

CAESAR: Modelling of the Sorption-Enhanced Water Gas Shift Process for Pre-combustion CO_2 Capture

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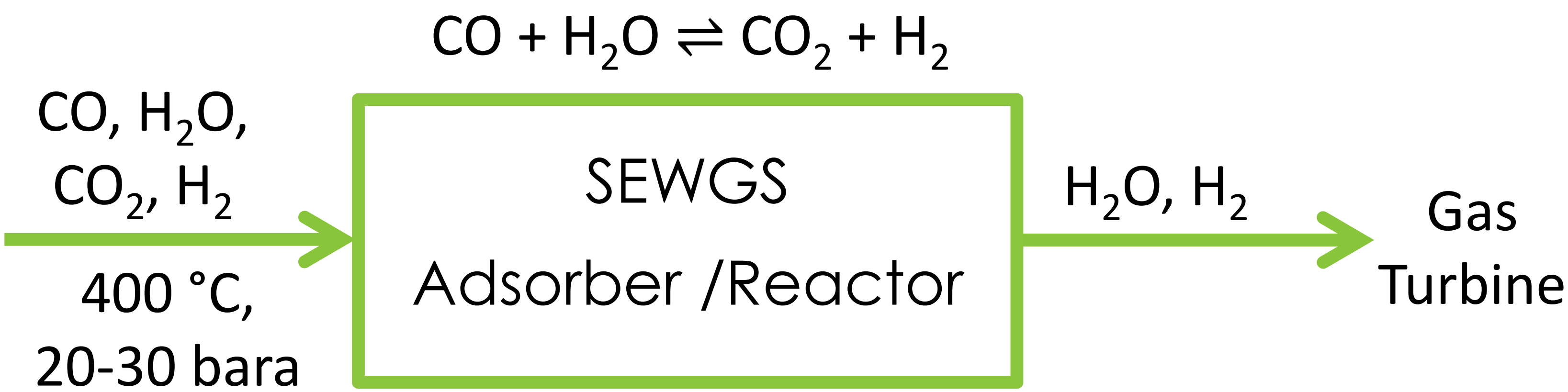
AIR PRODUCTS

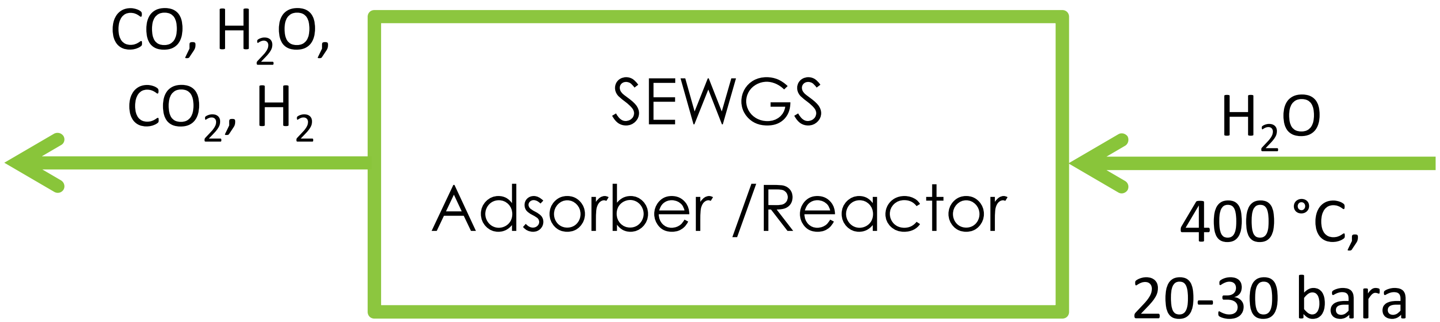
What is SEWGS?

- Sorption-Enhanced Water-Gas-Shift (SEWGS)
- Combines the Water-Gas-Shift reaction with sorbent material to simultaneously produce H_2 at high temperature whilst also capturing CO_2

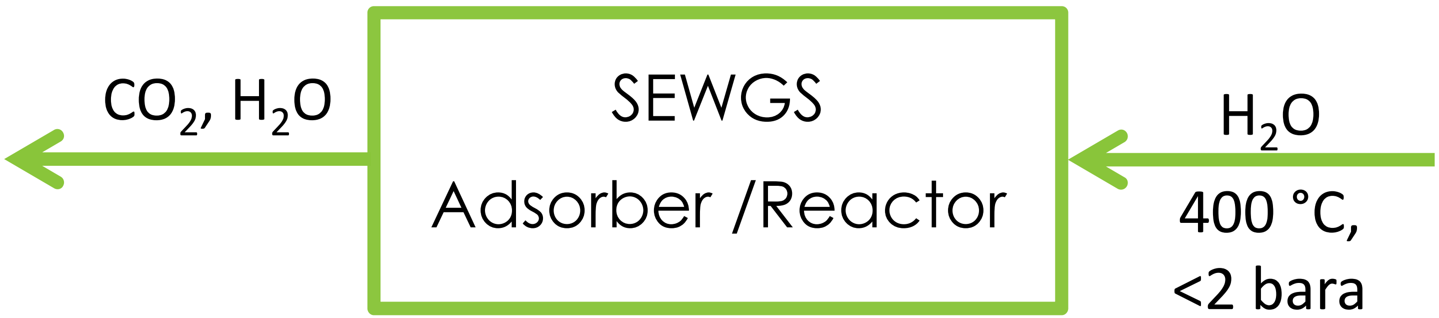


What is SEWGS?

- Before the CO_2 is regenerated from the sorbent, the vessel is **RINSED** using either steam or CO_2



- The CO_2 is regenerated from the sorbent by **PURGING** with low pressure steam



SEWGS and CAESAR

- Sorption-Enhanced Water Gas Shift (SEWGS)
  - Development started around 2000 by Air Products
  - CCP supported work
    - Material screening and technology feasibility study
  - CACHET
    - Construction and operation of test rig facilities
  - CAESAR
    - Material development, process optimisation, extension from natural gas to other feed-stocks

- CAESAR Consortium
  - Energy Research Centre of the Netherlands (ECN)
  - Air Products
  - SINTEF
  - Politecnico di Milano
  - BP

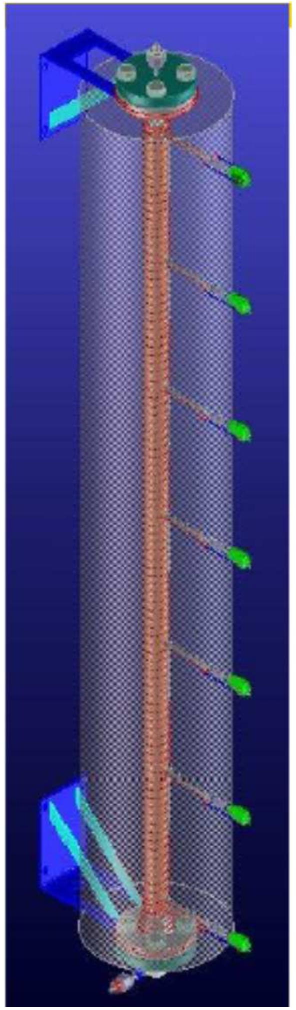
CAESAR Project

- Sorbent material used in previous studies was found not to be mechanically stable

- New material chosen for investigation in CAESAR
  - Physically more robust
  - Experimental data shows equivalent, if not better cyclic CO_2 capacity than original material

- Data collected on the sorbent material using various steady state and dynamic experiments
  - Gravimetric
  - Single column apparatus
  - Multi-column test rig

Test Rig Equipment



Single Column

2 metres tall

38 mm internal diameter

Multi-Column

6 vessels

6 metres tall

38 mm internal diameter

CAESAR: Scope of Work - Modelling

- Unfortunately, test rig data is not exactly representative of a full scale system
  - Heat management
  - Different numbers of vessels may be required
  - Different piping connections
  - Actual operating conditions may be different

- Therefore a full dynamic model of the SEWGS process is very useful for a number of reasons
  - Predict actual full-scale operation
  - Easier optimisation of the process
  - Evaluate benefit of further material development

- However model development is not a trivial task

Adsorption Process Modelling

- Air Products has developed extensive modelling capabilities for adsorption processes over several decades
  - PSA – H_2 production
  - VSA – O_2 production
  - TSA – Air drying

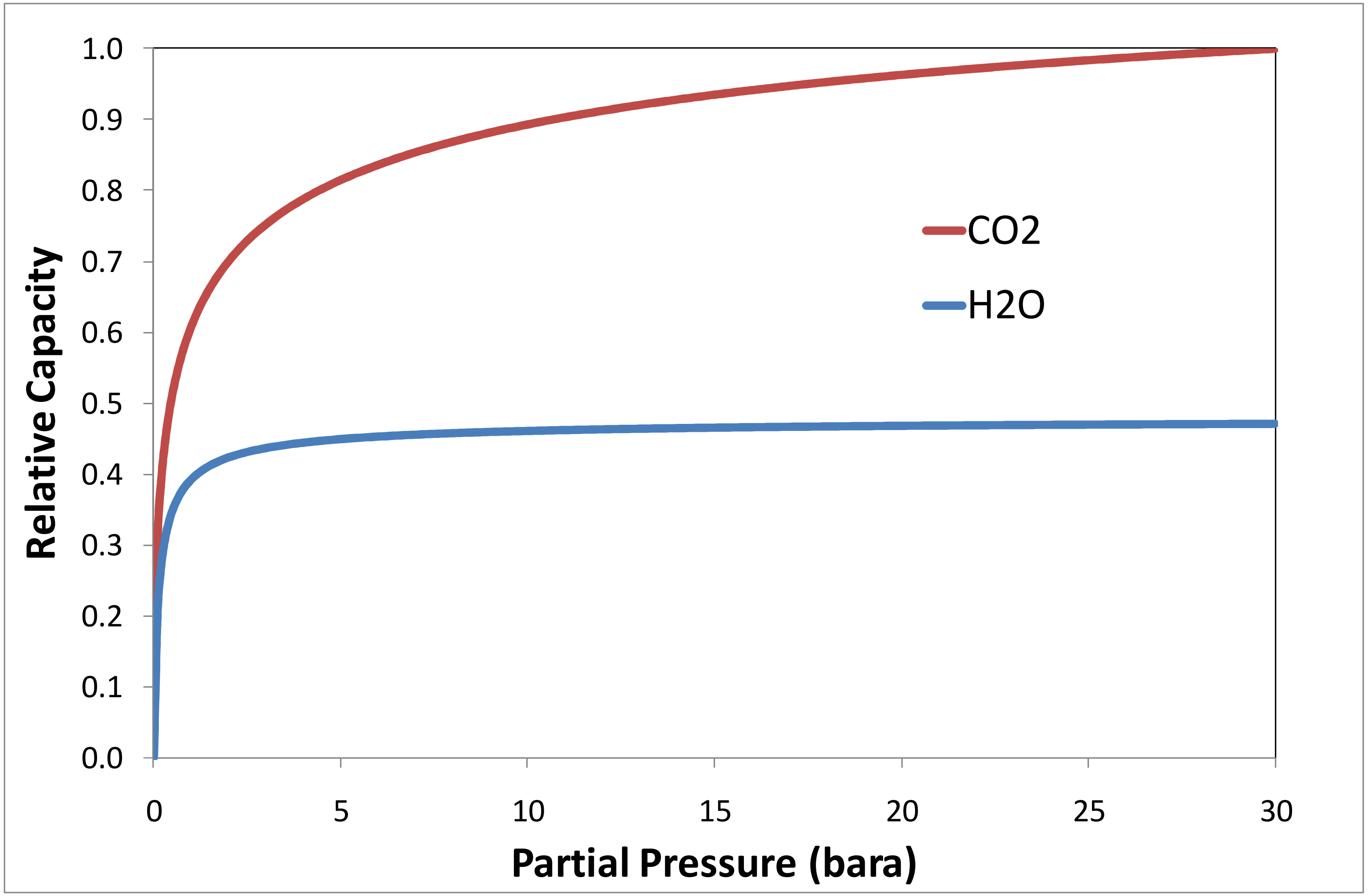
- SEWGS has unique challenges
  - Much higher temperature than normal
    - 400 °C compared with typically 40 °C
  - Includes WGS reaction
  - Sorbent does not behave like traditional materials

Adsorption Process Modelling

- Standard modelling building blocks still required
  - Overall heat and mass balance for the process
  - Material balances for all components
  - Momentum balance – i.e. Pressure drop
  - Equation of state (Ideal gas law)

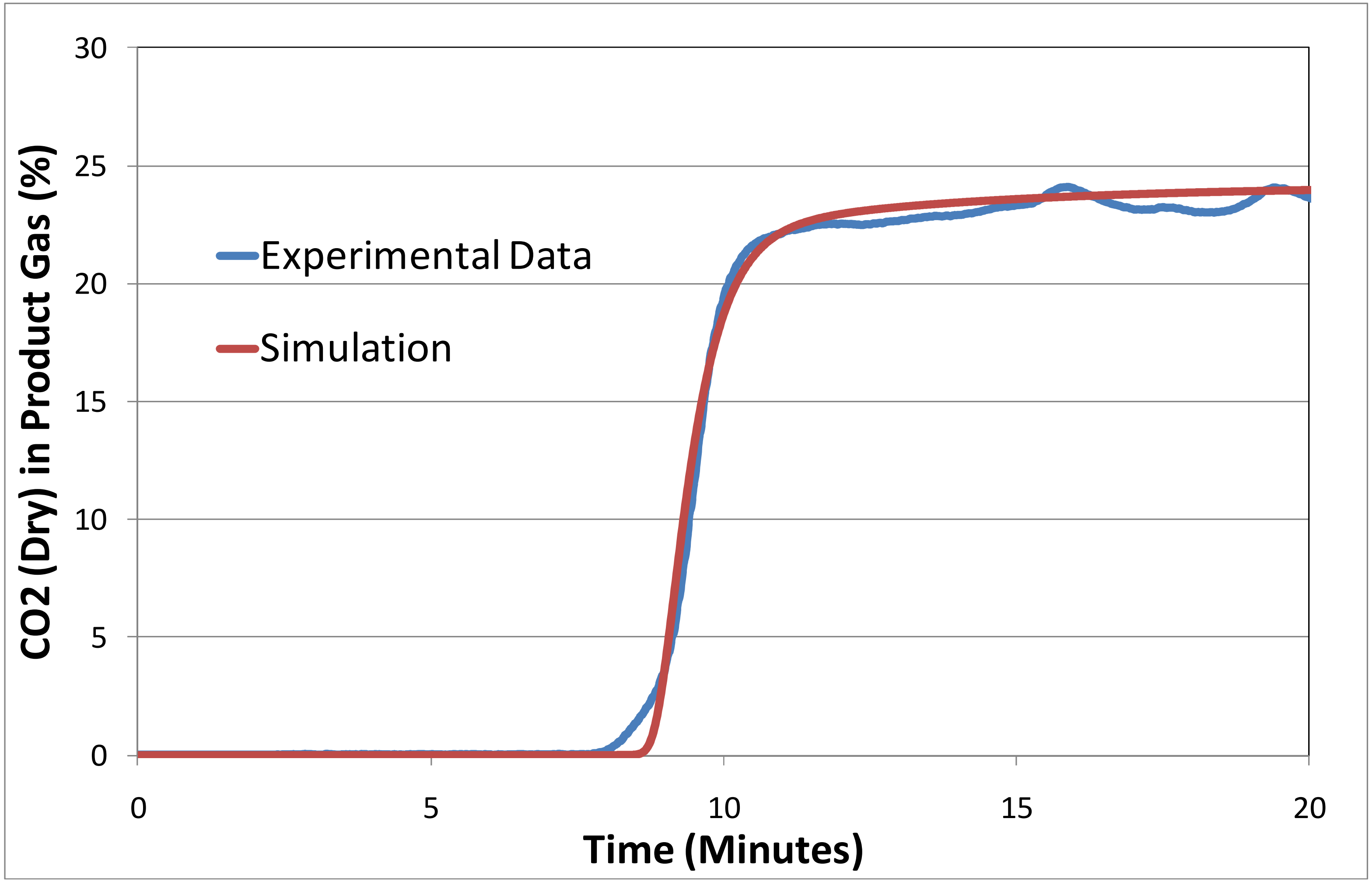
- Additional challenges
  - Small test rig equipment has large pipe volumes
  - Inclusion of reaction terms
    - Assumed always close to equilibrium
  - Accurate model of the sorbent required

Pure Component Isotherms (400 °C)



- Most of the capacity change is at low partial pressures

Breakthrough Experiment (400 °C)



- Adsorption mass transfer resistance of <1 second

Single Column Cyclic Experiments

Experimental Test Case	Cycle-Average Mass Transfer Resistance (s)
Steam-Rinse Test 1	95.2
Steam-Rinse Test 2	94.3
Steam-Rinse Test 3	120.5
Steam-rinse Test 3 (Repeat)	126.6
CO_2-Rinse	109.9

- Rate of desorption is much slower than adsorption

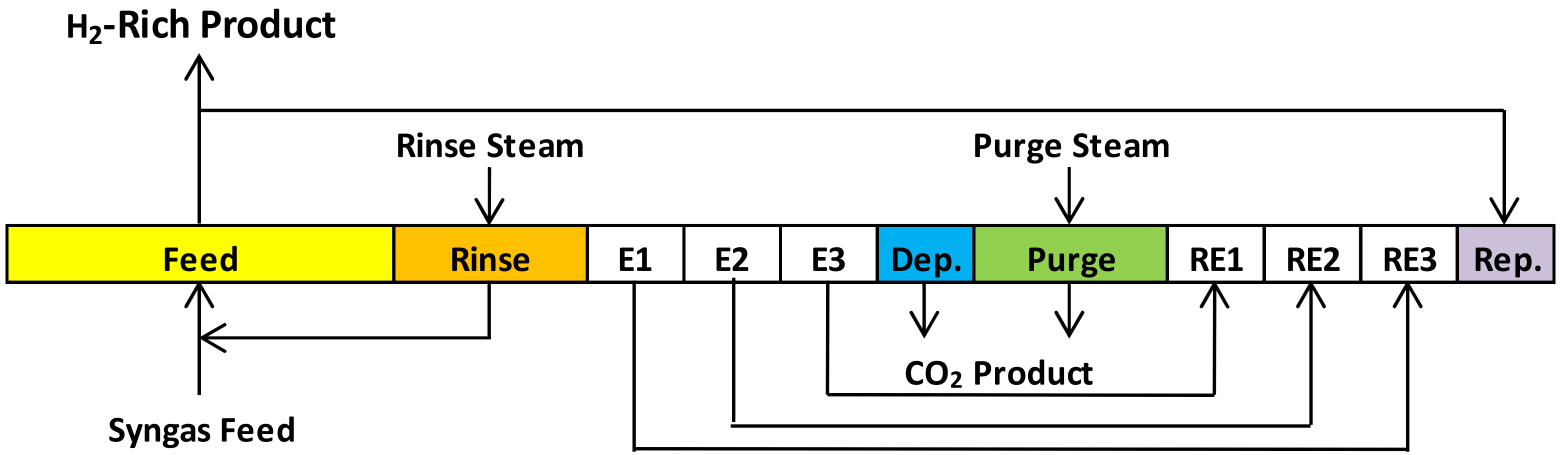
Full-Scale Design

- Example natural gas and coal based feed-stocks

	Natural Gas	IGCC
CO_2 (%)	12	24
CO (%)	5	6
H_2 (%)	42	35
H_2O (%)	8	31
N_2 (%)	32	3
Others (%)	1	1

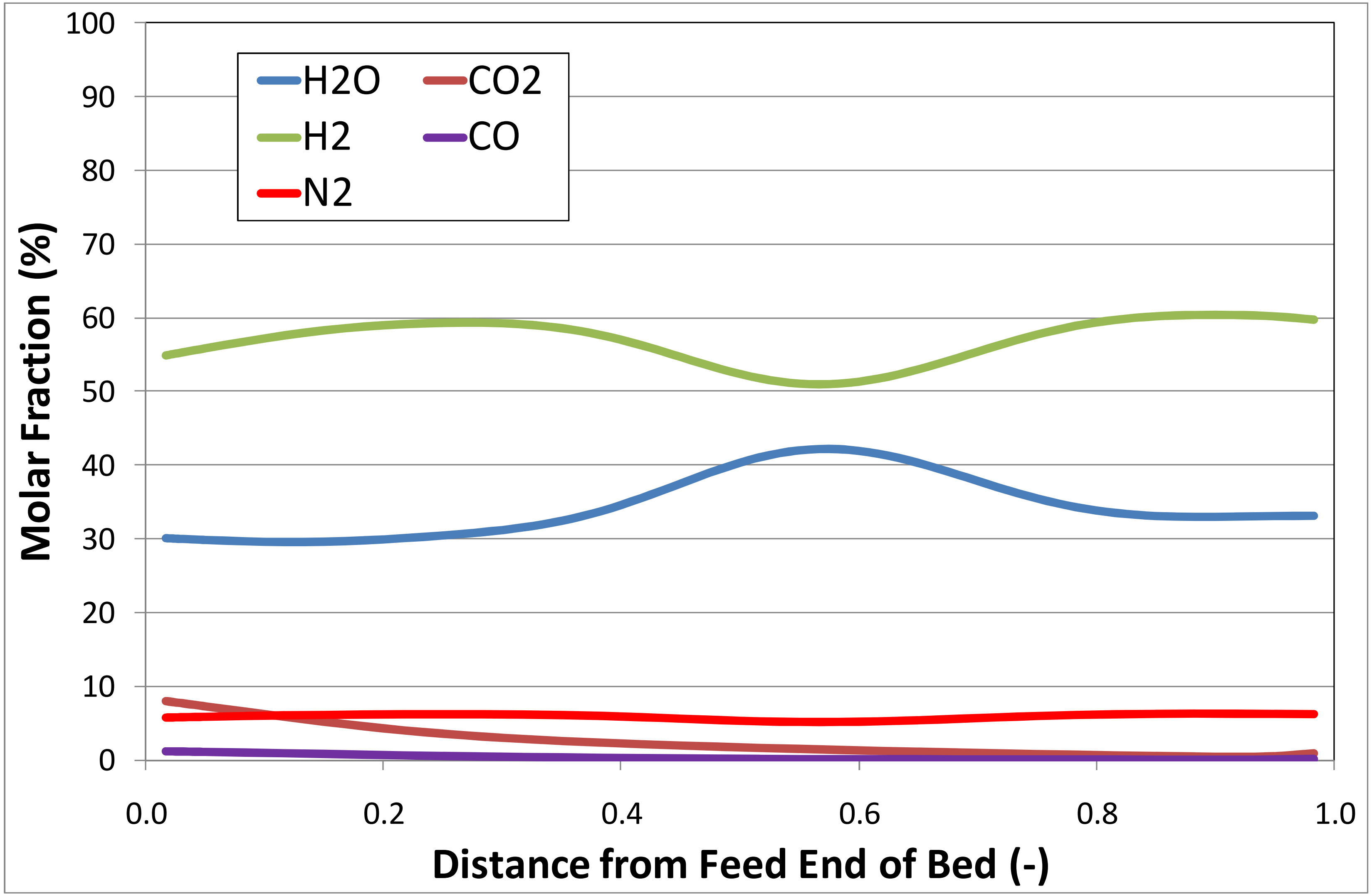
- Optimisation parameters available for investigation
  - Feed conditions, Bed length, Number of trains, Cycle time, CO_2 capture rate, CO_2 purity, Purge pressure, Cycle sequence, Sorbent physical properties, etc…

Full-Scale Design – Example Cycle

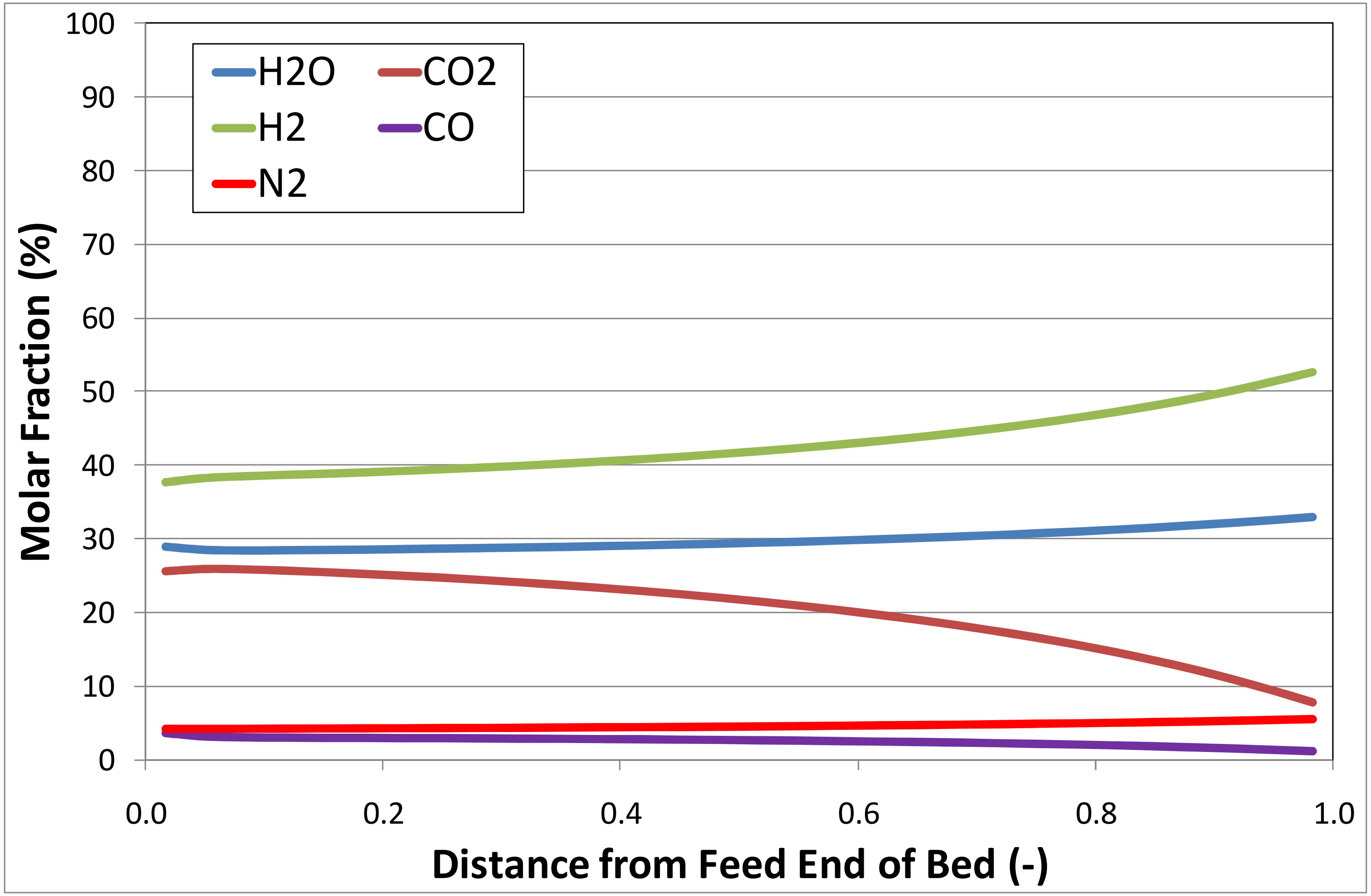


Sorption Vessel																
1	Feed				Rinse		E1	E2	E3	Dep.	Purge		RE1	RE2	RE3	Rep.
2	RE3	Rep.	Feed				Rinse		E1	E2	E3	Dep.	Purge		RE1	RE2
3	RE1	RE2	RE3	Rep.	Feed				Rinse		E1	E2	E3	Dep.	Purge	
4	Purge		RE1	RE2	RE3	Rep.	Feed				Rinse		E1	E2	E3	Dep.
5	E3	Dep.	Purge		RE1	RE2	RE3	Rep.	Feed				Rinse		E1	E2
6	E1	E2	E3	Dep.	Purge		RE1	RE2	RE3	Rep.	Feed				Rinse	
7	Rinse		E1	E2	E3	Dep.	Purge		RE1	RE2	RE3	Rep.	Feed			
8	Feed		Rinse		E1	E2	E3	Dep.	Purge		RE1	RE2	RE3	Rep.	Feed	

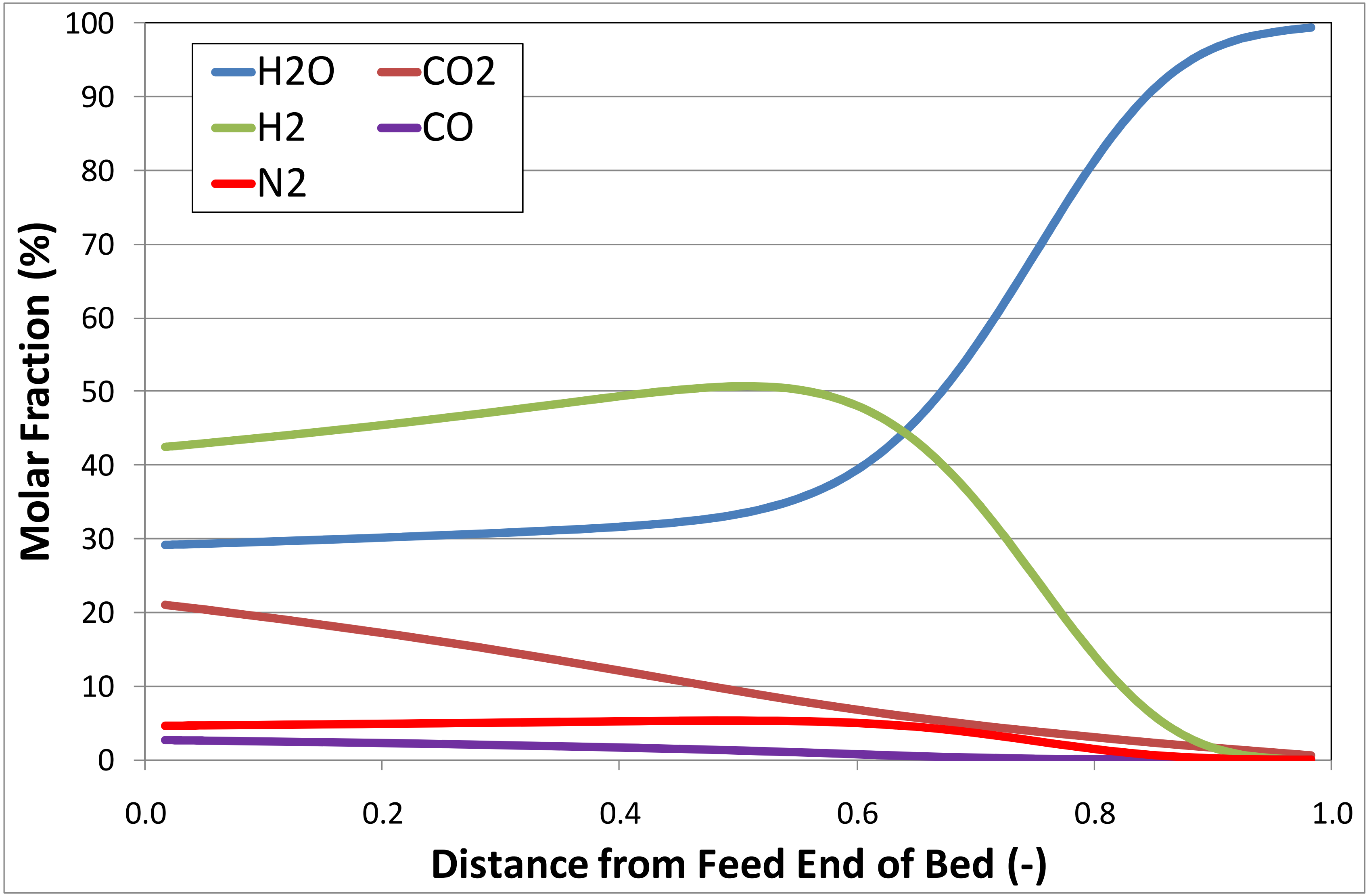
Example Cycle Modelling – Start of Feed



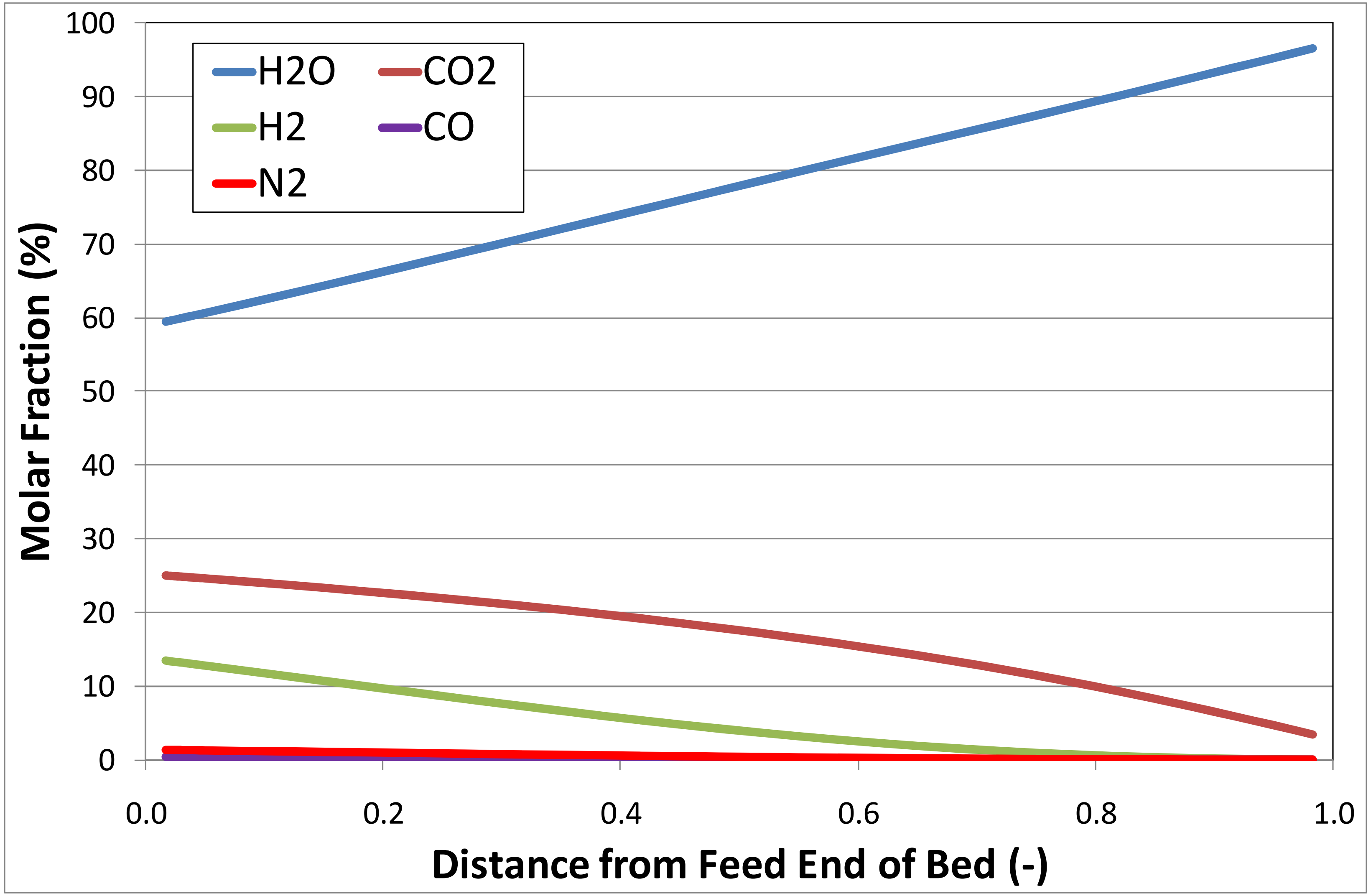
Example Cycle Modelling – End of Feed



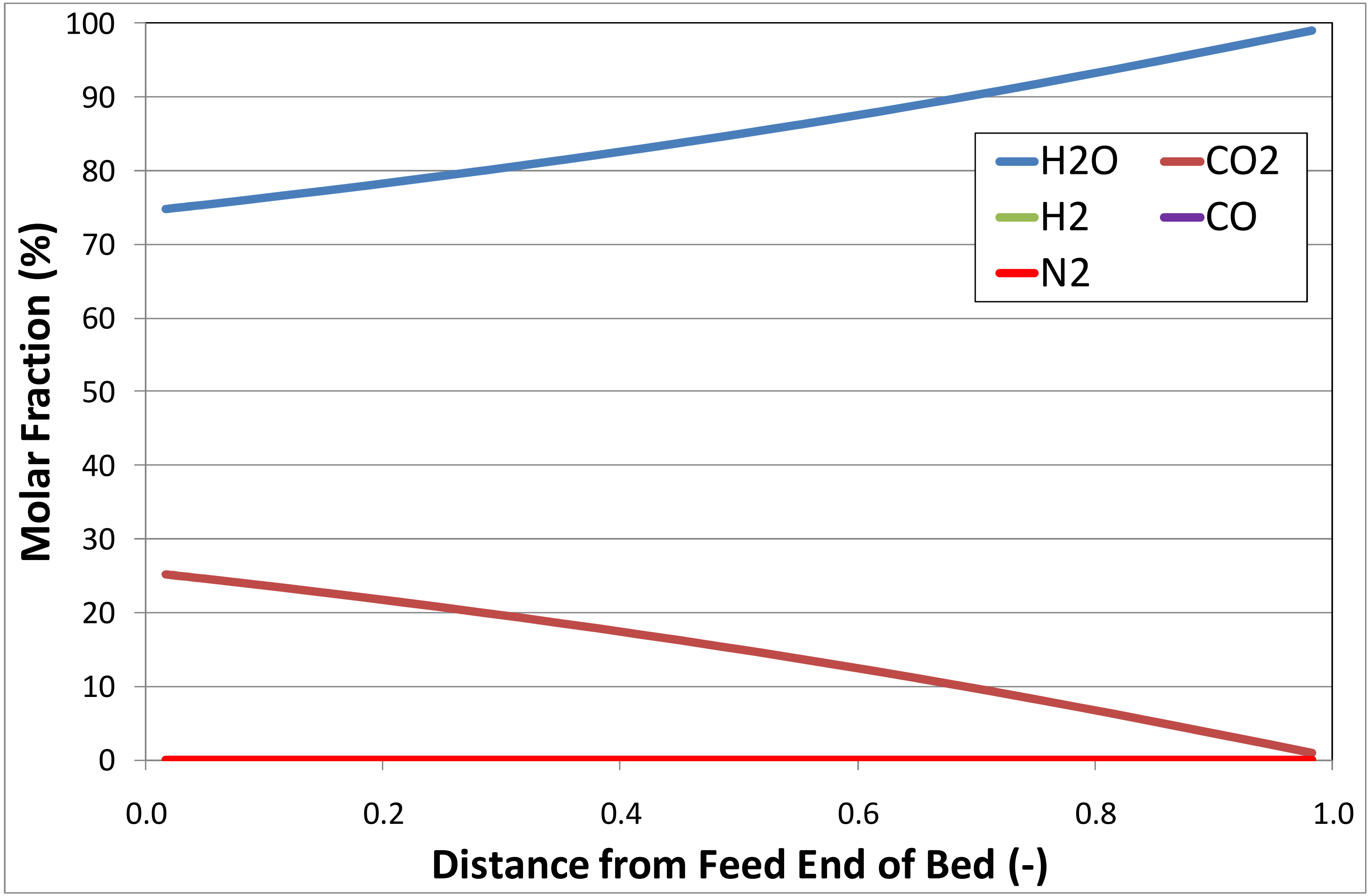
Example Cycle Modelling – Start of Rinse



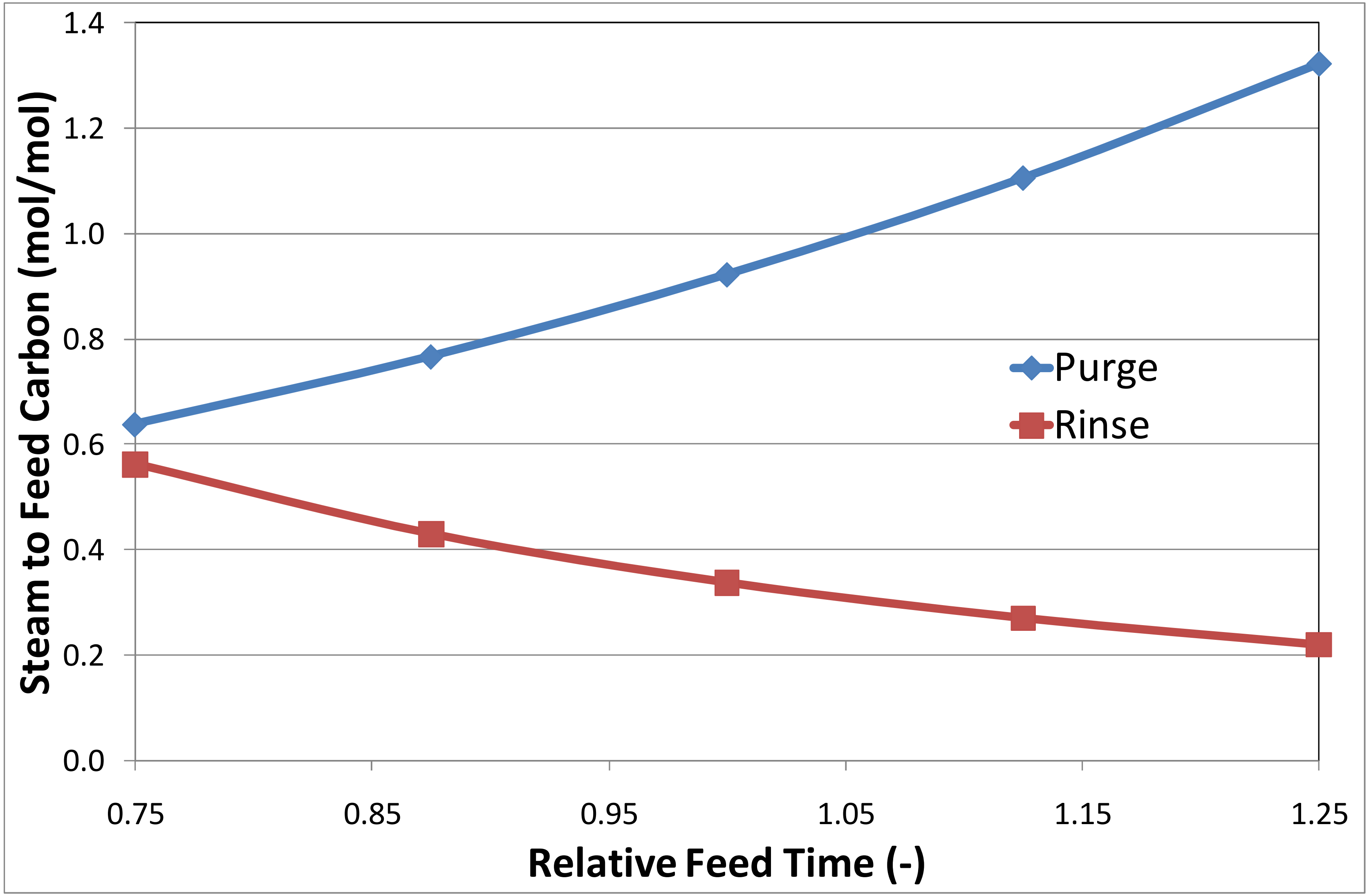
Example Cycle Modelling – End of Rinse



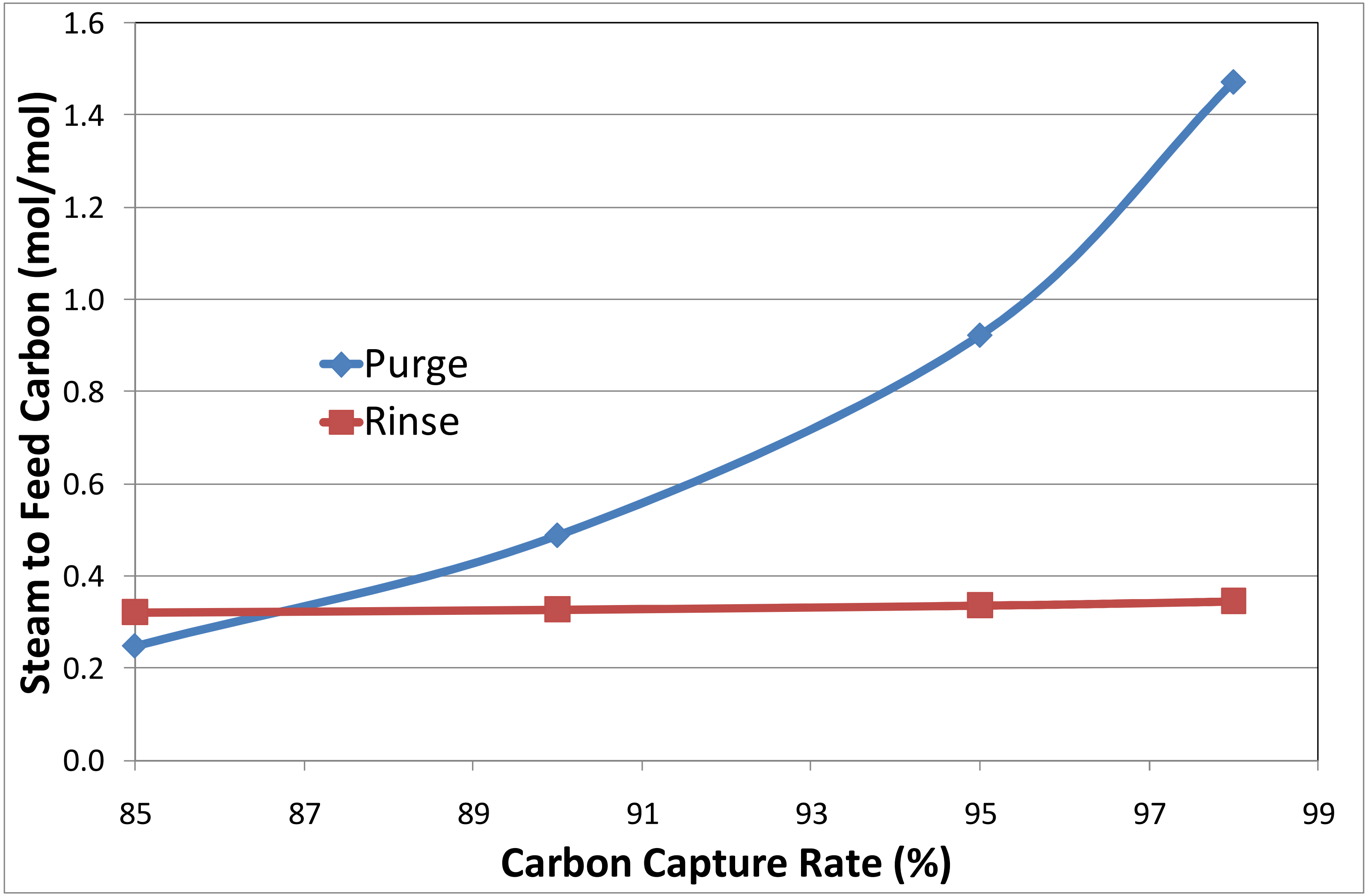
Example Cycle Modelling – End of Purge



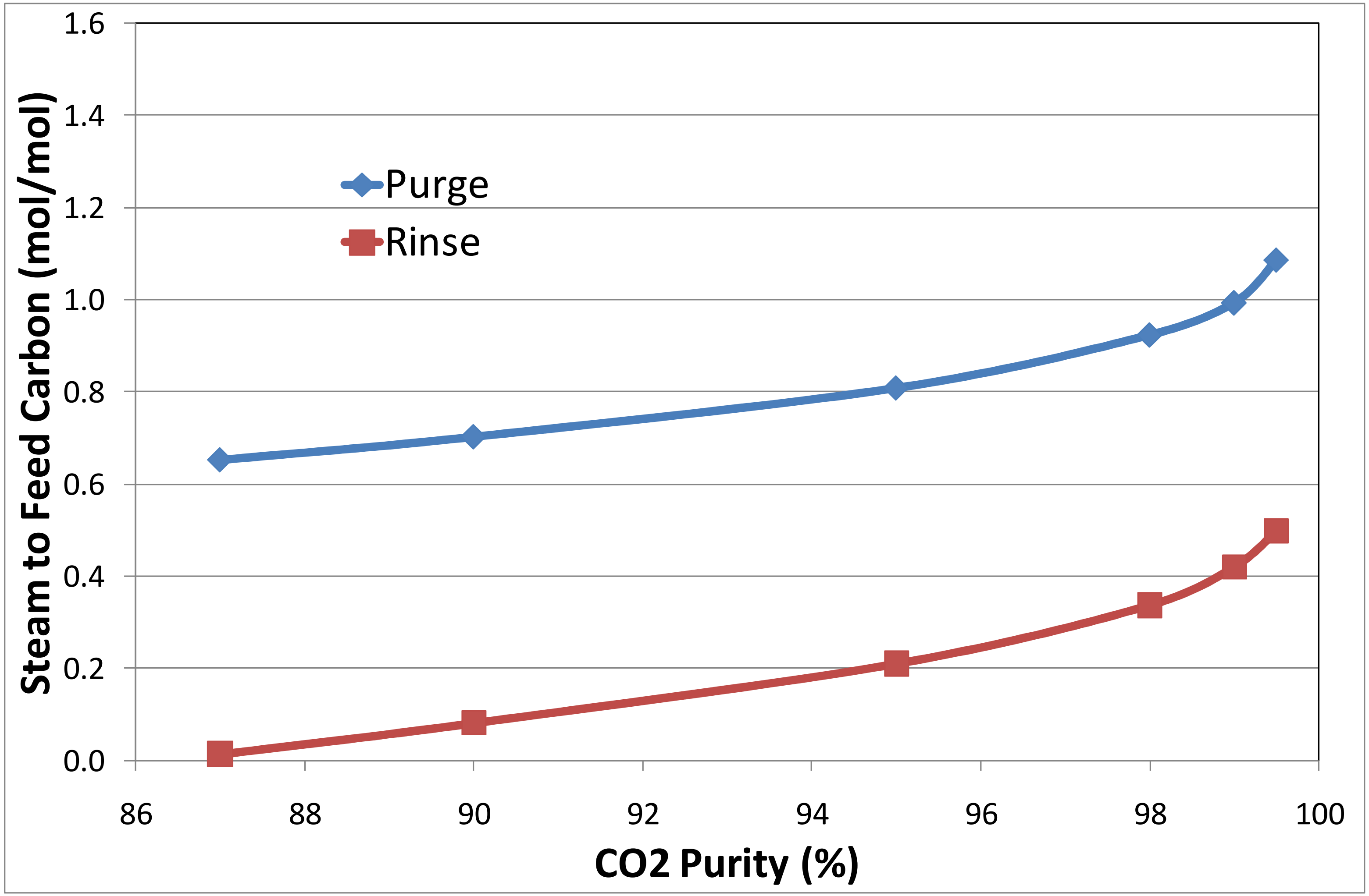
Cycle Time – IGCC Case



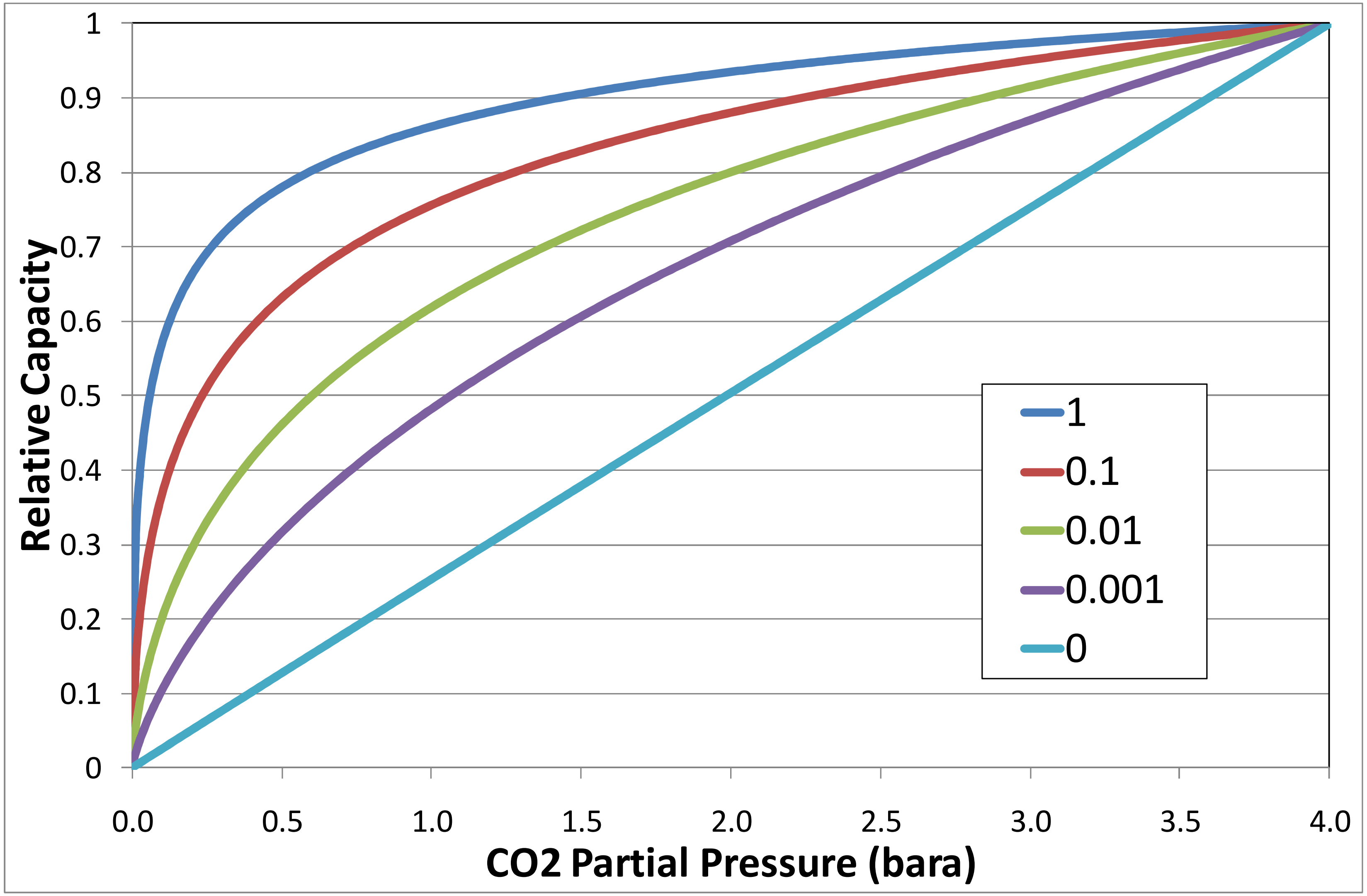
Carbon Capture Rate – IGCC Case



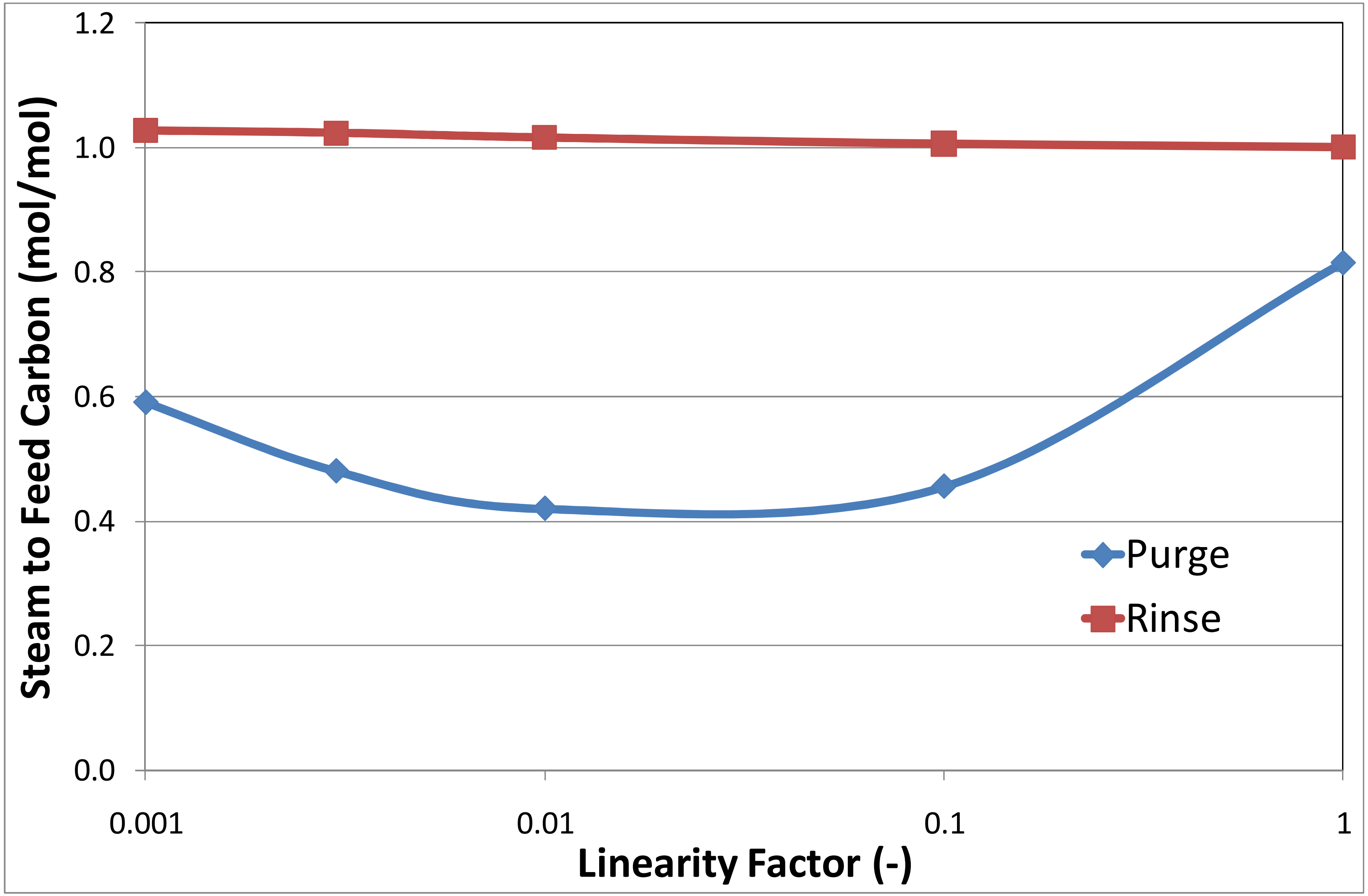
CO_2 Purity – IGCC Case



Material Development – Isotherm Shape



Linearity Factor – Natural Gas Case



Summary

- Within CAESAR, a model has been created for the SEWGS process based on a new sorbent material
- Predicted performance versus breakthrough and cyclic experiments in a single column unit show reasonable agreement over a range of conditions
- This model has been used to estimate the performance of a full-scale unit to evaluate changing different operating parameters
- Interesting results in regard to improved material formulation have arisen
- Next step is to optimise the SEWGS process as part of the entire power plant flow sheet
  - Preliminary results are encouraging

Summary

- The model needs further validation and to be improved based on cyclic data obtained from a larger multi-column test rig at ECN

- Key areas for improved modelling are:
  - A better understanding on kinetic versus equilibrium constraints affecting the rate of desorption of CO_2
  - Improved modelling of connecting pipes (particularly if high purity CO_2 is targeted)

Thank you

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