

1-D REACTOR MODELLING FOR HYDROGEN PRODUCTION FROM LOW-GRADE GAS STREAMS VIA CHEMICAL LOOPING

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CHALLENGE

Worldwide hydrogen production:

- 96% relies on fossil fuels
- 3% of global CO₂ emissions
- >70 Mton (pure, 2018) and rising [Source: IEA 2019]

Objective:

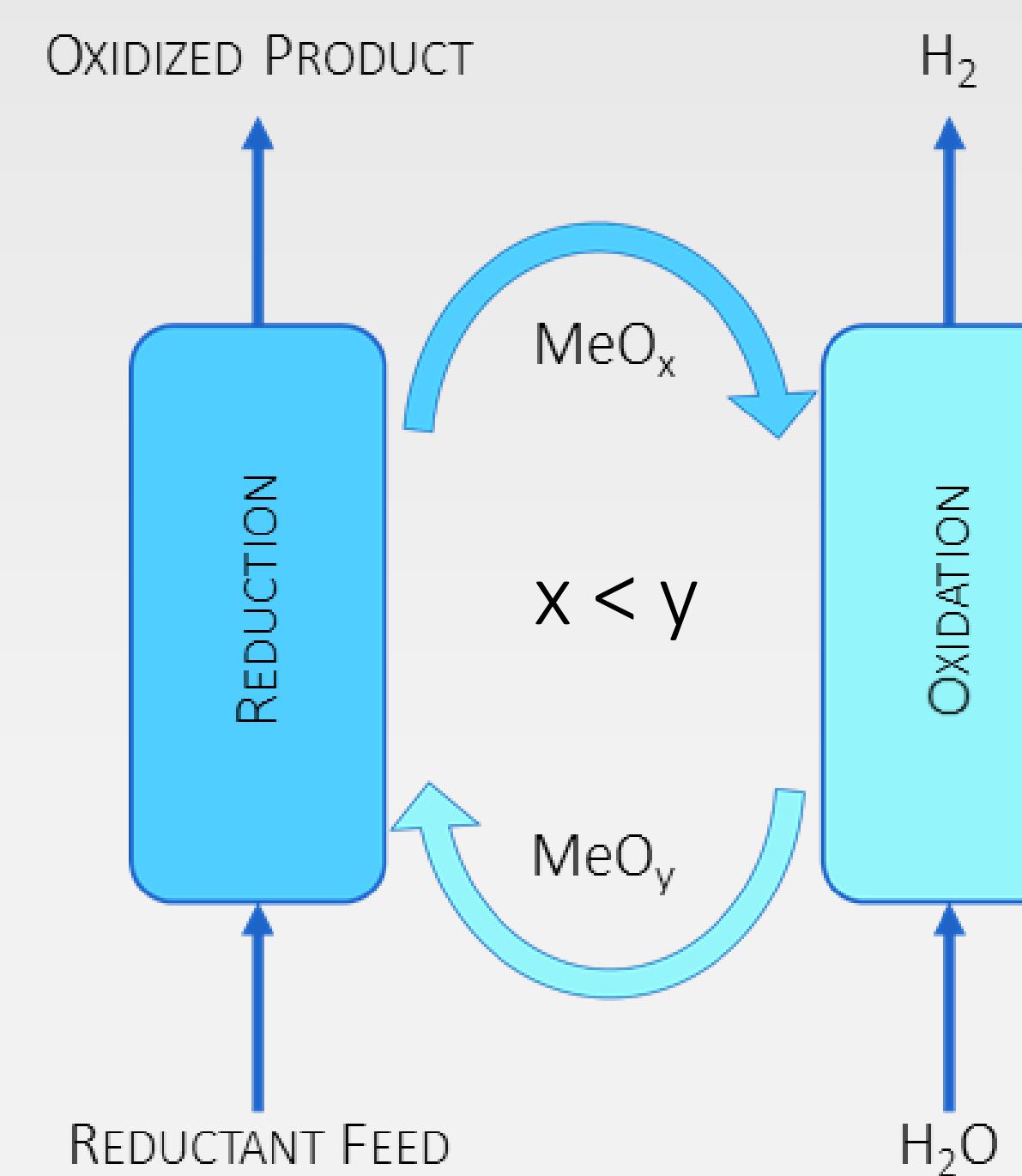
- Greener way to produce H₂ as a clean energy carrier

CHEMICAL LOOPING (CL)

- Solid intermediate
- Breaks down target reaction in steps
- Higher exergy efficiency

CL FOR H₂ PRODUCTION

- ✓ Possible inherent separation of CO₂
- ✓ Heat Integration
- ✓ High H₂ purity
- ✓ Easier post-processing



OXYGEN CARRIER MATERIAL

Iron oxide supported on magnesium aluminate spinel

- ✓ Non-toxicity
- ✓ Favorable redox characteristics
- ✓ Natural abundance

Reaction kinetics from literature.^[1,2,3]

REACTOR MODEL

1-D two phase reactor model (gas and solid)

Mass balance for gaseous phase:

$$\frac{\partial n_i}{\partial t} = -\frac{\partial(n_i u)}{\partial z} + (1-\varepsilon)V \sum_{j=1}^{N_R} v_{ij} r_{eff,j}$$

Mass balance for solid phase:

$$\frac{\partial x_i}{\partial t} = \frac{(1-\varepsilon)V \sum_{j=1}^{N_R} v_{ij} r_{eff,j}}{\rho_{bed,mol}}$$

Boundary conditions:

$$\forall z; t = 0, n_i = n_i^0, x_i = x_i^0$$

$$\forall t; z = 0, n_i = n_{i,in}$$

$$\forall t; z = L, \frac{\partial n_i}{\partial z} \Big|_{z=L} = 0$$

Isothermal reactor

Energy balance:

$$\frac{\partial T}{\partial t} = 0$$

Adiabatic reactor

Energy balance for the gas phase:

$$\frac{\partial T_f}{\partial t} = -\frac{\partial(T_f u)}{\partial z} + \frac{ha_e(1-\varepsilon)}{\varepsilon C_t C_{P_f}} (T_s - T_f)$$

Energy balance for the solid phase:

$$\frac{\partial T_s}{\partial t} = \frac{(1-\varepsilon)}{\rho_{bed,mol} C_{P_s}} \sum_{j=1}^{N_R} (-\Delta H_j) v_{ij} r_{eff,j} + \frac{(1-\varepsilon)}{\rho_{bed,mol} C_{P_s}} ha_e (T_f - T_s)$$

Boundary conditions:

$$\forall z; t = 0, T_f = T_f^0, T_s = T_s^0 \quad \forall t; z = L, \frac{\partial T_f}{\partial z} \Big|_{z=L} = 0$$

SOLUTION METHOD

- Method of lines
- First order upwind scheme
- MATLAB ode15s solver

REACTOR PARAMETERS

- 0.5 m diameter
- 3 m length

SIZE OF THE PELLETS

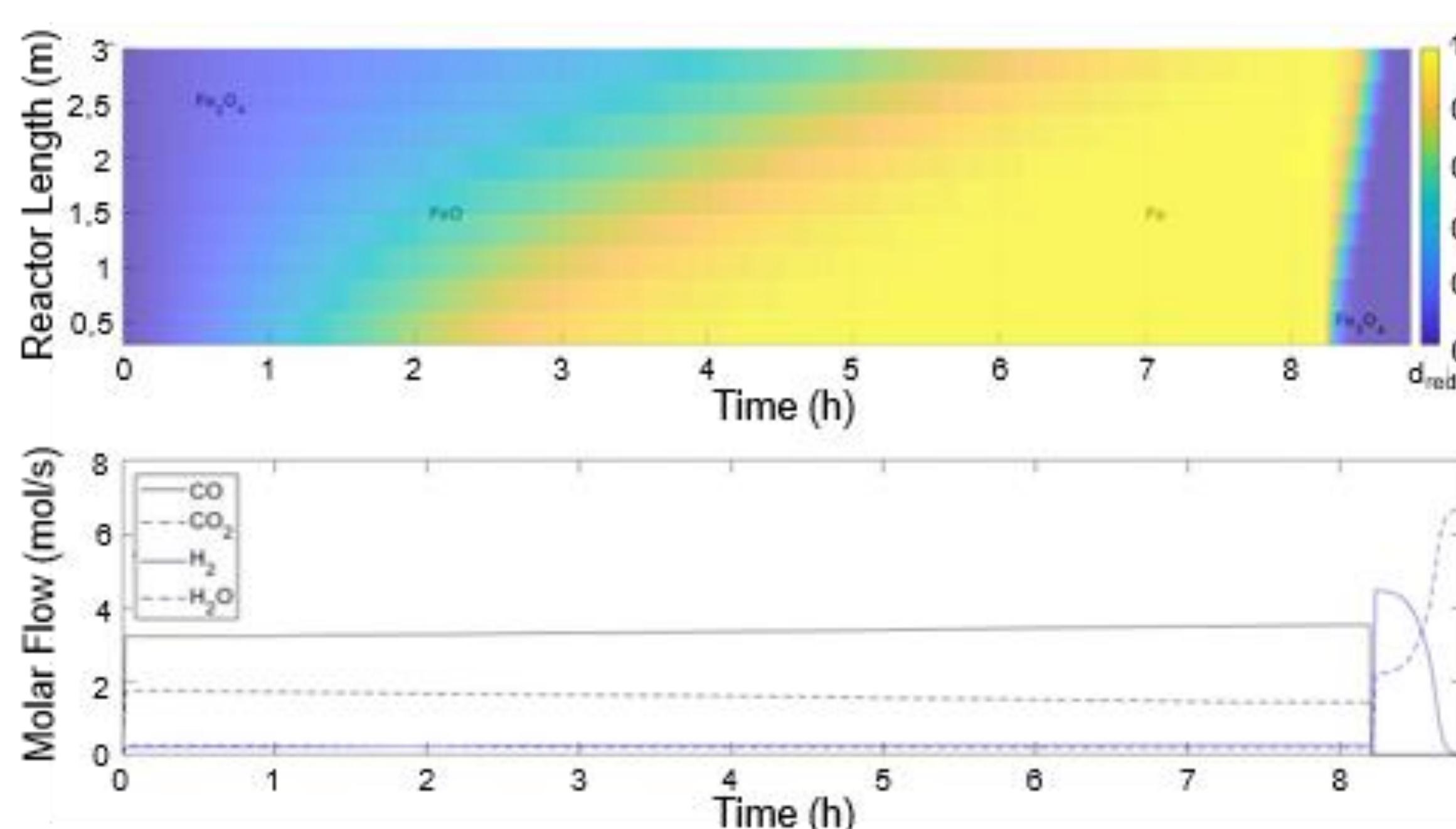
- 8 x 10⁻³ m

REDUCTANT FEEDS TESTED^[4,5]

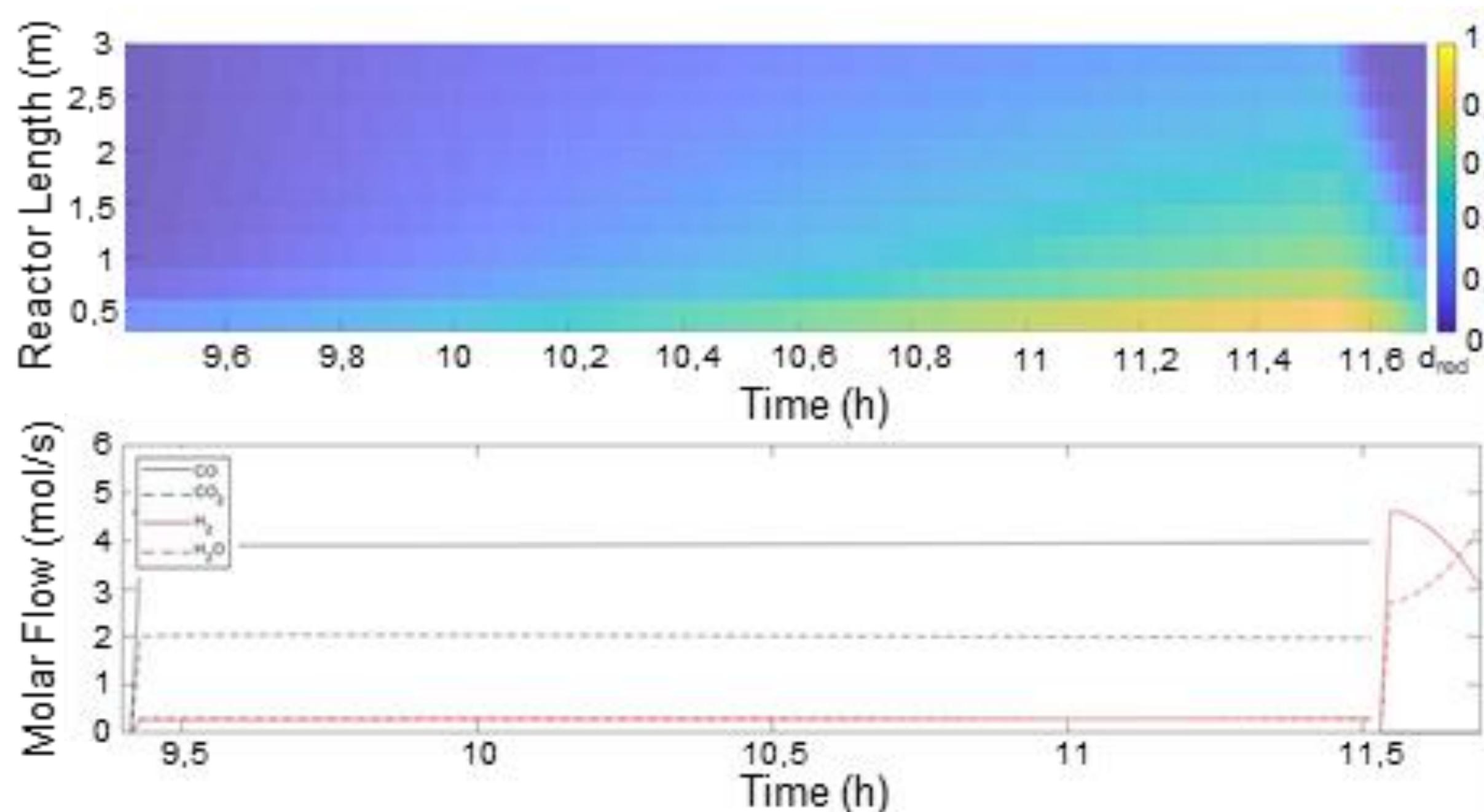
- Blast Furnace Gas (BFG) from iron and steel industry
- Blast Oxygen Furnace Gas (BOFG) from iron and steel industry
- Waste gaseous stream from pyrolysis (py-gas) of Municipal Solid Waste

ISOTHERMAL REACTOR

Simulation results for full reduction and oxidation using BOFG at a superficial velocity of 3 m/s at 1073 K and ambient pressure



Simulation results for cyclic steady state of the reactor using BOFG and reverse-flow operation mode at 3.6 m/s and 1073 K.

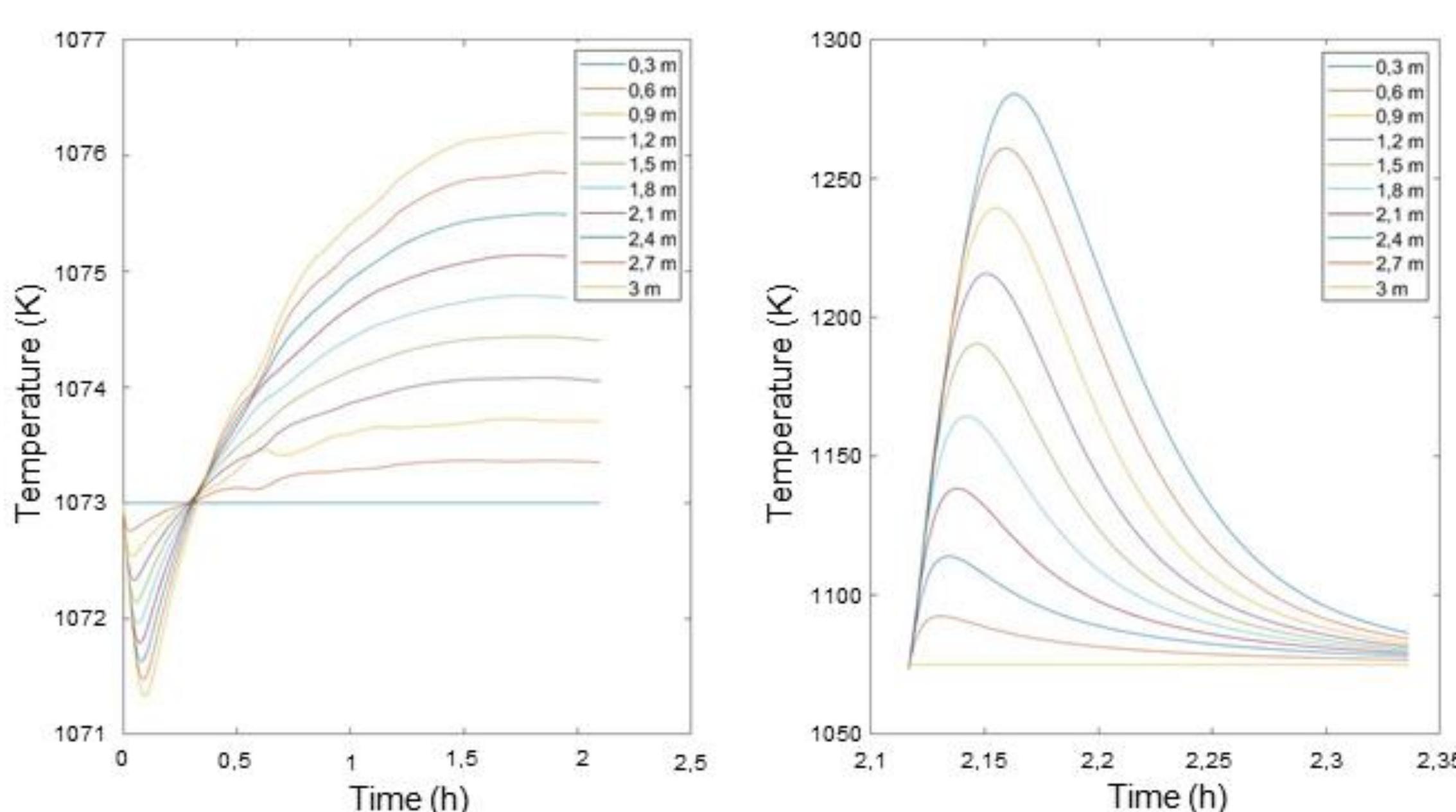


MAIN RESULTS

- Faster reduction is facilitated by a higher ratio of reductants to oxidants in the feed gas
- BFG is incapable of reducing FeO to Fe
- None of the reductant feeds can be fully utilized (i.e. oxidized)
- Reverse-flow indicates slightly better performance

ADIASTATIC REACTOR

Temperature profile in the reactor during reduction (left) and oxidation (right) while using BOFG as the feed gas in adiabatic mode and with reverse-flow operation.



MAIN RESULTS

- Difficult heat management
- Possible heat integration
- Worse performance when compared to the isothermal reactor

CONCLUSION AND OUTLOOK

- ✓ Chemical looping (CL) is suitable for hydrogen production
- ✓ CL can produce H₂ from all three waste streams with basic oxygen furnace gas and pyrolysis gas performing the best.
- ✓ The simulator is robust, expandable and can be used in further optimization of the process
- ✓ Productivity of 0.6 mol/m³/s achieved (comparable to catalytic industrial processes)

REFERENCES

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