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Modelling study of two chemical looping reforming reactor configurations: Looping vs. switching

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Modelling study of two Chemical Looping Reforming reactor configurations: Looping vs. Switching

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Outline

1. Objective
2. CLR vs. GSR principles
3. Simulations
4. Results and discussion
5. Conclusions

2. Objective of the work

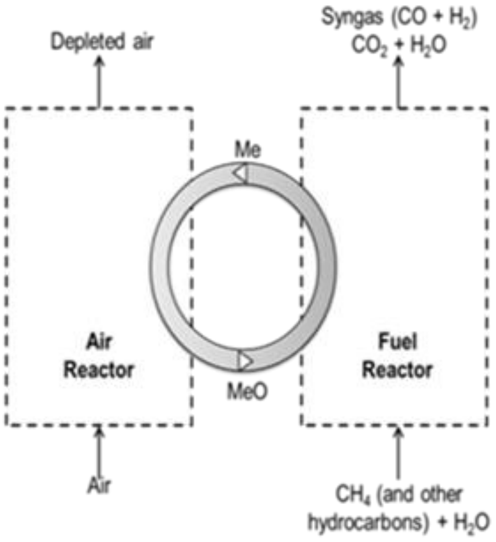
To compare the performance of two pre-combustion reactor concepts

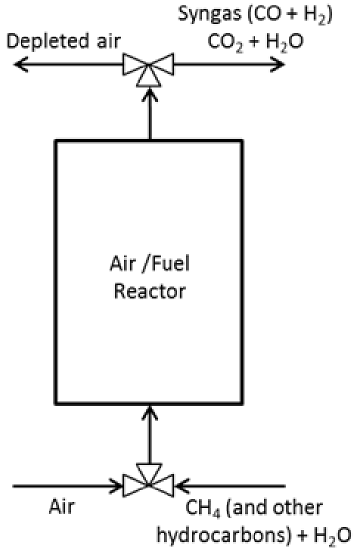
Chemical Looping Reforming (CLR)

Gas Switching Reforming (GSR)

3. CLR vs. GSR

CLR	GSR
Two interconnected FBR reactors (AR and FR);	**One FBR** for oxidation and reduction of the OC – **switching concept**;
OC continuously transported between AR and FR;	**Alternating feed** of air and fuel to the reactor unit;
No mixing between N_2 and fuel;	**Undesired mixing** between N_2 and fuel;
Scale-up and operational challenges.	**Facilitates scaling-up** under pressurized conditions.





4. Simulations

Single formulation is used!

1-D phenomenological model for FBR

- **Generic formulation** based on the generic model developed by Abba *et al.* (2003)[1];
- Uses an **averaging probabilistic approach** by Thompson *et al.* (1999)[2];
- **Two-phase** model by Toomey and Johnstone (**L- and H-phases**) [3,4];

Differential Balances

- **Mass balance**
  - Gas total mass balance
  - Gas species mass balance for each phase
  - Total solids species mass balance
- **Total Energy balance**
- **Pressure Balance**

Numerical scheme:

- Method of lines (MATLAB routine *ode15s*)
- Finite volume method (discretization in space)
  - **Non-uniform grid**
  - **Convective term**: 1st order upwind scheme
  - **Diffusion term**: central differences scheme

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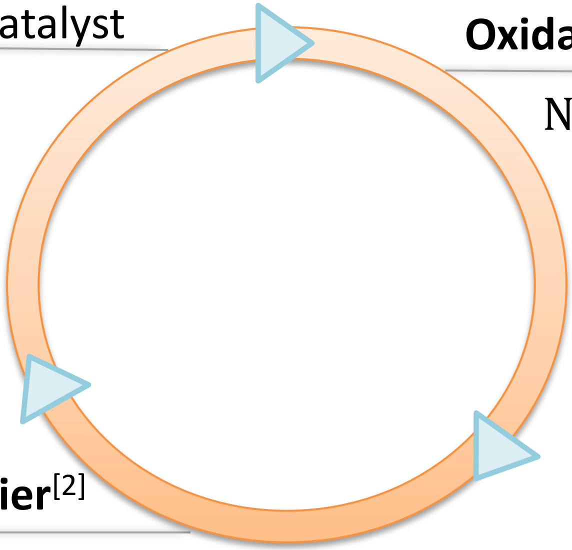
1. Abba, I.a., et al., *Spanning the flow regimes: Generic fluidized-bed reactor model.* AIChE Journal, 2003. **49**: p. 1838-1848.
2. Thompson, M.L., H. Bi, and J.R. Grace, A generalized bubbling / turbulent fuidized-bed reactor model. Chemical Engineering Science, 1999. 54: p. 3-10.
3. Kunii, D. and O. Levenspiel, *Fluidization Engineering*. second ed. 1991: Butterworth-Heinemann.
4. Mahecha-Botero, A., et al., *Pure hydrogen generation in a fluidized bed membrane reactor: Application of the generalized comprehensive reactor model.* Chemical Engineering Science, 2009. **64**(17): p. 3826-3846.

4. Simulations

Reactions and Kinetics



Reforming stage

Reforming[1] Ni as catalyst

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2$$

Fuel Reactor

Oxidation of the oxygen carrier[2]

$$Ni + 1/2\,O_2 \leftrightarrow NiO$$

Air Reactor

Oxidation stage

Reduction of the oxygen carrier[2]

$$CH_4 + 4NiO \leftrightarrow 4Ni + CO_2 + 2H_2O$$

$$H_2 + NiO \leftrightarrow Ni + H_2O$$

$$CO + NiO \leftrightarrow CO_2 + Ni$$

Reduction stage

🟩 CLR
🟦 GSR

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1. Xu, J. and G.F. Froment, *Methane steam reforming, methanation and water-gas shift: I. Intrinsic kinetics.* AIChE Journal, 1989. **35**(1): p. 88-96.
2. Abad, A., et al., *Mapping of the range of operational conditions for Cu-, Fe-, and Ni-based oxygen carriers in chemical-looping combustion.* Chemical Engineering Science, 2007. **62**(1-2): p. 533-549.

4. Simulations

Simulation Parameters

Steam flowrate	170 ton/h
Fuel flowrate	250 ton/h
Maximum temperature	1100 °C
Fuel inlet temperature	205 °C
Steam inlet temperature	400 °C
Operating pressure	17.3 bar
OC density	3446 kg/m3
Particle diameter	250 µm
Reactor diameter	6 m
Reactor height	7 m
Axial resolution	20 cells

How to compare these two technologies?

Same simulation parameters and physical properties

Study variable: Degree of Oxygen Carrier utilization

How to adjust this parameter?

4. Simulations

CLR: Oxygen carrier flux

↓ OC flux: ↑ OC residence time

GSR: Cycle time flux

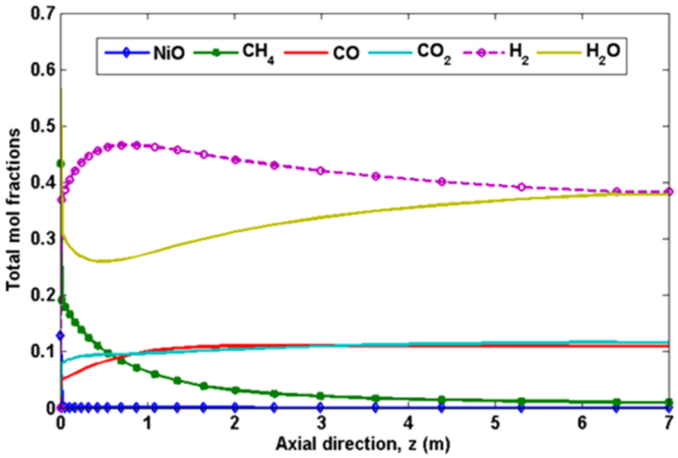
↑ cycle time: ↑ reduction + ↑ oxidation

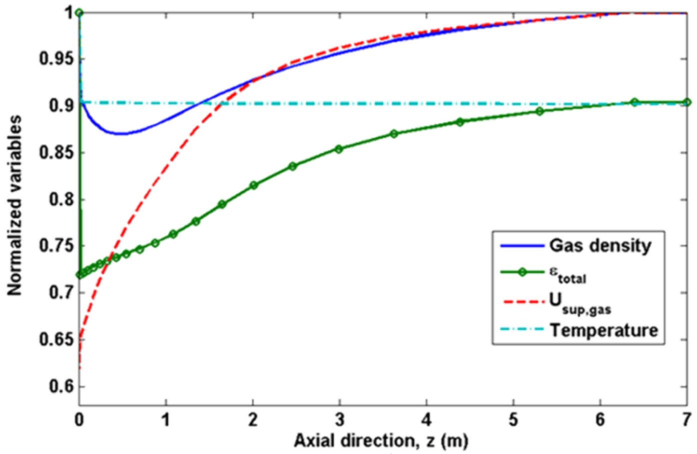
Higher oxygen carrier conversion

Degree of OC utilization (%)	CLR	GSR		
	OC flux (kg/m^2 s)	Oxidation stage time (s)	Reduction stage time (s)	Reforming stage time (s)
10	466	25	13	25
20	233	68	34	68
40	116.5	198	99	198
60	82.4	400	200	400
80	58.25	-	-	-

5. Results: Profiles

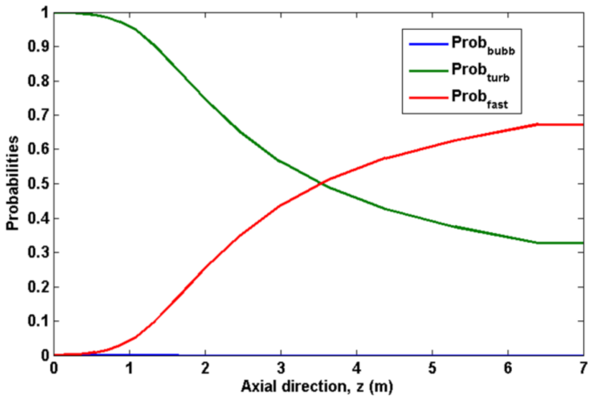
Chemical Looping Reforming: Fuel Reactor





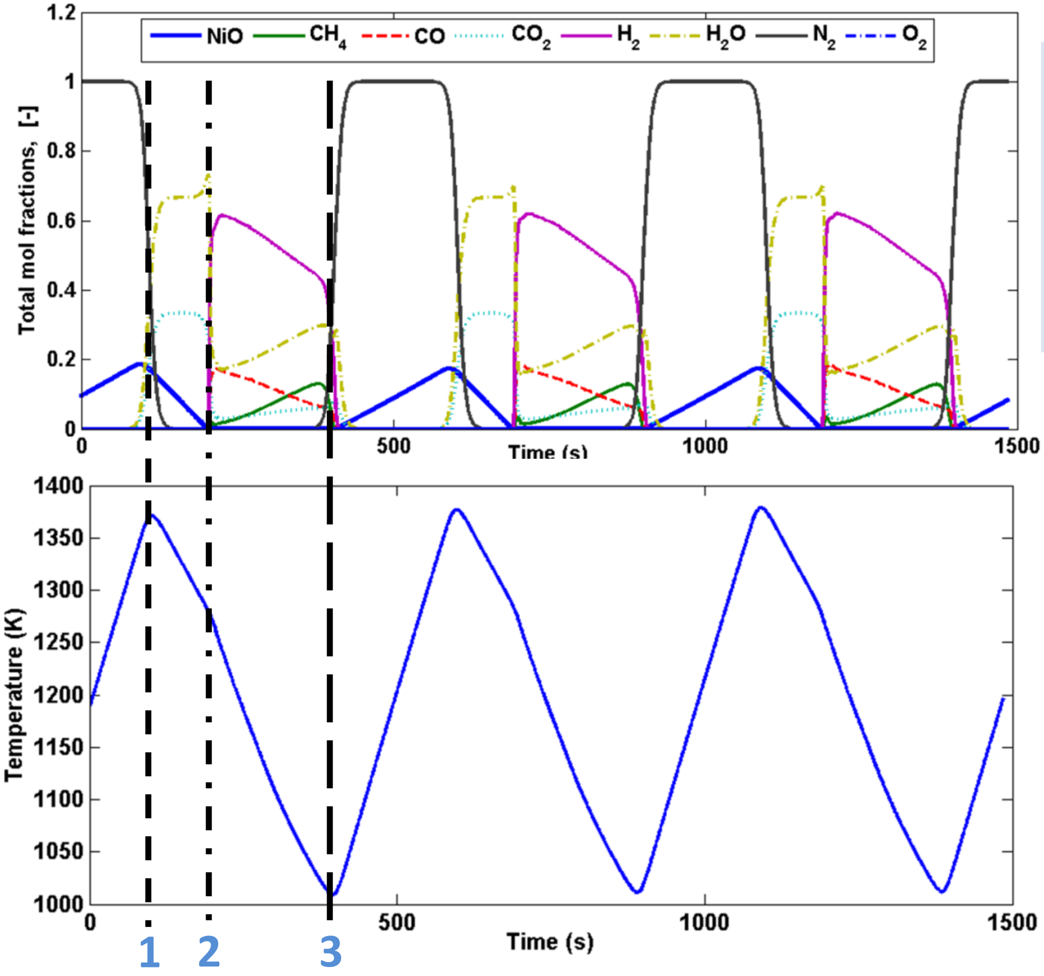
Maximum values: 2.94 kg/m3 for the gas density, 1 for the void fraction, 2.4 m/s for the superficial velocity and 989 °C for the temperature

- Reforming reactions dominate at the beginning of the reactor → system far from equilibrium conditions → production of H_2 → density decrease
- Reduction reactions dominate at the end;
- Low amount of NiO through the bed;
- Temperature almost constant → good axial mixing

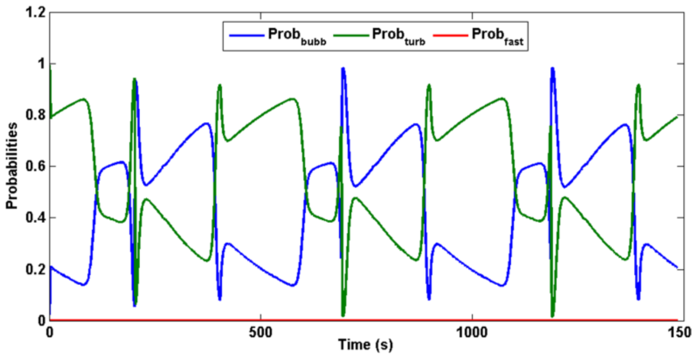


5. Results

Gas Switching Reforming



- O_2 totally consumed in the oxidation stage;
- Undesired mixture of N_2 with fuel → reduces CO_2 capture performance;



1. **Oxidation**
2. **Reduction**
3. **Reforming**

5. Results

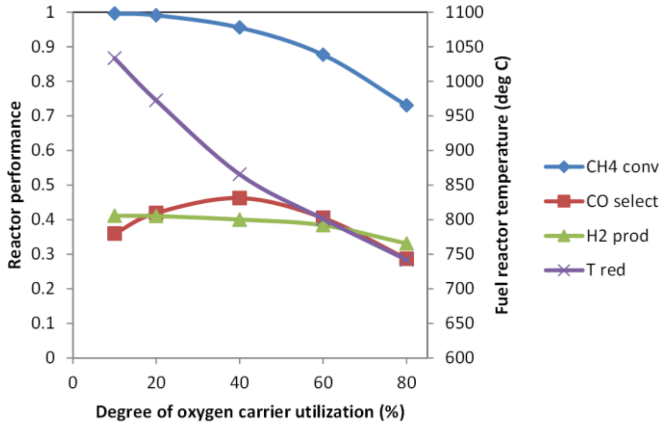
Performance Measures

CH_4 conversion

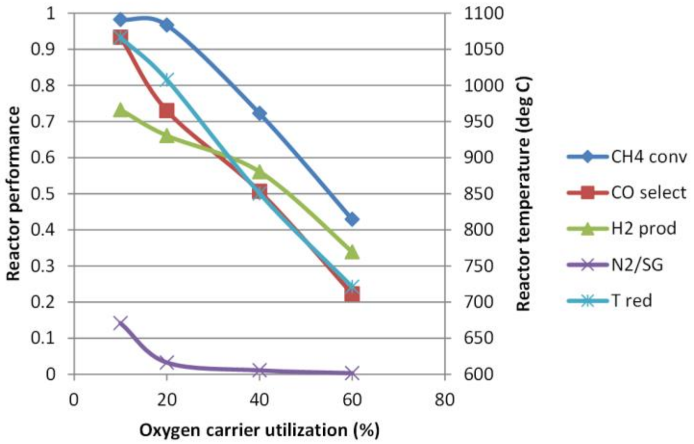
CO selectivity

H_2 production performance

CLR



GSR



Higher OC utilization

- Lower reduction temperature → low CH_4 conversion (by reforming endothermic reactions)→productivity of H_2 decreases
- Lower CO selectivity → WGS reaction

Lower OC utilization

- Lower CO selectivity → To supply heat

Higher OC utilization

- Lower CH_4 conversion → Reforming stage is higher
- Lower H_2 productivity → lower CH_4 conversion

Lower OC utilization

- Higher amount of N_2 mixed with fuel → Short cycle times

6. Conclusions

1. CLR

- Lower degree of OC utilization (higher OC circulation rate) → higher temperature in fuel reactor → better reforming performance
- However, high OC circulation rate can bring practical and economic challenges

2. GSR

- Lower degree of OC utilization (shorter stage times) → higher temperature in reforming stage → higher CH_4 conversion and H_2 production
- However, undesired mixing of N_2 with CO_2 and syngas increases with shorter stage times

6. Conclusions

3. CLR vs. GSR

- H_2 production and CO conversion is higher in GSR
- Fuel conversion is higher for CLR with higher CO_2 content
- CLR is best suited to thermal power production with pre-combustion CO_2 capture and GSR to pure H_2 production

Thank you for your Patience!!!

Questions?