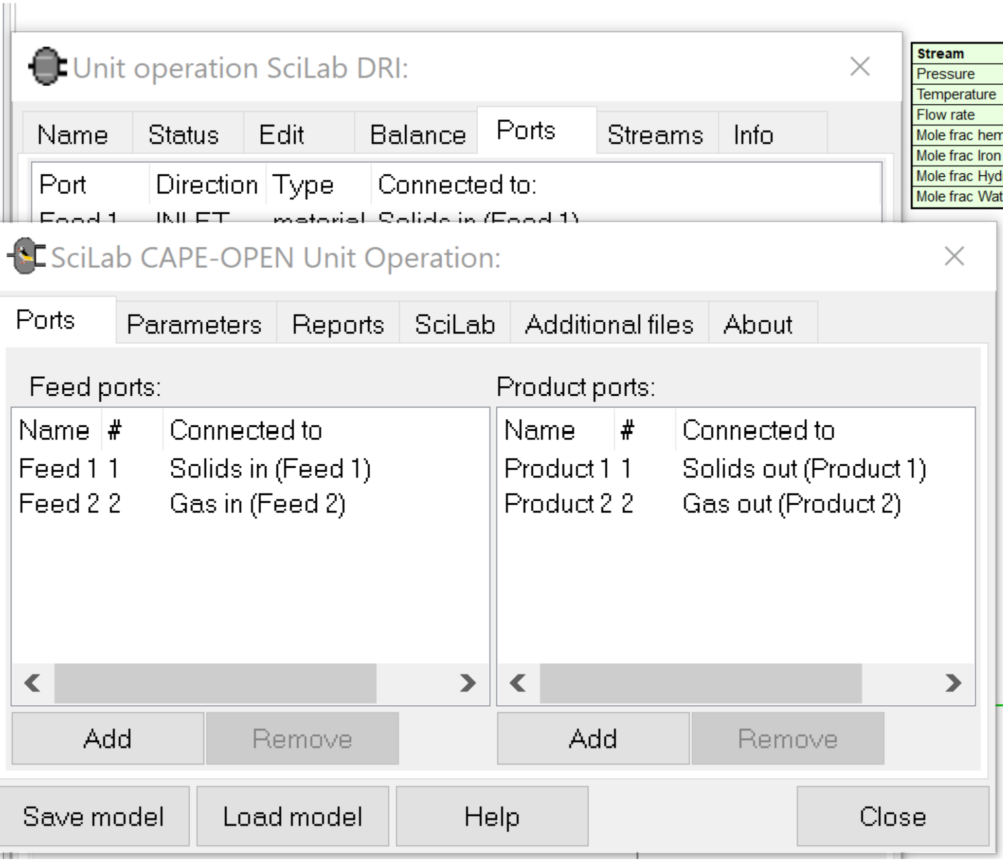

Stream	Solids in (Feed 1)	Gas in (Feed 2)	Solids out (Product 1)	Gas out (Product 2)	Unit
Pressure	101325	101325	101325	101325	Pa
Temperature	298.15	1073.15	1041.82	601.335	K
Flow rate	1000	10000	1753.83	10000	mol / s
Mole frac hematite	1	0	0.140364	0	
Mole frac Iron	0	0	0.859636	0	
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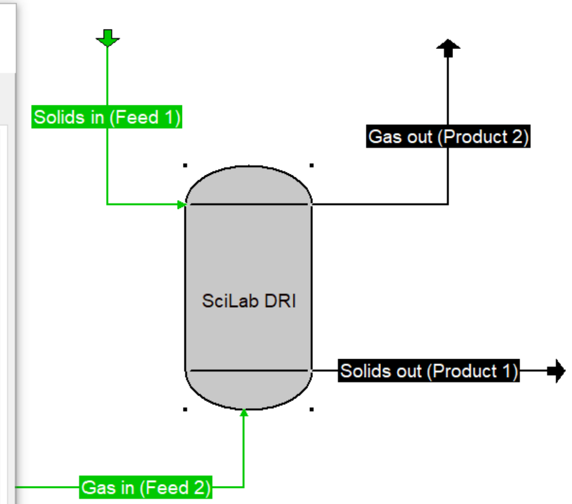

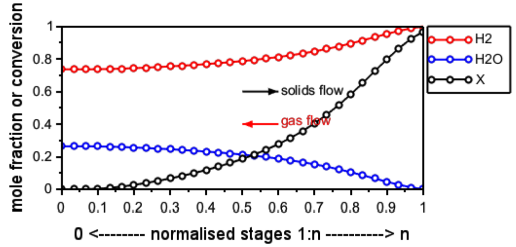

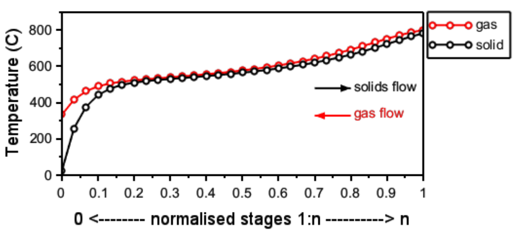

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Vapor phase					
phase fraction	1			1	
Solid phase					
phase fraction		1	1		

- **Embedded tanks in series model**

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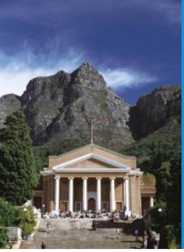

Future work

Scilab unit operation

- Refinement of tanks in series approximations
- Refine performance

Use in techno-economic study of H2 iron processing

Thank you for your attention