NTNU – Trondheim
Norwegian University of Science and Technology

DEVELOPMENT OF NANO-STRUCTURED MATERIALS THROUGH A NOVEL MULTI-SCALE MODELLING FRAMEWORK FOR ENERGY CONVERSION WITH CO_2 CAPTURE

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Outline

- Background and introduction
- Different modeling scales
  - Atomistic level modeling
  - 1D modeling (reactor scale)
  - Process modeling (plant scale)
- Description of the method – flow and type of data
- Results
- Summary

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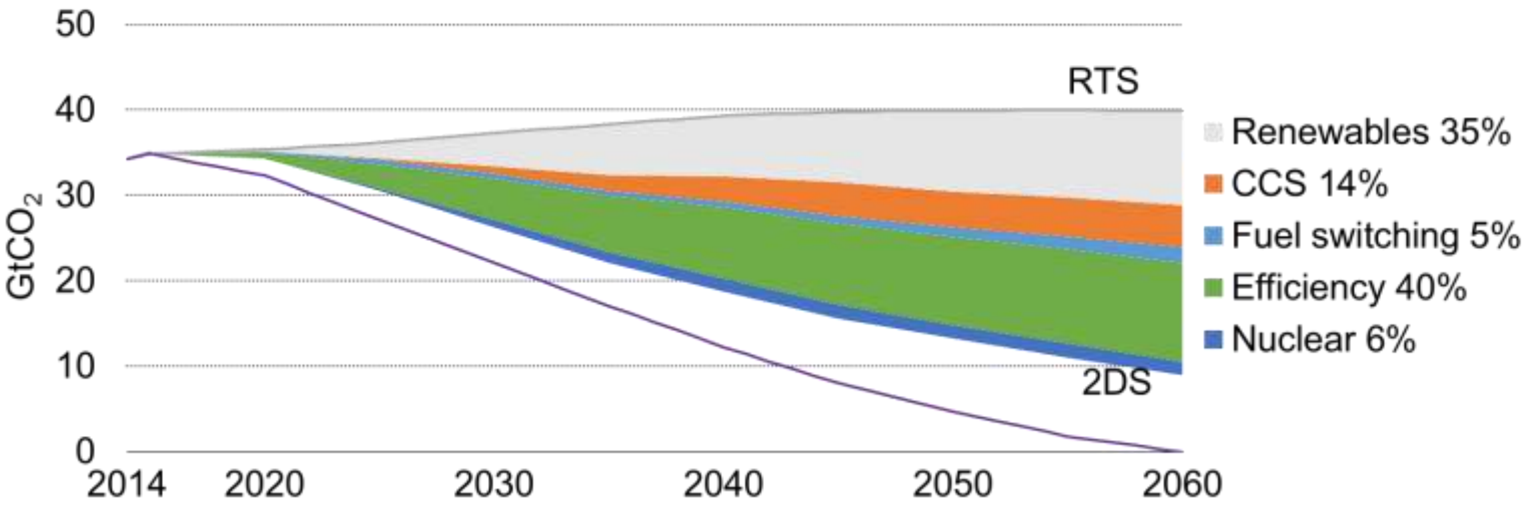
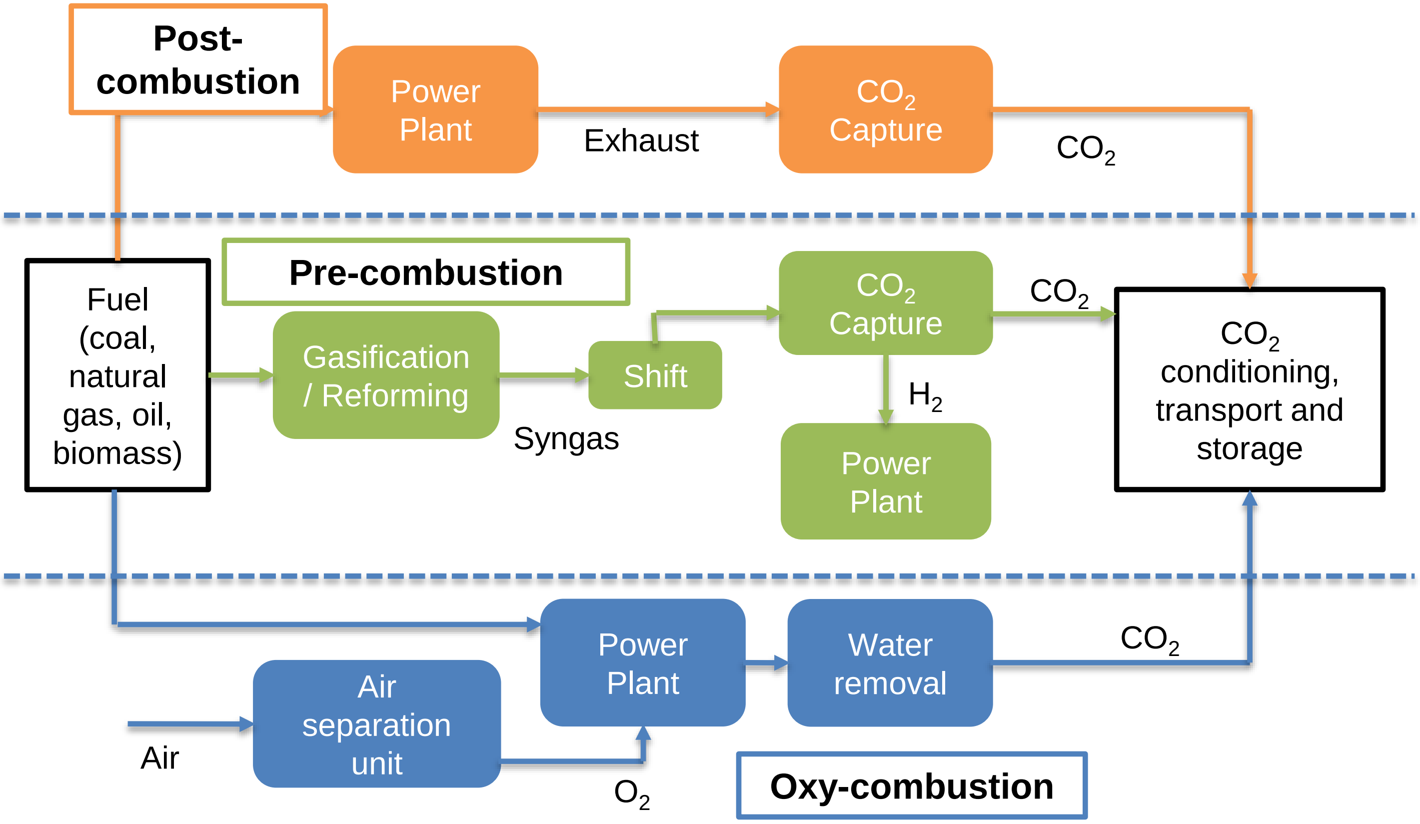
Background



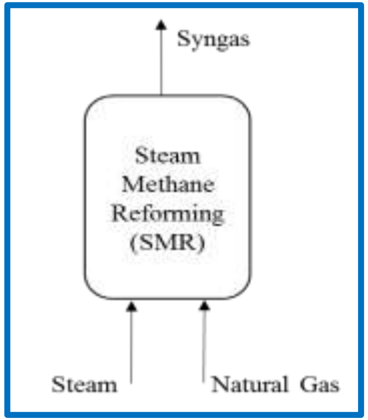
Source: International Energy Agency (2017), Energy Technology Perspectives 2017, OECD/IEA, Paris

CO_2 capture methods

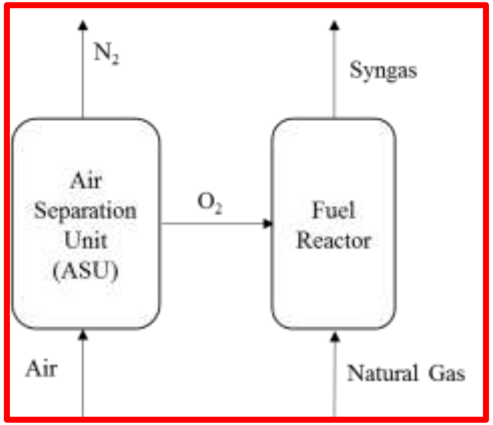


Reforming methods

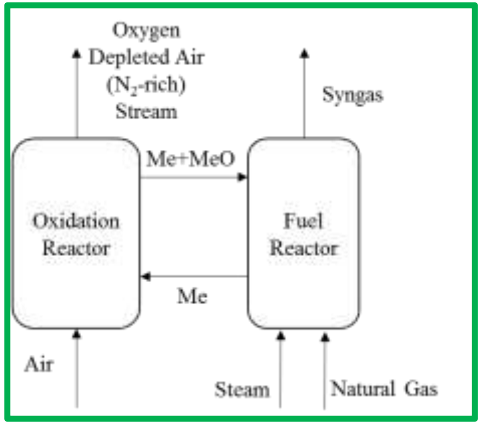
Steam Methane Reforming (SMR)



Partial Oxidation (POX)



Chemical Looping Reforming (CLR)



SMR $CH_4 + H_2O \rightleftharpoons CO + H_2$

POX $CH_4 + O_2 \rightleftharpoons CO + H_2$

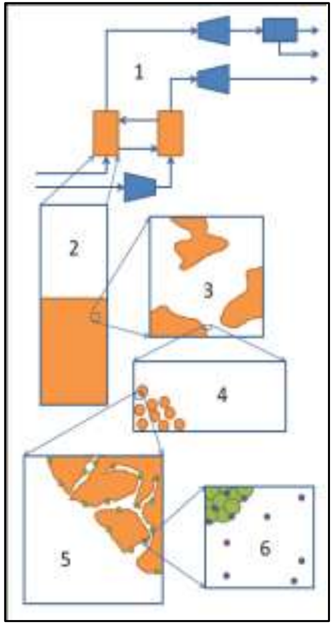
CLR $CH_4 + MeO \rightleftharpoons CO + H_2$

- CLR has less thermodynamic losses and has inherent air separation
- CLR reforms CH_4 to a product gas with higher H_2/CO ratio when compared to conventional POX

Earlier project

Project **NanoSim**: A Multiscale Simulation-Based Design Platform for Cost-Effective CO_2 Capture Processes using Nano-Structured Materials (EU FP7 framework)

https://www.sintef.no/projectweb/nanosim/



1. System Scale
2. Equipment Scale
3. Cluster Scale
4. Particle Scale
5. Intra-particle pore scale
6. Atomistic scale

Consortium

1. SINTEF Industry
2. TU Graz
3. University College London
4. INPT Toulouse
5. NTNU
6. DCS Computing GmbH
7. Andritz Energy and Environment GmbH
8. University de Coimbra

- Develop an open-source computational platform that will allow the rational design of the second generation of gas-particle CO_2 capture technologies based on nano-structured materials
- Design and manufacture nano-structured material and shorten the development process of nano-enabled products based on the multi-scale modelling
- Design and demonstrate an energy conversion reactor with CO_2 capture based on the superior performance of nano-structured materials

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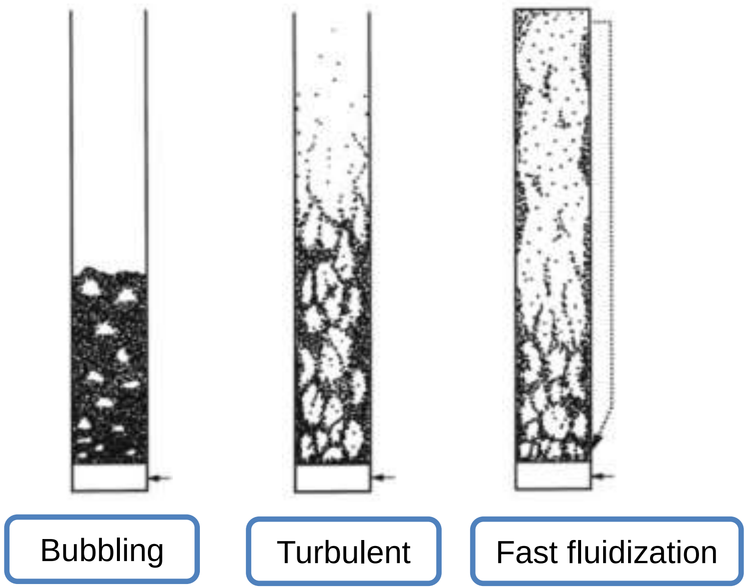
Atomistic and cluster scale modeling

- Reactivity of nanoparticles at the atomic scale/nanoscale, is estimated through kinetic Monte Carlo (kMC) modeling, guided by Density Functional Theory (DFT) calculations, on the detailed kinetics of the CH_4 conversion to products as a function of temperature.

- Cluster scale:
  - Intra-particle transport model
  - Fluid-Particle flow model (Tools: LIGGGHTS for particle motion and CFDEM for fluid flow)

Reference: Andersson, S., et al., *Towards rigorous multiscale flow models of nanoparticle reactivity in chemical looping applications.* Catalysis Today, 2019.

Equipment scale - 1D Model of CLR



- Rapid convergence
- Wide range of applicability (reasonably generic)
- User friendly
- Accommodate reactor clusters
- Handle dynamic and stationary simulations

“Generalized fluidized bed reactor” (GFBR) model

1-D model for fluidized bed reactors

Generic formulation based on the generic model developed by Abba *et al.* (2003)

- uses an **averaging probabilistic approach**
- **Two-phase** model

Single formulation is used!

Differential Balances

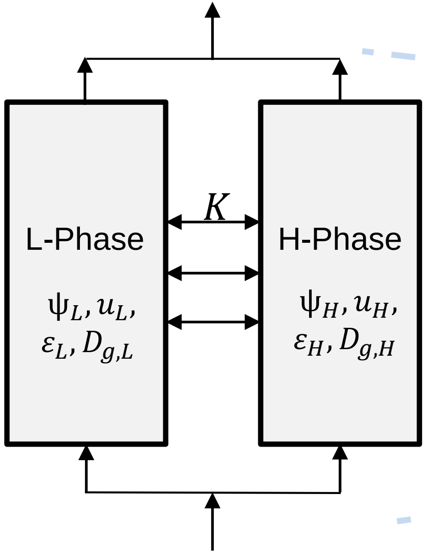
- **Mass balance**
  - Gas total mass balance
  - Gas species mass balance for each phase
  - Total solids species mass balance
- **Total Energy balance**
- **Pressure Balance**

Numerical scheme:

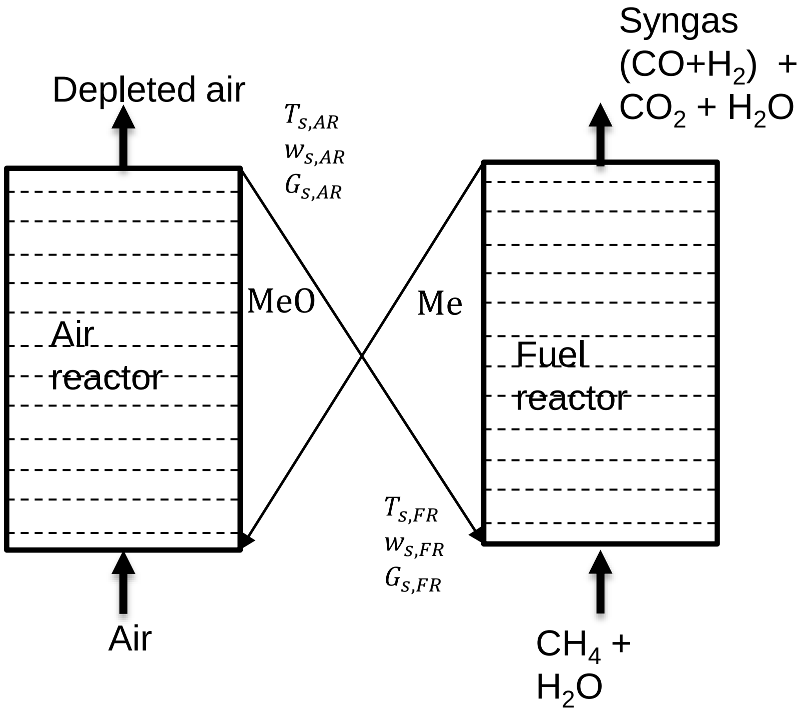
- Method of lines (MATLAB routine *ode15s*)
- Finite volume method (discretization in space)
  - **Non-uniform grid**
  - **Convective term**: 1^{st} order upwind scheme
  - **Diffusion term**: central differences scheme

Reference: Abba, I.a., et al., *Spanning the flow regimes: Generic fluidized-bed reactor model.* AIChE Journal, 2003. **49**: p. 1838-1848.

Two phases



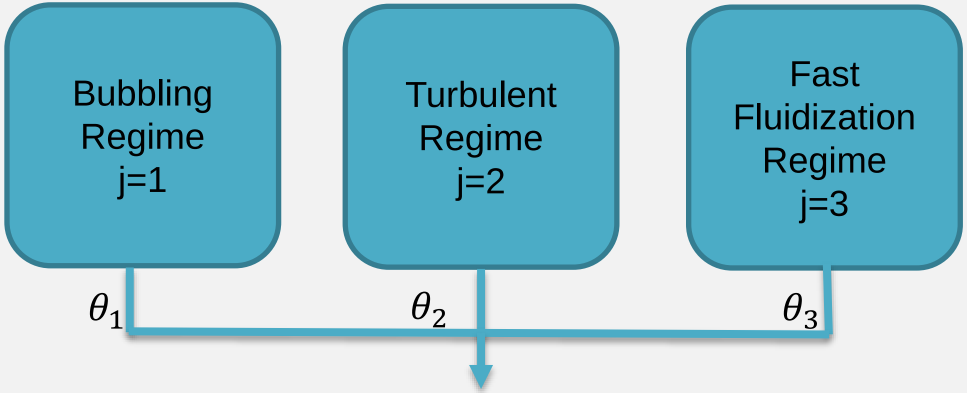
Sketch of the two-phase approach for a fluidized bed reactor



Simulation domain

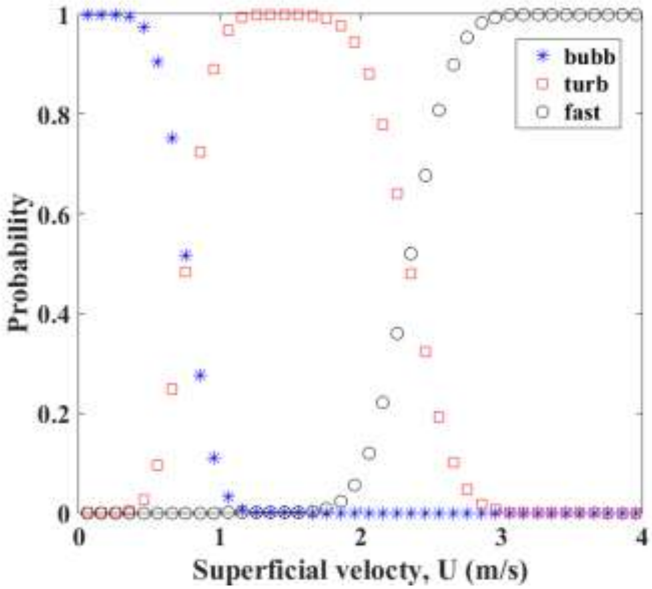
Averaging probabilistic approach

- Library of closures for different fluidization regimes



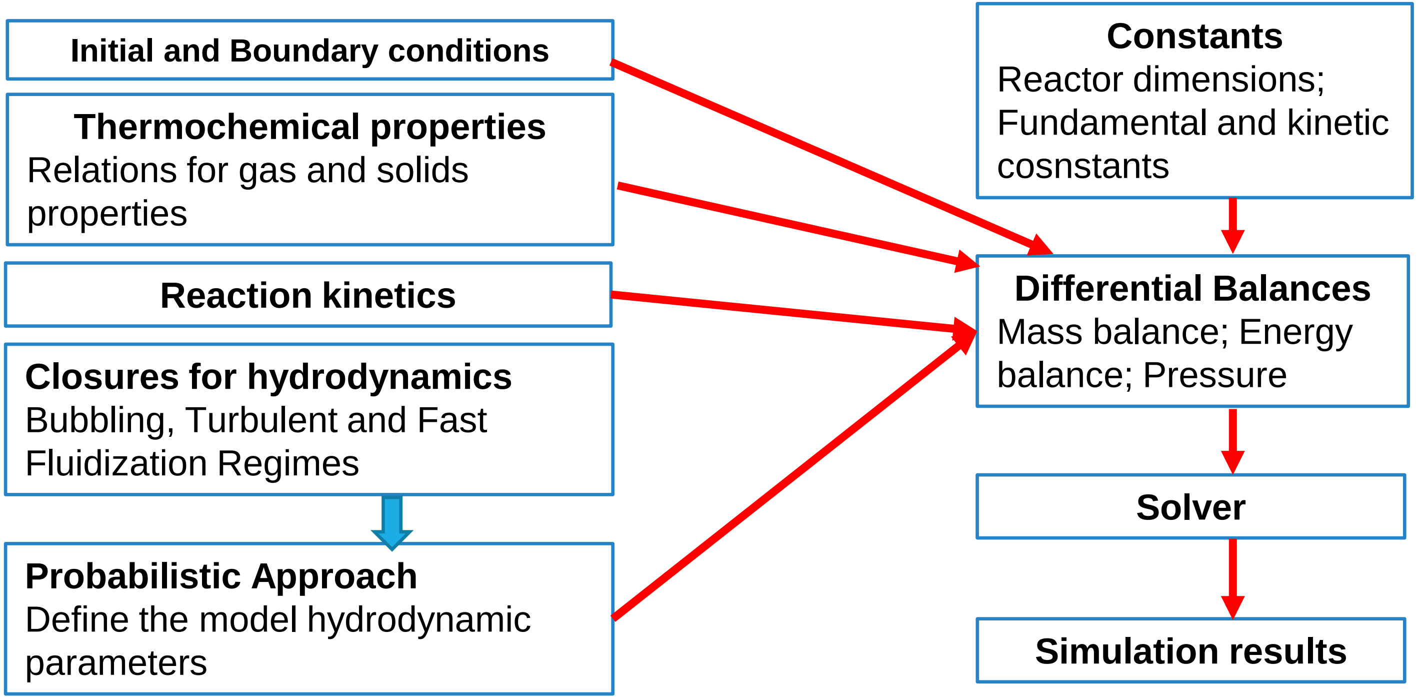
$$\hat{\theta} = \boldsymbol{P_1}\theta_1 + \boldsymbol{P_2}\theta_2 + \boldsymbol{P_3}\theta_3$$

$\boldsymbol{P_j}$ Probability of being under regime *j*



Reference: Abba, I.a., et al., AIChE Journal, 2003. **49**: p. 1838-1848.

1D Model outline



Parameter interaction in 1D-Model

KMC – Kinetic Monte Carlo

- Kinetic parameters (Arrehnius parameters)

Gas physical properties/conditions

- Flowrate
- Density
- Composition
- Heat capacity

→

Affects:
Gas velocities
Void fraction
Temperature
Reaction rate ($R = \mathbf{k}C^n$)
Pressure drop

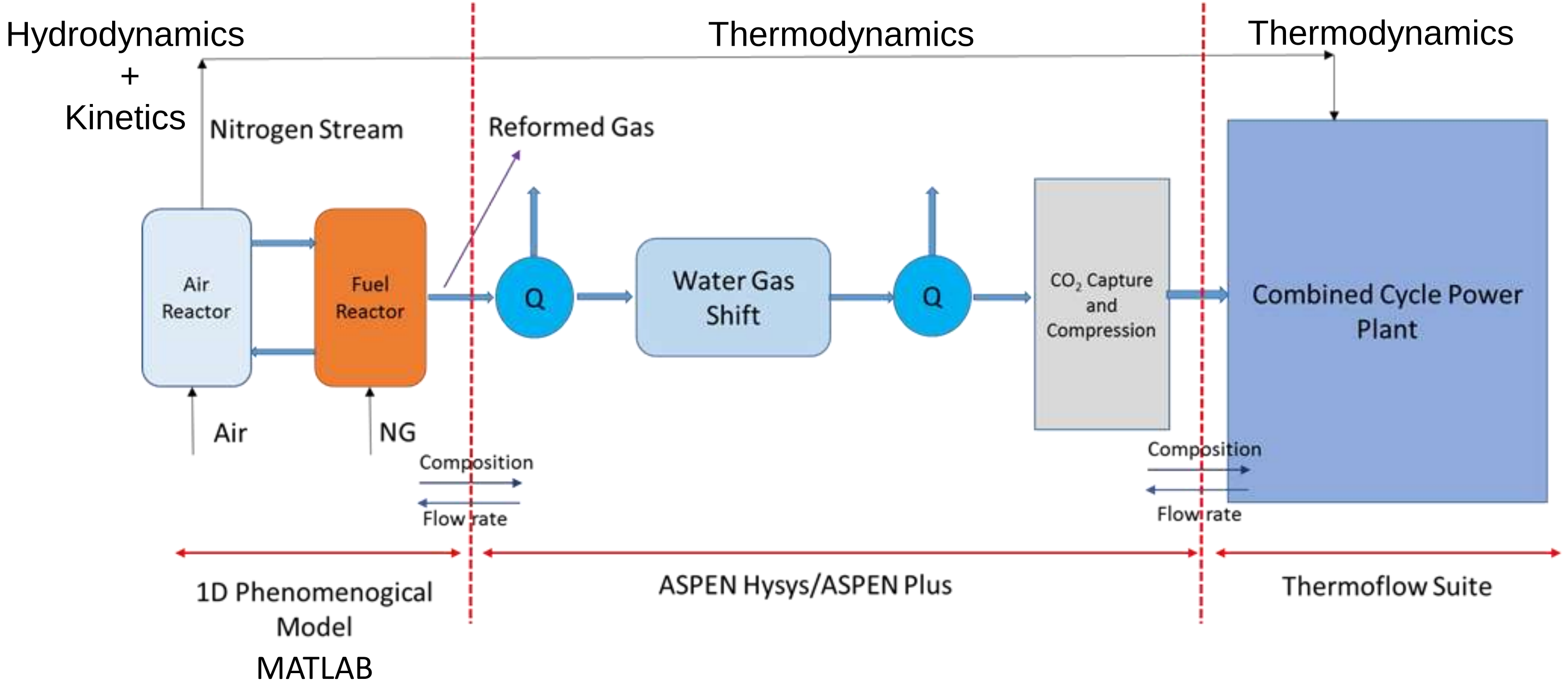
Solid physical properties/conditions

- Flowrate
- Density
- Composition
- Temperature
- Heat capacity
- Particle size

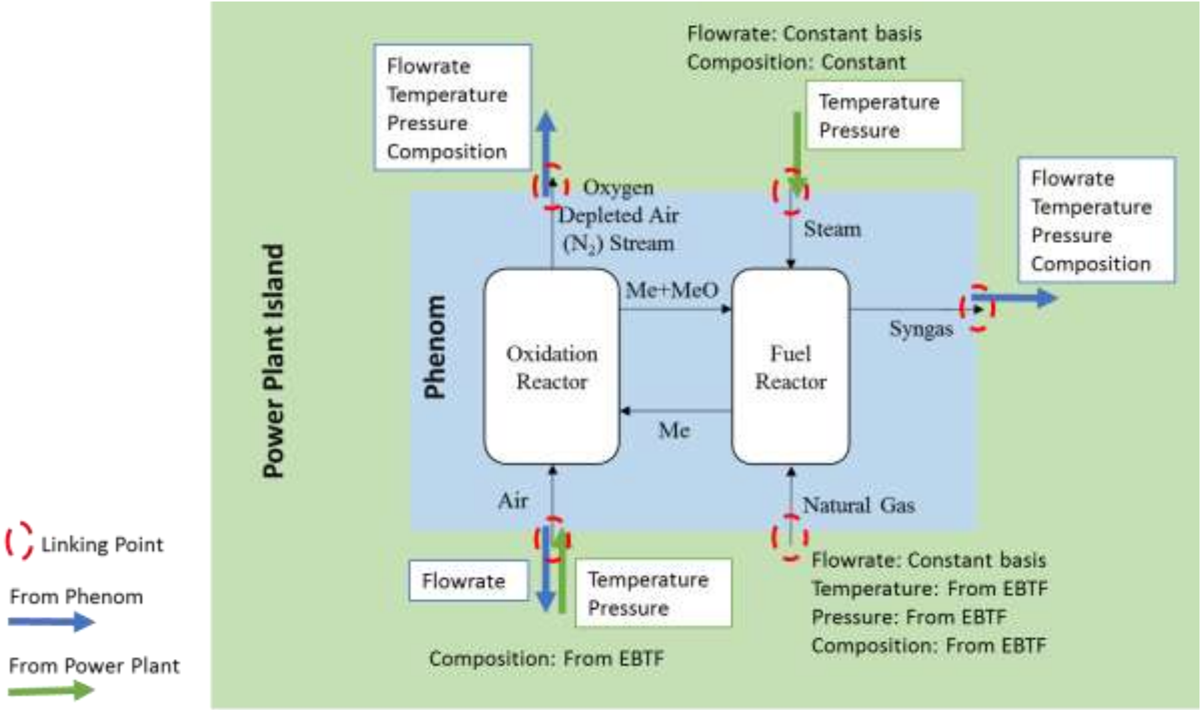
→

Affects:
Solids velocities
Void fraction
Temperature
Reaction rate ($R = \mathbf{k}C^n$)
Pressure drop
Solid recirculation rate

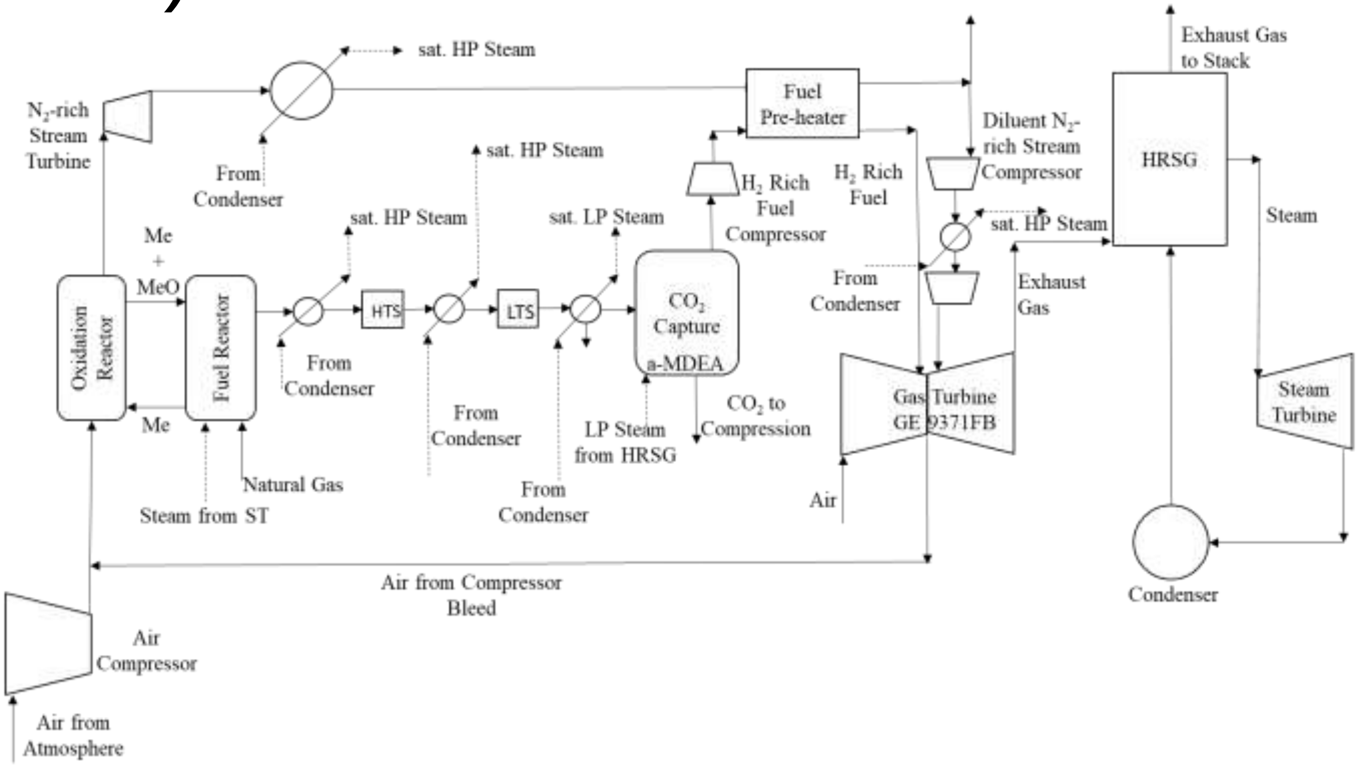
System (process plant) scale model



Interaction between 1d model and plant scale simulations



Pre-combustion combined cycle with CLR (CLR-CC)



Key performance indicators

CO_2 Capture (%) $= \frac{CO_2\ Captured}{CO_2\ generated\ in\ the\ process} \times 100$

CO_2 Avoidance (%) $= \frac{CO_2\ (emitted\ by\ ref.plant) - CO_2\ (emitted\ by\ process)}{CO_2\ (emitted\ by\ ref.plant)} \times 100$

Net Electrical Efficiency (%-LHV input) $= \frac{Net\ Electricity\ Produced}{LHV\ of\ fuel\ inout\ to\ process} \times 100$

Key performance indicators

Levelised cost of electricity ($/MWh)

$$LCOE = \frac{(TCR)(FCF) + FOM}{(MW)(CF \times 8766)} + VOM + (HR)(FC)$$

TCR – Total capital requirement

FC – Fuel costs

HR – Heat Rate

FOM – Fixed operating & maintenance costs

VOM – Variable operating & maintenance costs

Cost of CO_2 avoided

$$= \frac{LCOE_{CLR\_CC} - LCOE_{NGCC}}{\left(\frac{tCO_2}{MWh}\right)_{NGCC} - \left(\frac{tCO_2}{MWh}\right)_{CLR\_CC}}$$

*GCCSI. 2013. Global CCS Institute - TOWARD A COMMON METHOD OF COST ESTIMATION FOR CO_2 CAPTURE AND STORAGE AT FOSSIL FUEL POWER PLANTS.

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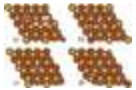
Flow of data

Atomic/Particle Scale

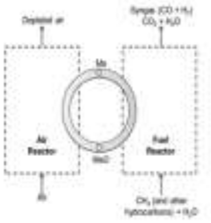
Physics and Chemistry



- Kinetic data from atomic/molecular simulations
- Particle size and shape

Equipment Scale

Chemical Engineering

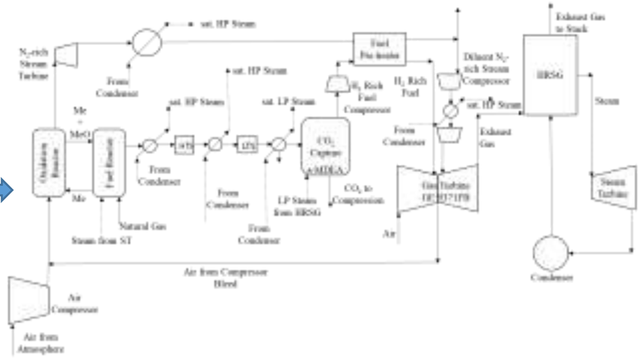


Physical phenomenological modeling at equipment scale with closures derived at atomic/cluster level

- Heat transfer
- Mass transfer
- Hydrodynamics
- Reactions

Plant Scale

Process Systems Engineering



Process modeling and simulation by linking the equipments together

- Thermodynamics
- Process integration
- Process efficiency
- Optimization

Global Scale

Economics

Environment and Market

- Cost of electricity
- CO_2 captured and avoided
- Cost of CO_2 avoided

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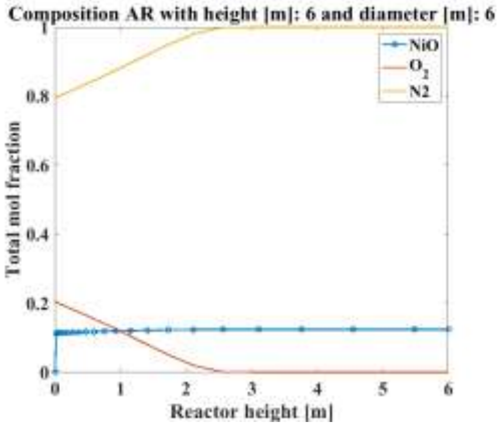
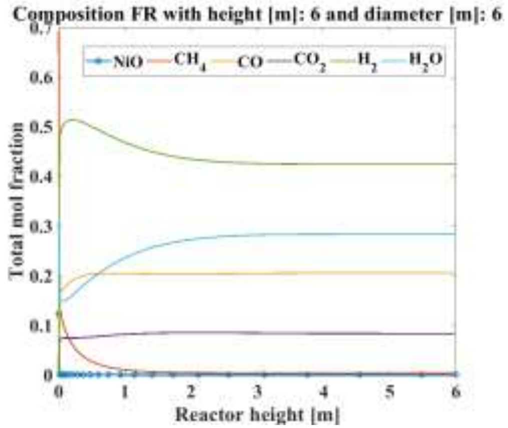
Conversion profiles in CLR – 1D Model

Base case kinetic data from literature

Installed cost of CLR = 49 M€

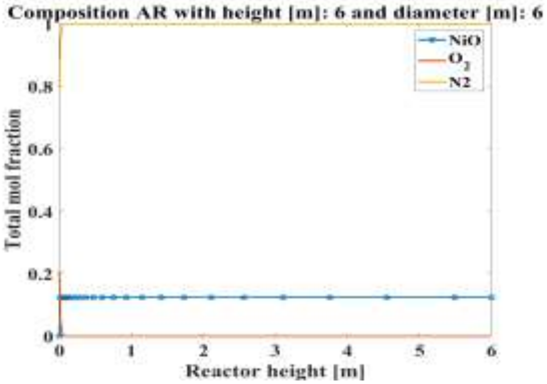


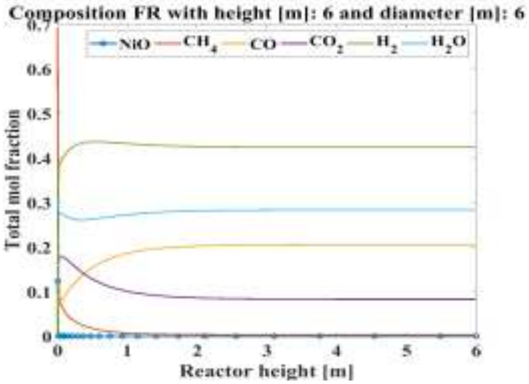


Support particle size: 250 microns

Assuming 50x times faster kinetics

Installed cost of CLR = 41 M€

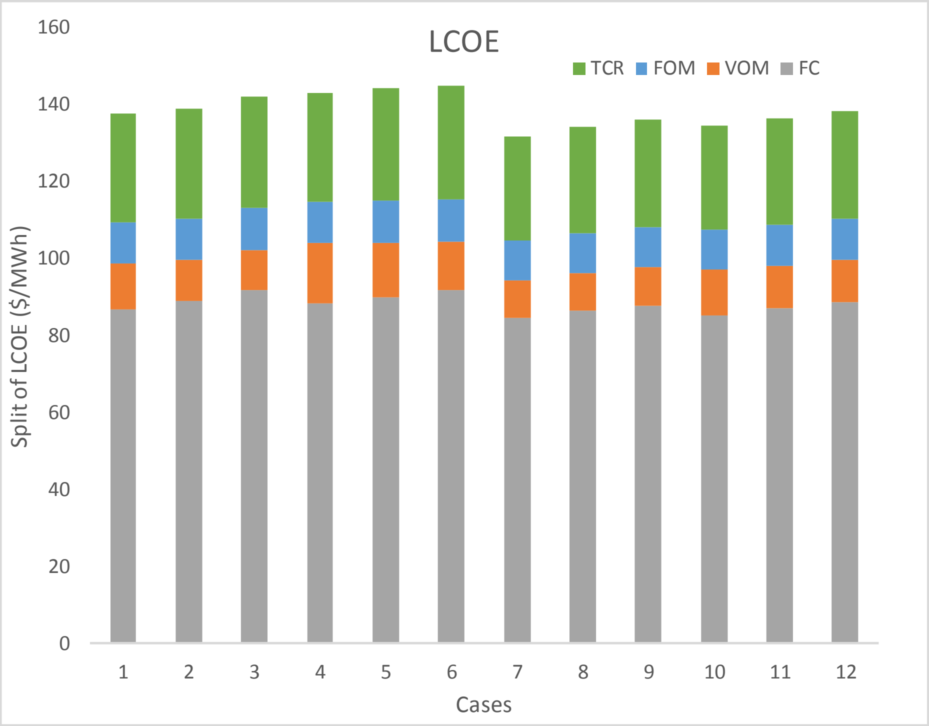




Sensitivity study for techno-economic analysis

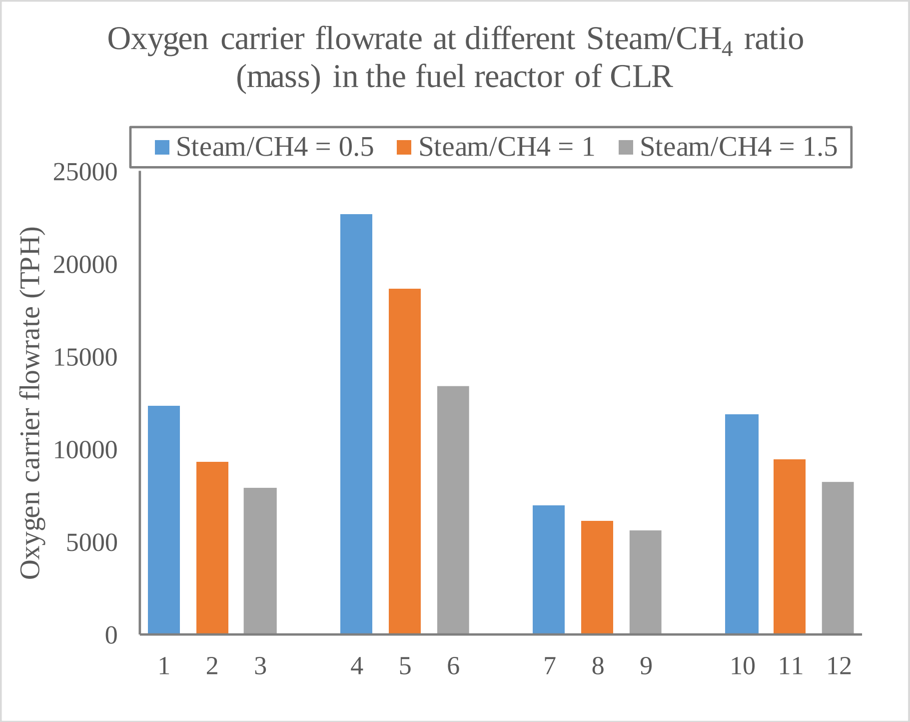
Cases	O_2/CH_4 by moles	Steam/CH_4 by mass	Oxidation Reactor Outlet Temperature (°C)	CH_4 flow (TPH)
1	0.9	0.5	1200	170
2	0.9	1	1200	170
3	0.9	1.5	1200	172
4	0.9	0.5	1100	170
5	0.9	1	1100	170
6	0.9	1.5	1100	170
7	0.8	0.5	1200	160
8	0.8	1	1200	160
9	0.8	1.5	1200	160
10	0.8	0.5	1100	160
11	0.8	1	1100	160
12	0.8	1.5	1100	160

Techno-economic performance



*Nazir, S.M., et al., Techno-economic assessment of chemical looping reforming of natural gas for hydrogen production and power generation with integrated CO2 capture. International Journal of Greenhouse Gas Control, 2018. 78: p. 7-20

Oxygen carrier related costs



Oxygen carrier flow in case 1 = 12289 TPH

Lifetime: 5 years
Variable O&M cost from oxygen carrier ~1.4 €/MWh

Lifetime: 0.5 years
Variable O&M cost from oxygen carrier ~ 14 €/MWh

*Considering cost of Ni-NiO oxygen carriers

*Nazir, S.M., et al., Techno-economic assessment of chemical looping reforming of natural gas for hydrogen production and power generation with integrated CO2 capture. International Journal of Greenhouse Gas Control, 2018. 78: p. 7-20

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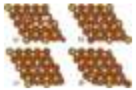
Summary

- A method to develop oxygen carrier materials for chemical looping systems from a techno-economic perspective is discussed.
- The method aims to reduce the time required to test different materials experimentally.
- The tools at atomic, equipment and plant scale have been developed and tested.
- Future work will focus on mapping techno-economic process peformance with different material properties. This chart could then be used a starting point to consider oxygen carrier materials for respective chemical looping systems.

Opportunities

Atomic/Particle Scale

Physics and Chemistry



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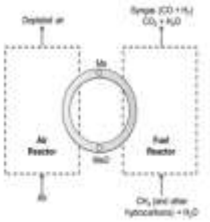

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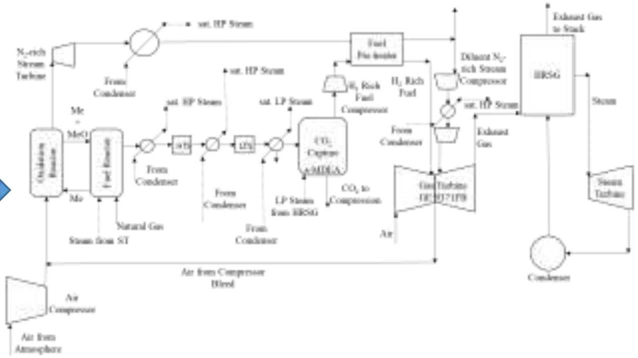

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Thank you

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