SIMULATION-BASED DESIGN
OF
CO_2 CAPTURE REACTORS

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Agenda

- Why simulations?
- Why CO_2 capture processes?
- Accelerated development

- Model development
- Model validation
- Simulation-based reactor design

- Conclusions & future work

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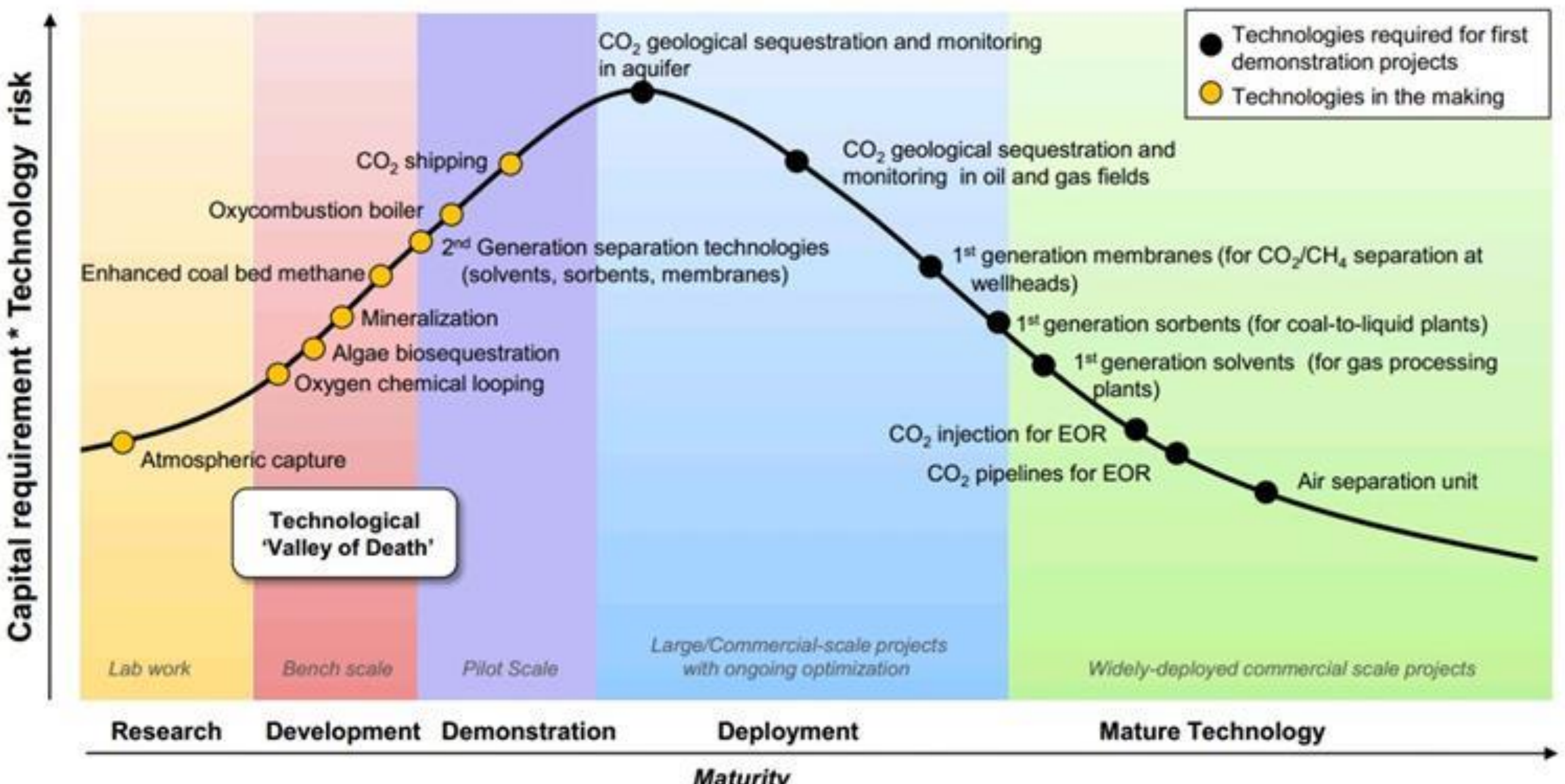
Why simulations?

- Not subject to any physical limitations
  - Change any design/operating variable
  - Simulate real scales and operating conditions
  - Extract any flow variable from anywhere in space/time
- Ideal for:
  - Process optimization and scale-up studies
  - Prototyping of novel concepts
  - Troubleshooting of existing reactors

Why simulate CO_2 capture systems?

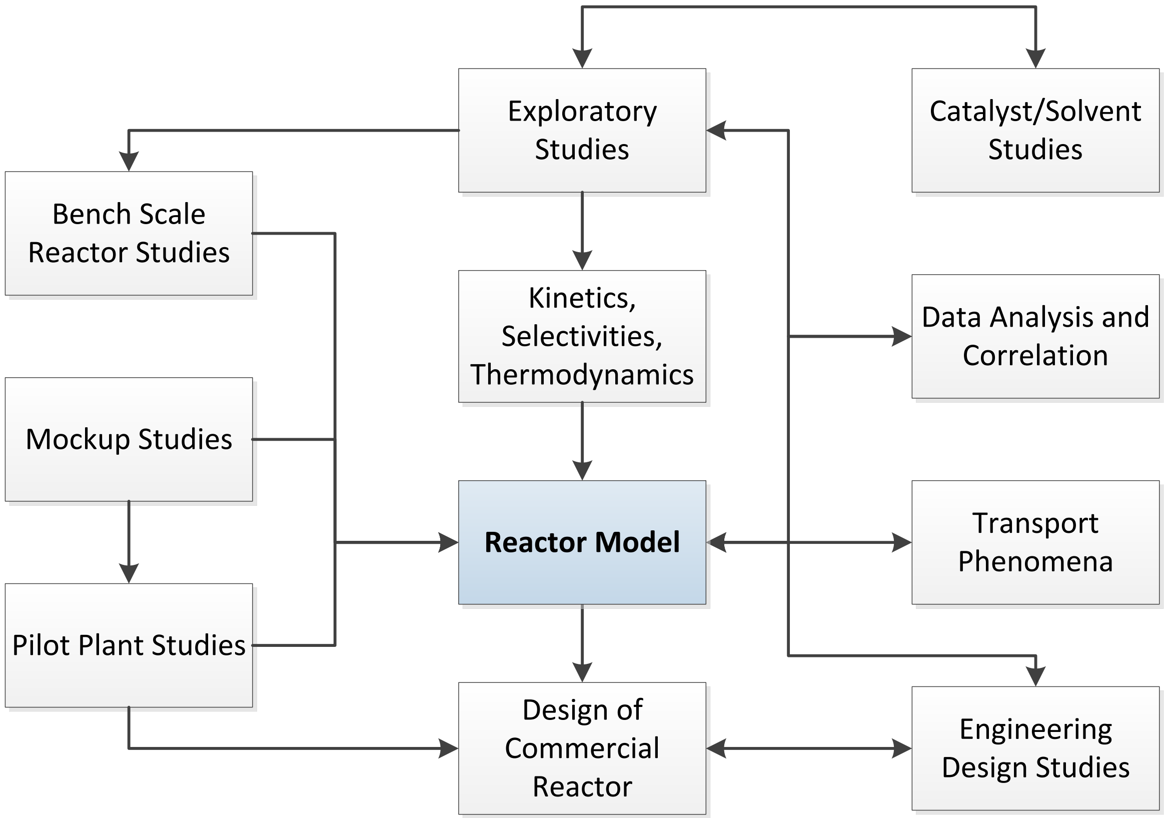
- Relatively small amount of funding available
- Large number of candidate technologies
- Limited time to traverse the technology risk peak



http://cdn.globalccsinstitute.com/publications/factbook-bringing-carbon-capture-and-storage-market

Classical process development

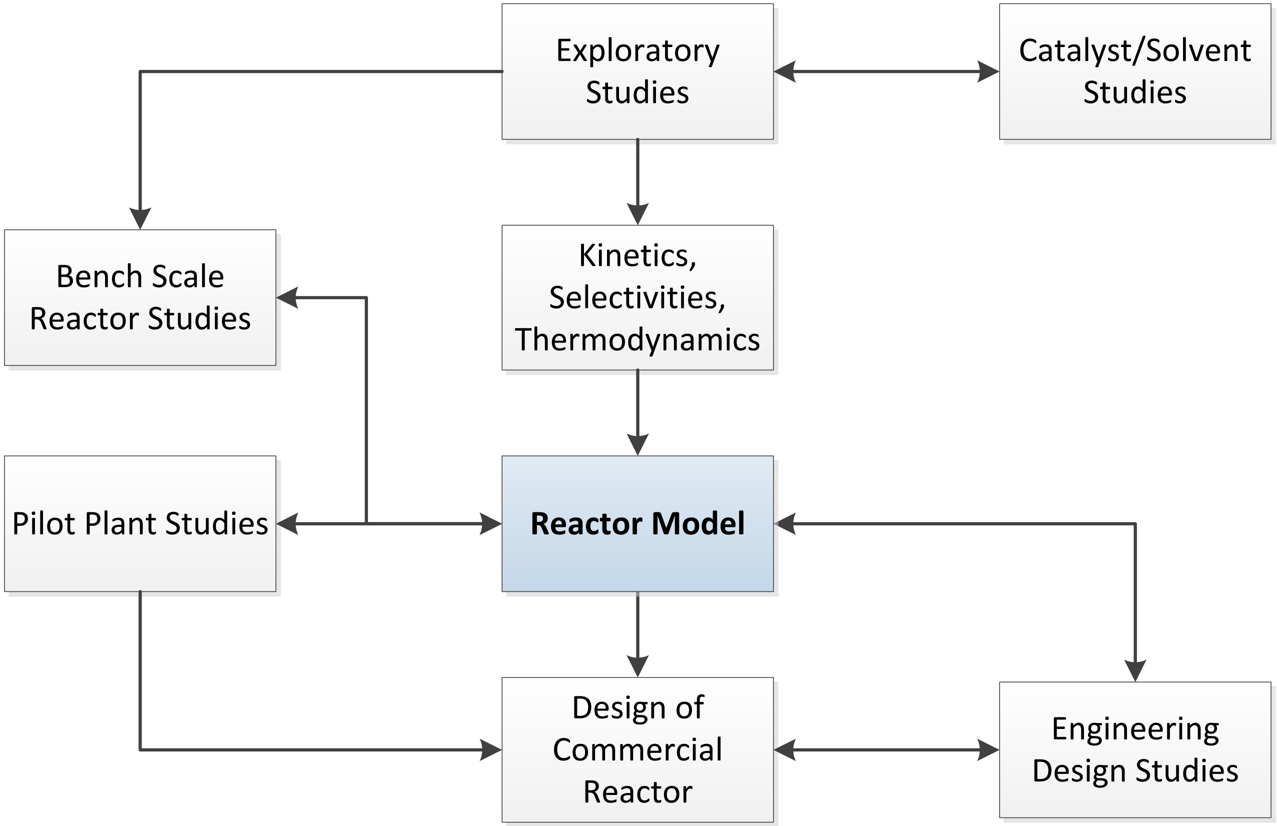
- Chemical engineers have used models for a very long time
- Model is a vehicle to condense state of the art knowledge



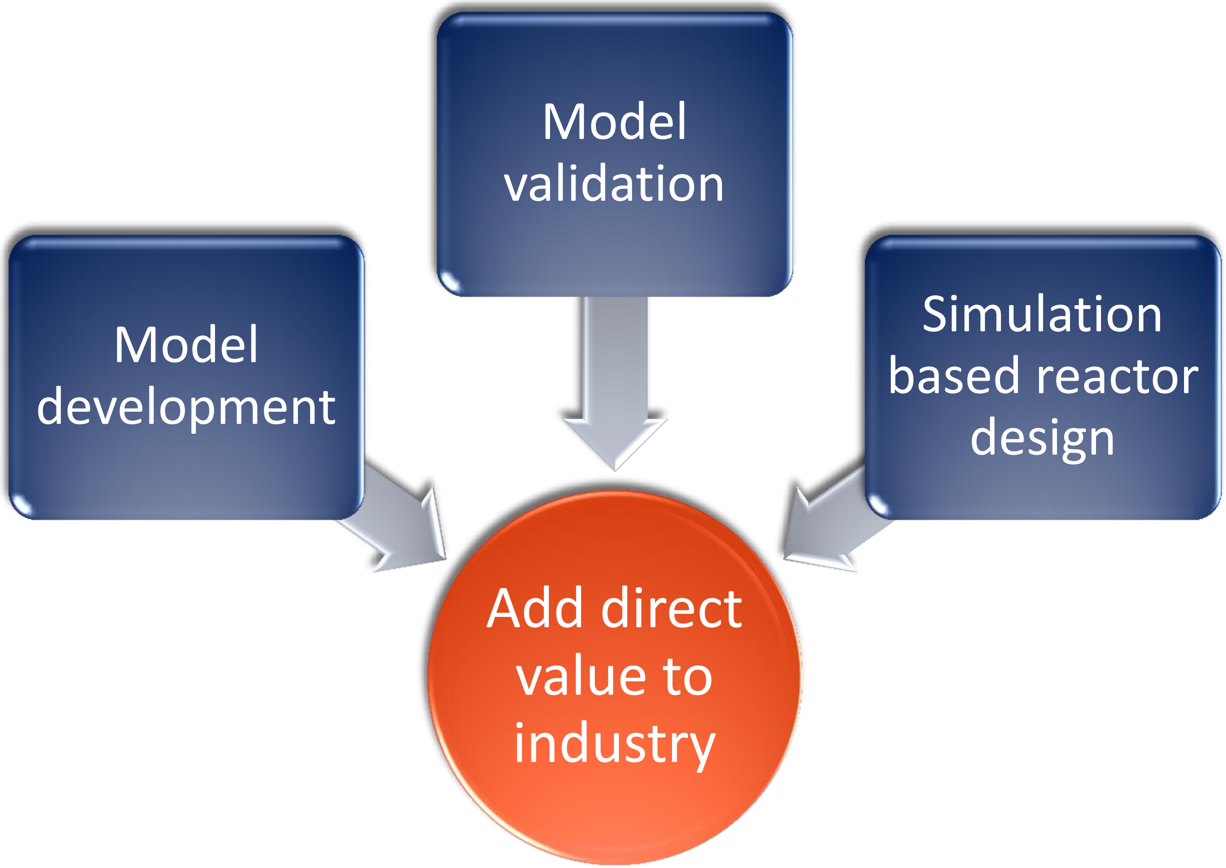
Johnsen *et al.* Energy Procedia 2009:1

Accelerated process development-potentials for low risk – high return

- More trustworthy model = larger scale-up steps
- Potential to greatly accelerate and optimize



Accelerated development: Big picture



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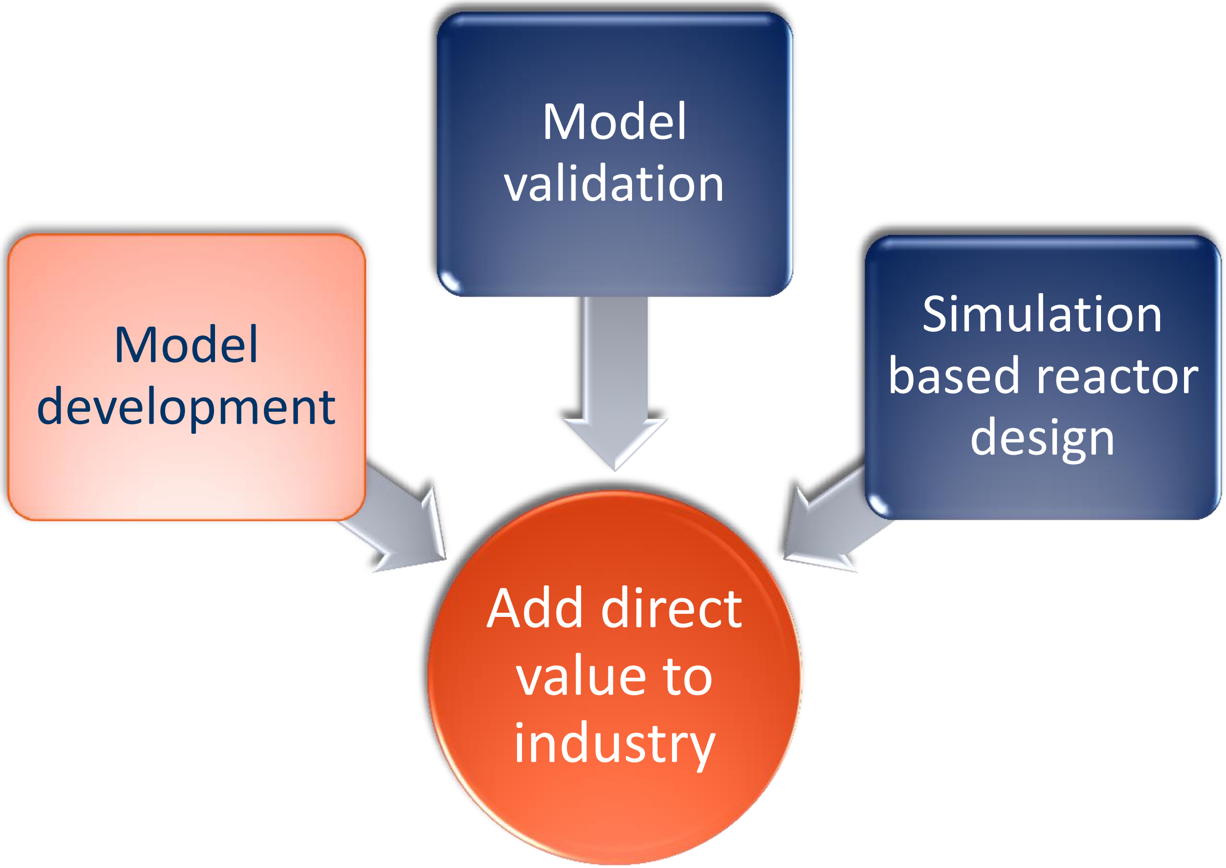
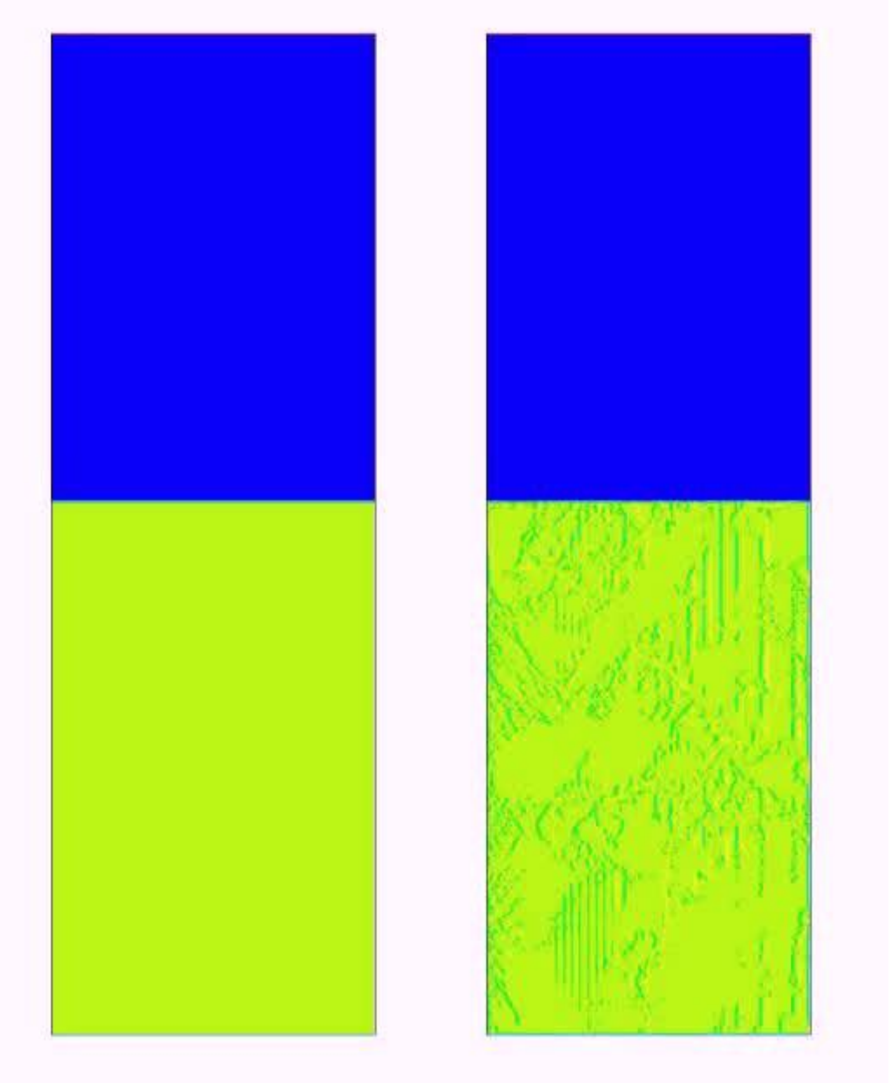
Accelerated development: Big picture



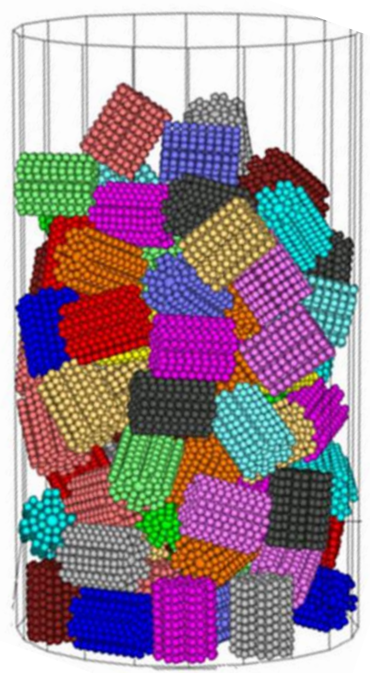
Model development: Fluidized beds

- Challenge: Good accuracy required at low computational costs
- The use of super computers
- Current works on large scale models:
  - Dense Discrete Phase Model (DDPM)
  - Filtered Two Fluid Model (fTFM)

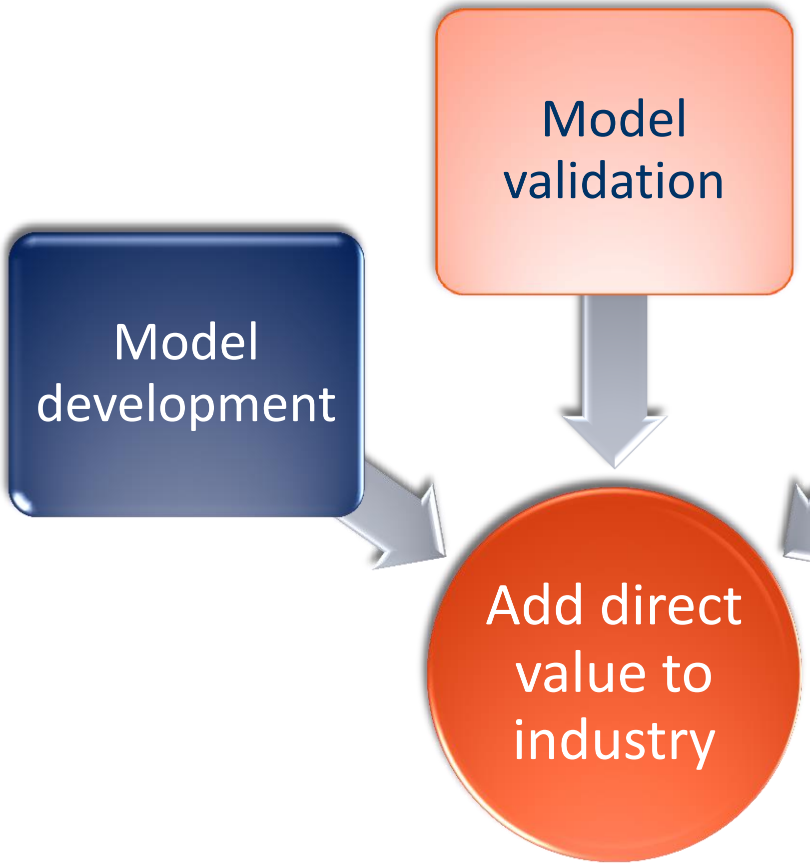


Model development: Packed beds

- Simpler flow problem
- More sensitive to accurate material and kinetic data
  - Large temperature variations
  - Large chemical composition changes
  - Diffusion resistance within larger pellets must be accurately modelled
- 1D models well developed – ready for industrial applications (DemoCLOCK)
- Further development required:
  - Multi-dimensional models for special cases

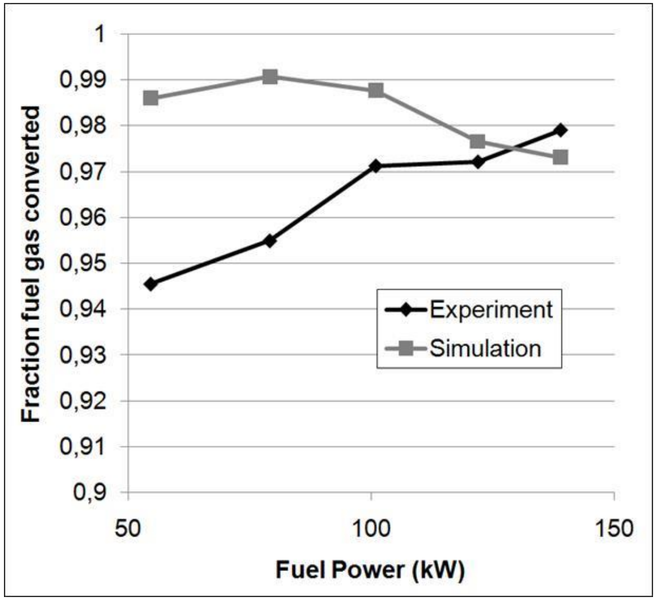


Accelerated development: Big picture



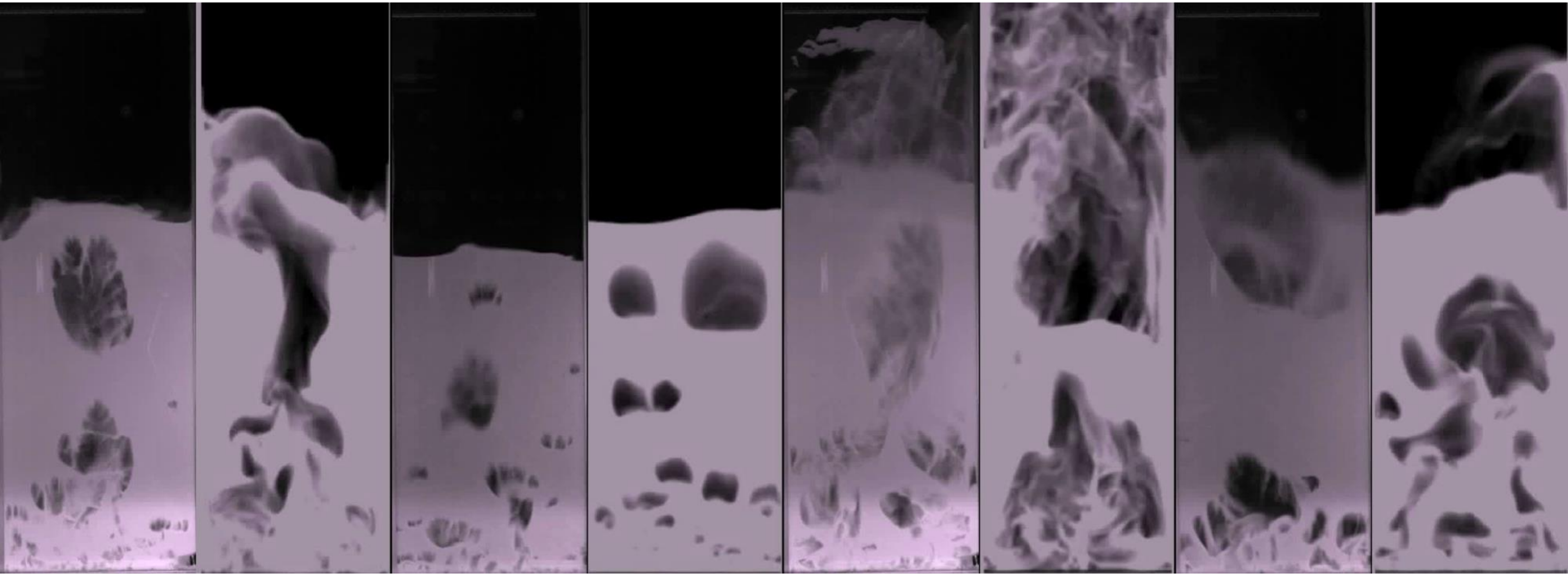
Model validation: Principle

- Model generality must be explicitly demonstrated
  - Will inevitably be used far from validation conditions
  - Will be used as a basis for multi-scale modelling
- Dedicated experimental campaigns required
  - Collect data over a wide range of flow variables
  - Collect detailed local measurements
  - Separate hydrodynamics, species transfer, heat transfer and reactions



Model validation: Hydrodynamics

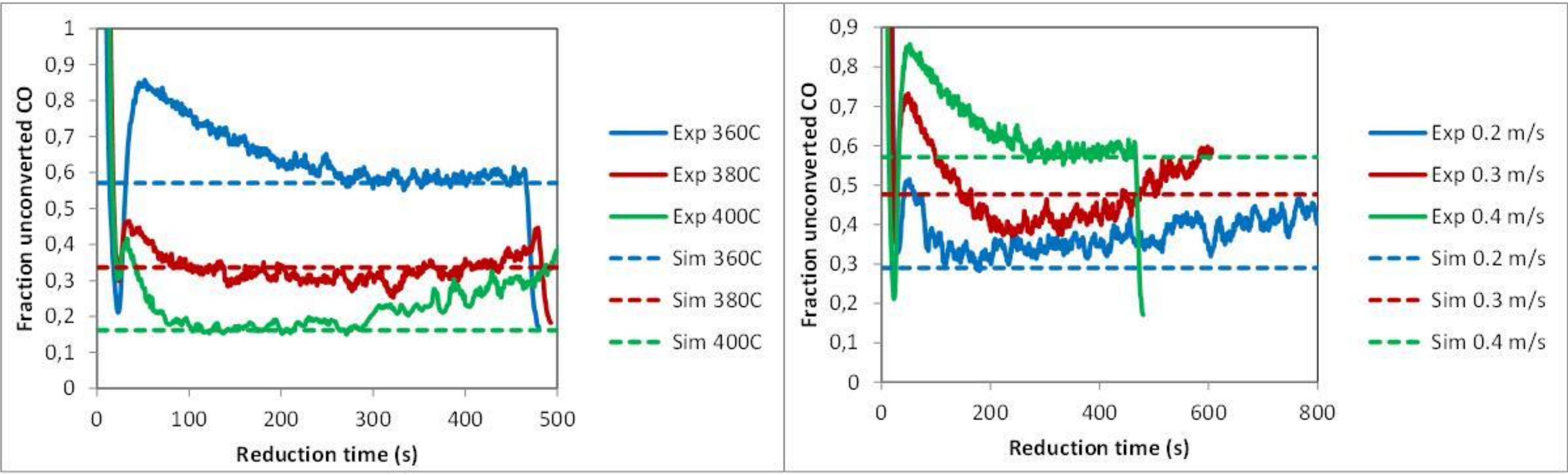
- In collaboration with Eindhoven University of Technology



Particle size: 150 µm Fluidization velocity: 0.4 m/s	Particle size: 350 µm Fluidization velocity: 0.4 m/s	Particle size: 150 µm Fluidization velocity: 0.8 m/s	Particle size: 350 µm Fluidization velocity: 0.8 m/s

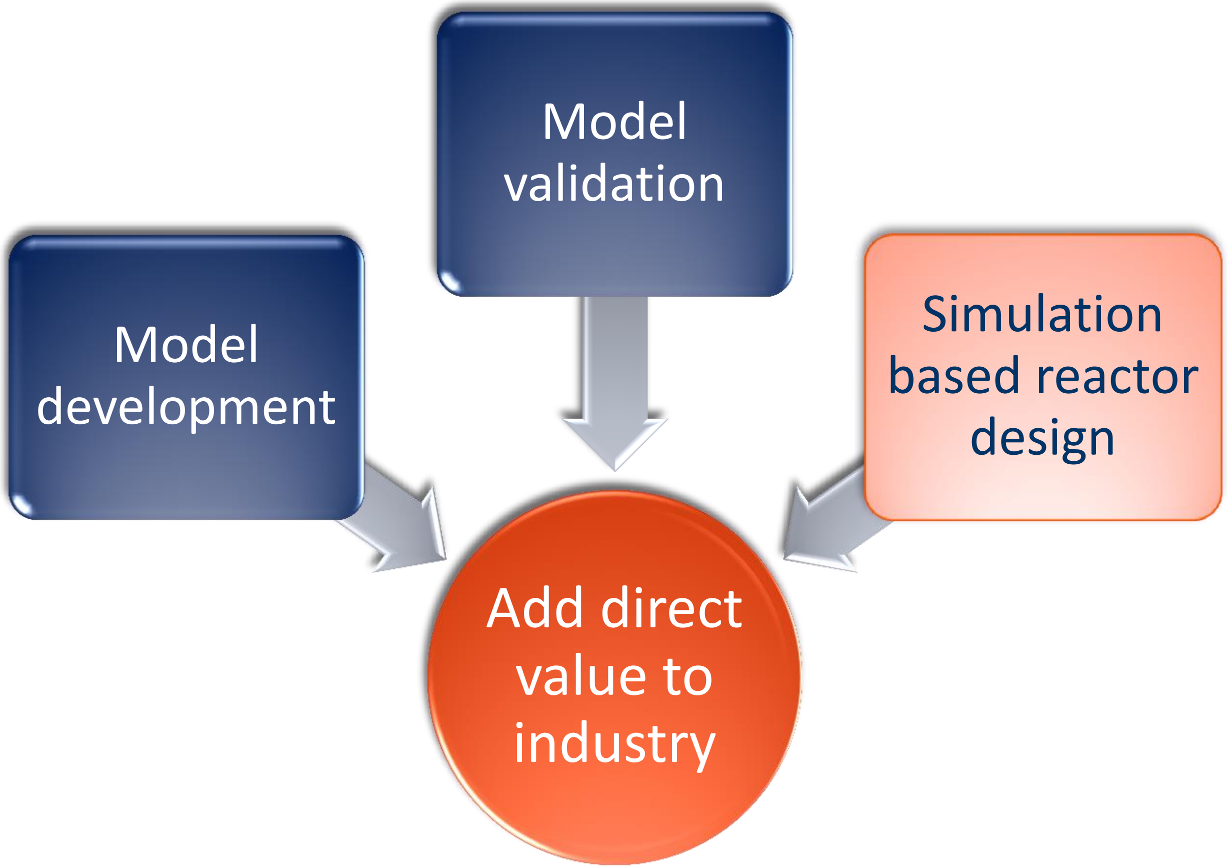
Model validation: Reaction kinetics

- In collaboration with Eindhoven University of Technology
- Appear to be on the right track, but more work needed



- Two variables in this case: temperature and fluidization velocity
- Simulations averaged over 30 seconds

Accelerated development: Big picture

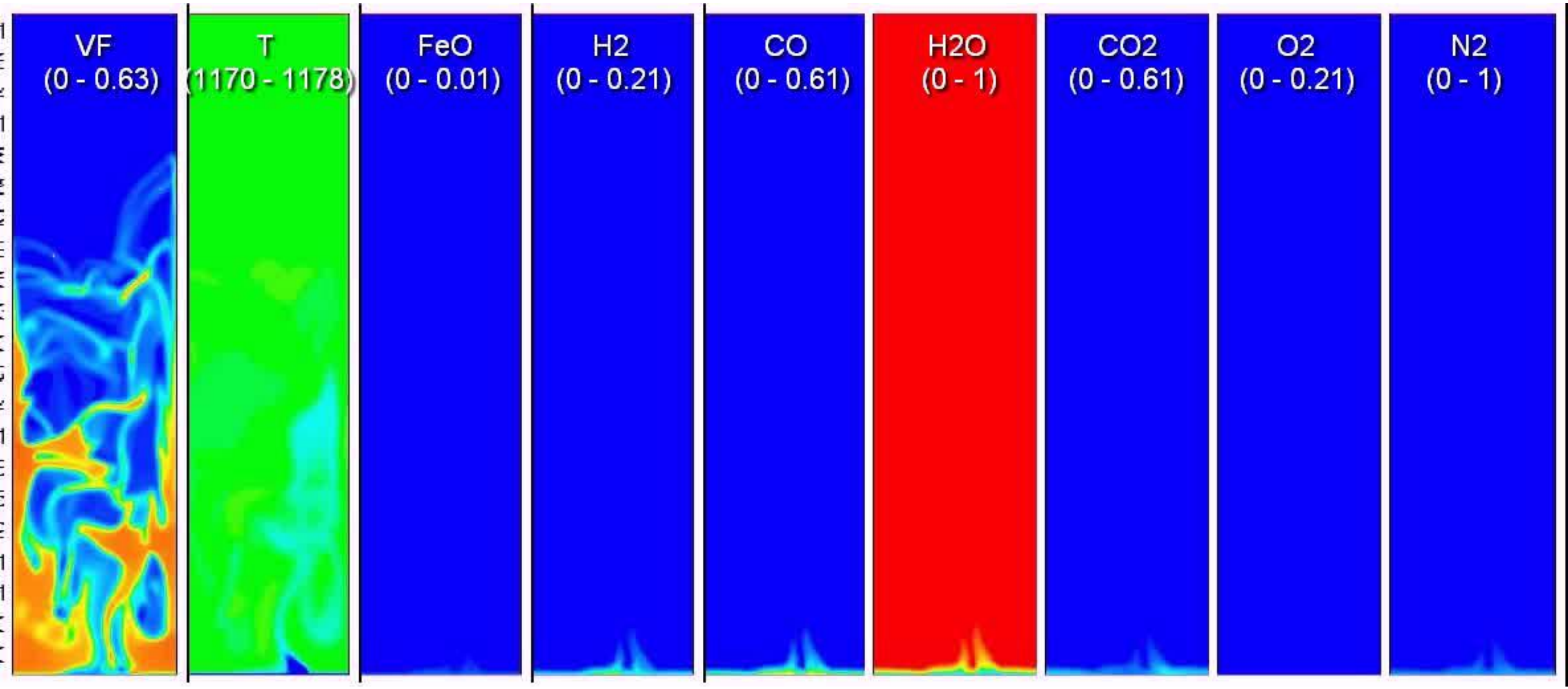


Simulation based reactor design: Principle

- Develop methods on the assumption of high model fidelity
- Allows for full utilization of the fundamental advantages of simulation based reactor design:
  - Detailed process behaviour under any operating conditions
  - Ideal for optimization over a wide range of operating and design parameters
  - Complete creative freedom for developing novel reactor concepts
- Models will eventually live up to these expectations

Process behaviour: Fluidized bed

- Bubbling bed CLC with periodic gas switching



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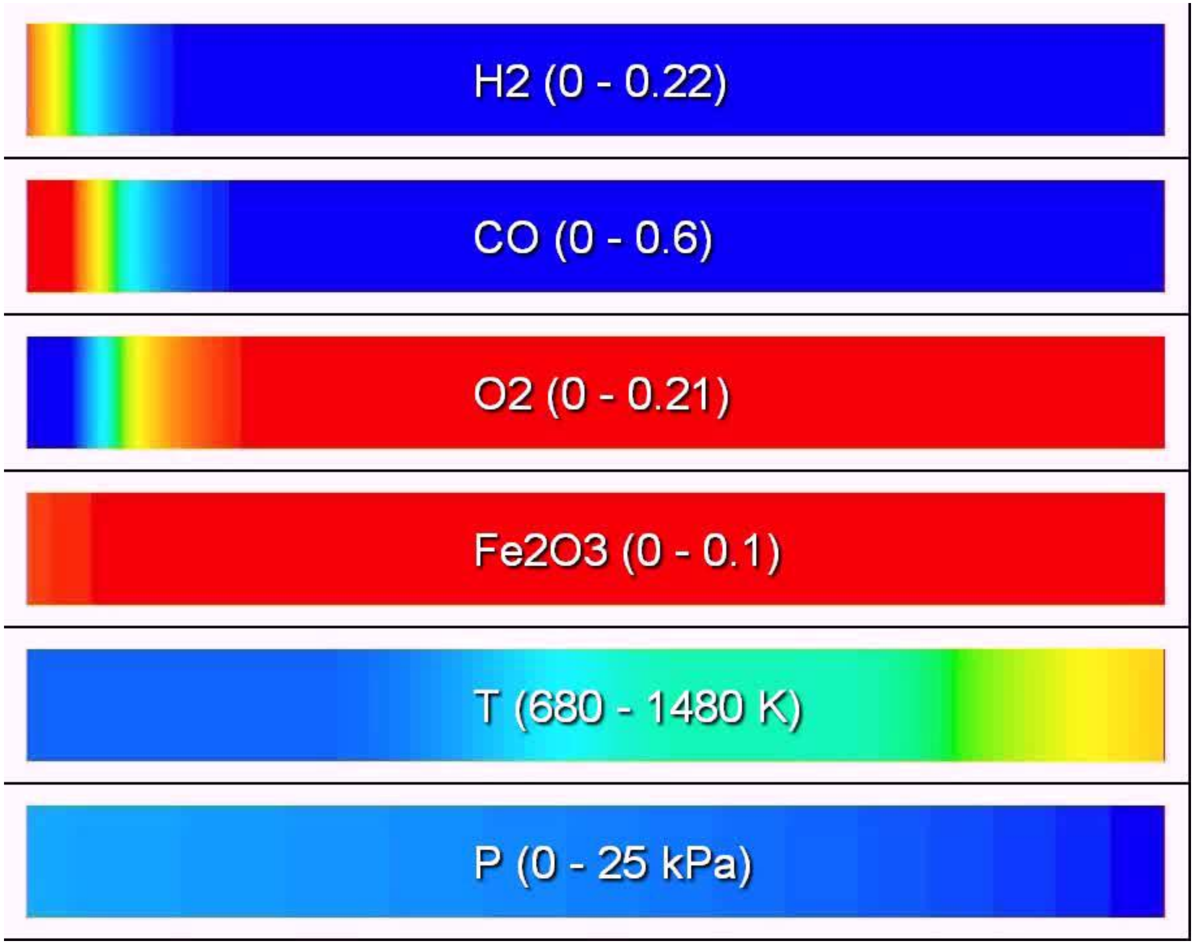
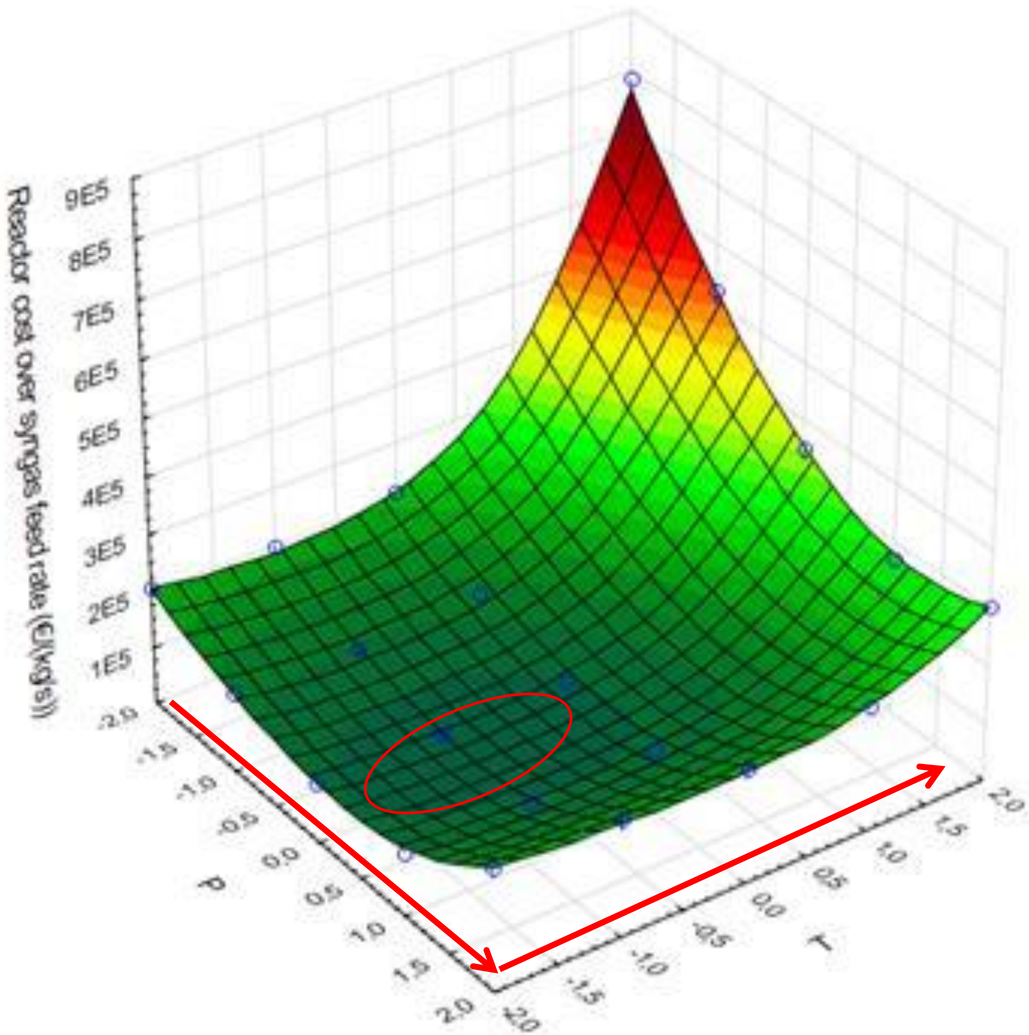


Optimization: Lowest cost operation

- Simplified example for finding lowest cost reactor P & T
- Challenge: Highly dependent on accurate cost estimates as a function of all independent variables



$$T_{actual} = 900 + 200T$$

$$P_{actual} = 5 \times 2.5^{P}$$

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Conclusions & future work

- Simulation-based reactor design shows great promise especially for application to second generation CO_2 capture processes
- Dedicated experimental validation is key
- Model development and more widespread utilization will follow swiftly from such campaigns

- On the horizon for future work:
  - Reactive model validation
  - Reactive filtering for large scale simulations
  - Representative cost-functions for optimization studies
  - Increased application to real engineering problems

Thank you