Solid Oxide Fuel Cell Research at the University of Waterloo

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Introduction

- UW and CANMET have been involved in research on clean energy from fossil fuels for many years/decades
- Focus in recent years has been on CO_2 mitigation technologies from fossil-fuel based power plants
  - Higher efficiency power plant
  - CO_2 capture and storage (energy intensive, costly)
- SOFC appears very promising in terms of efficiency and reduced cost of capturing CO_2

SOFC Research at Waterloo

- SOFC Research at Waterloo started in 2001
  - 2 published research papers and 1 about to be submitted
- Main activity: computer simulation
  - Process simulation (Aspen Plus)
  - Fundamental single cell modeling (Matlab, Femlab)
- Current focus:
  - SOFC power generation from coal/natural gas
  - Effect of mixtures of CO/H_2 on cell performance
  - CO_2 capture from SOFC systems
- Collaboration with CANMET Energy Technology Centre

SOFC Research at Waterloo - Personnel

- Supervisors:
  - Eric Croiset, assistant professor
  - Peter Douglas, professor
  - Michael Fowler, lecturer
  - Evgueniy Entchev, research scientist, CANMET
- Graduate students:
  - Rapeepong Suwanwarangkul, Ph.D. candidate
  - Wei Zhang, M.A.Sc. candidate
  - Leslie Backham, M.A.Sc. candidate

Overall Research Objective

Investigate/develop SOFC-based power generation processes that can simultaneously:

- achieve high electricity generation efficiencies
- generate pure CO_2 with minimum energy/cost penalty

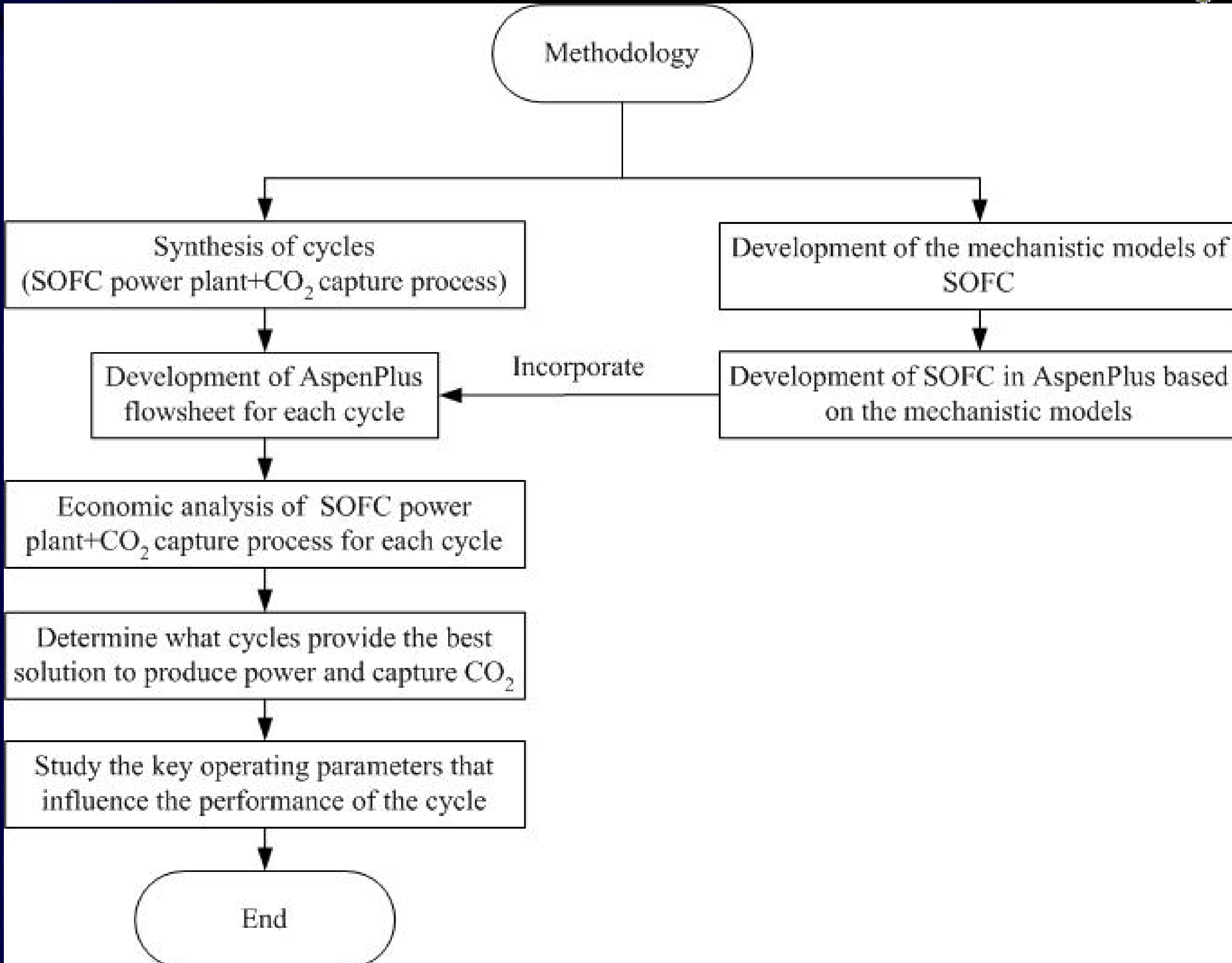
Key Issues to be Investigated

- Key operating variables:
  - fuel composition (Especially H_2 and CO mixtures)
  - utilization factor
  - temperature
  - pressure
  - operating cell voltage or current density
- Cycle options for CO_2 capture and concentration
  - oxygen enrichment, chemical absorption
- Efficiency and cost

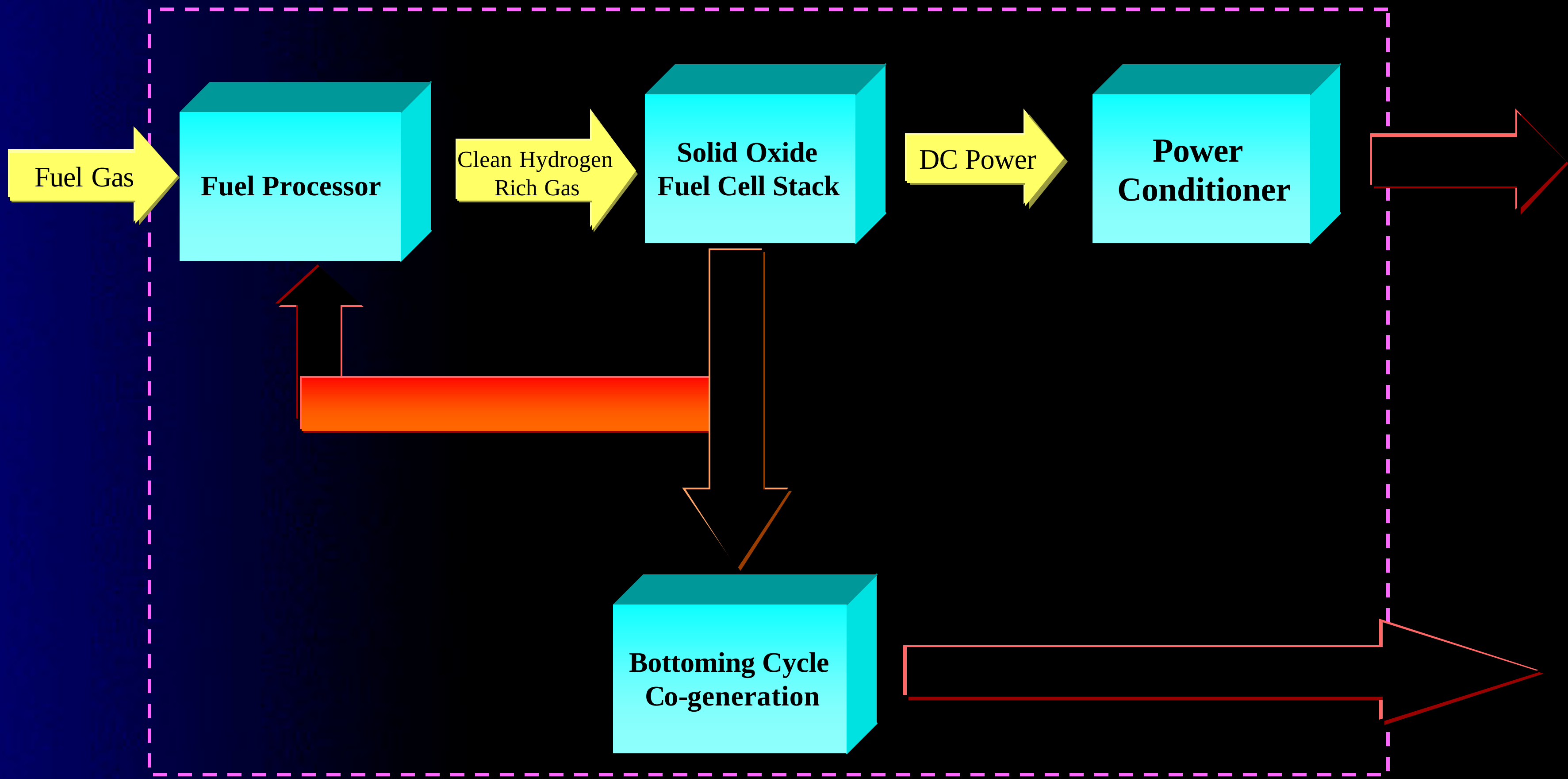
Overall Research Methodology

- Synthesis:
  - examine potential SOFC-based power generation/CO_2 capture cycles at conceptual level
- SOFC cycle models in Aspen Plus:
  - develop SOFC (empirical) and process cycles models into Aspen Plus, allowing for integration, optimization and, eventually, costing
- Mechanistic Model
  - develop a fundamental model to simulate fuel cell performance over a wide range of operating conditions, fuel compositions, and cell designs

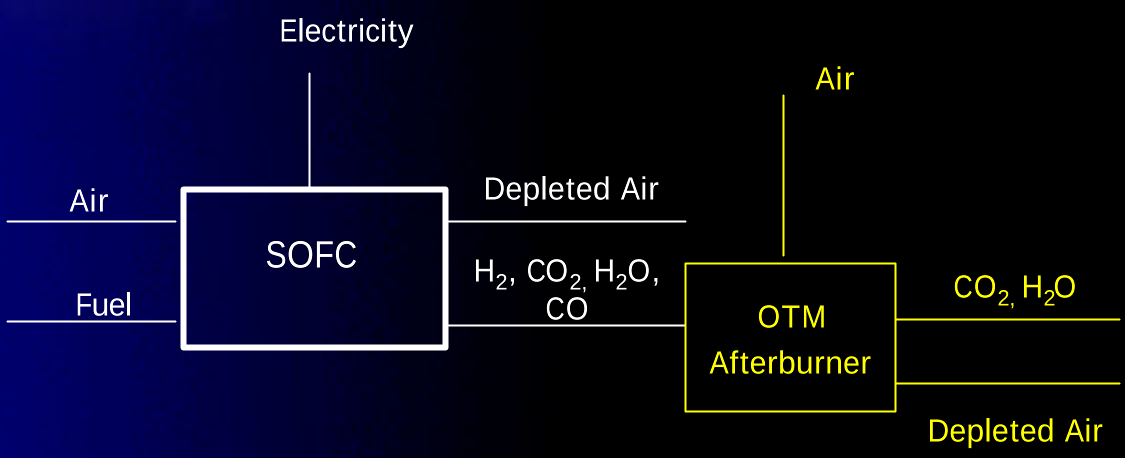
Overall Research Methodologies (Cont'd)

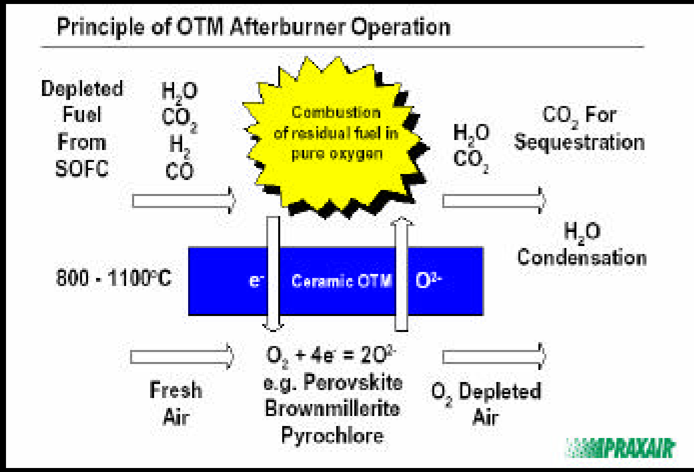


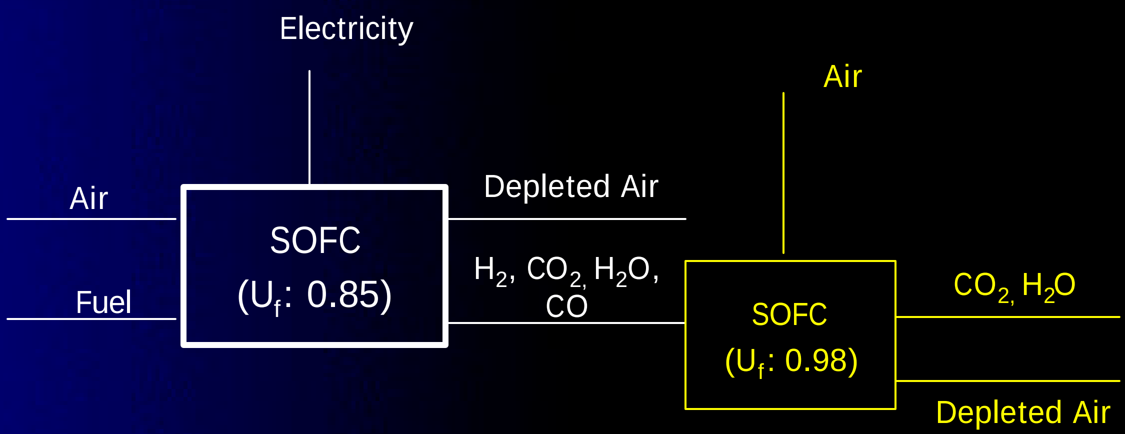
SOFC System Concept

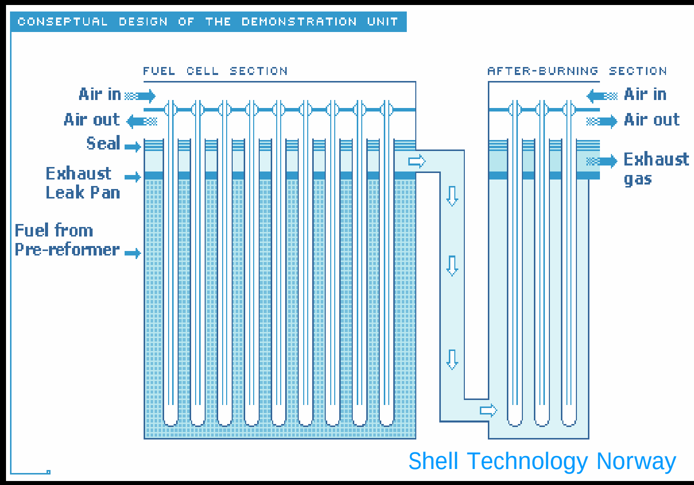


CO_2 Capture Using SOFC

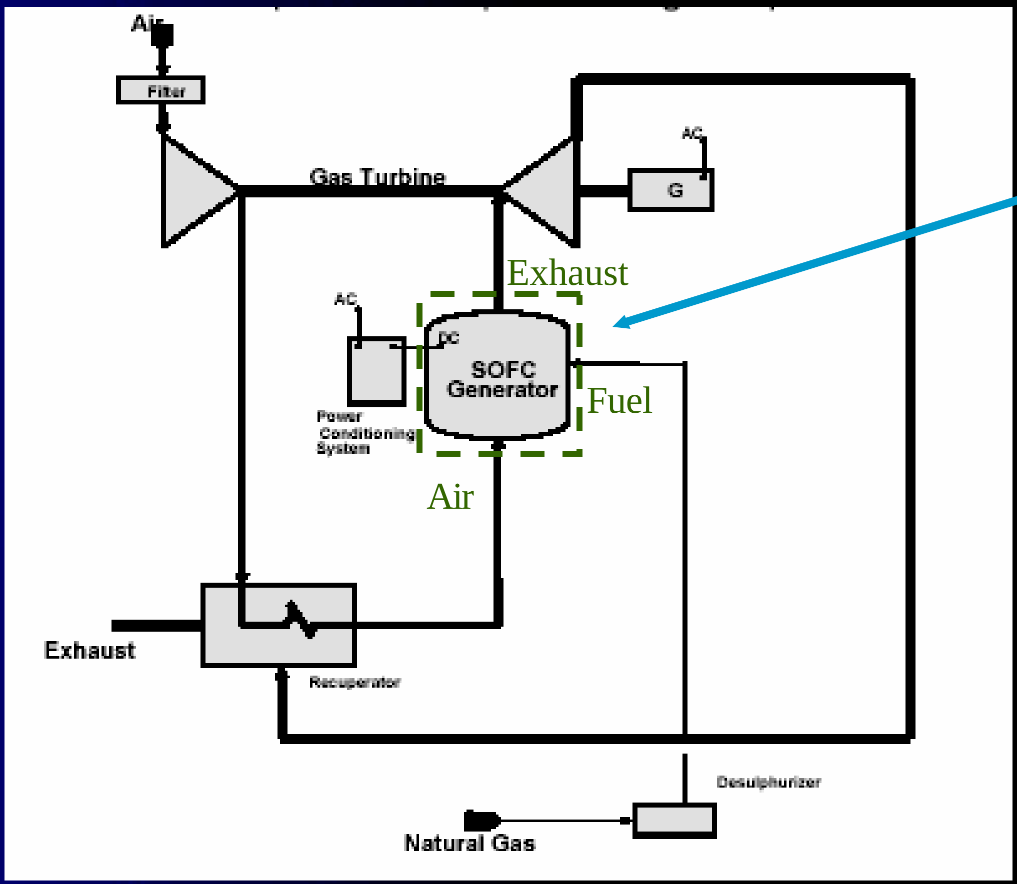








SOFC Modeling in Aspen Plus: Challenge

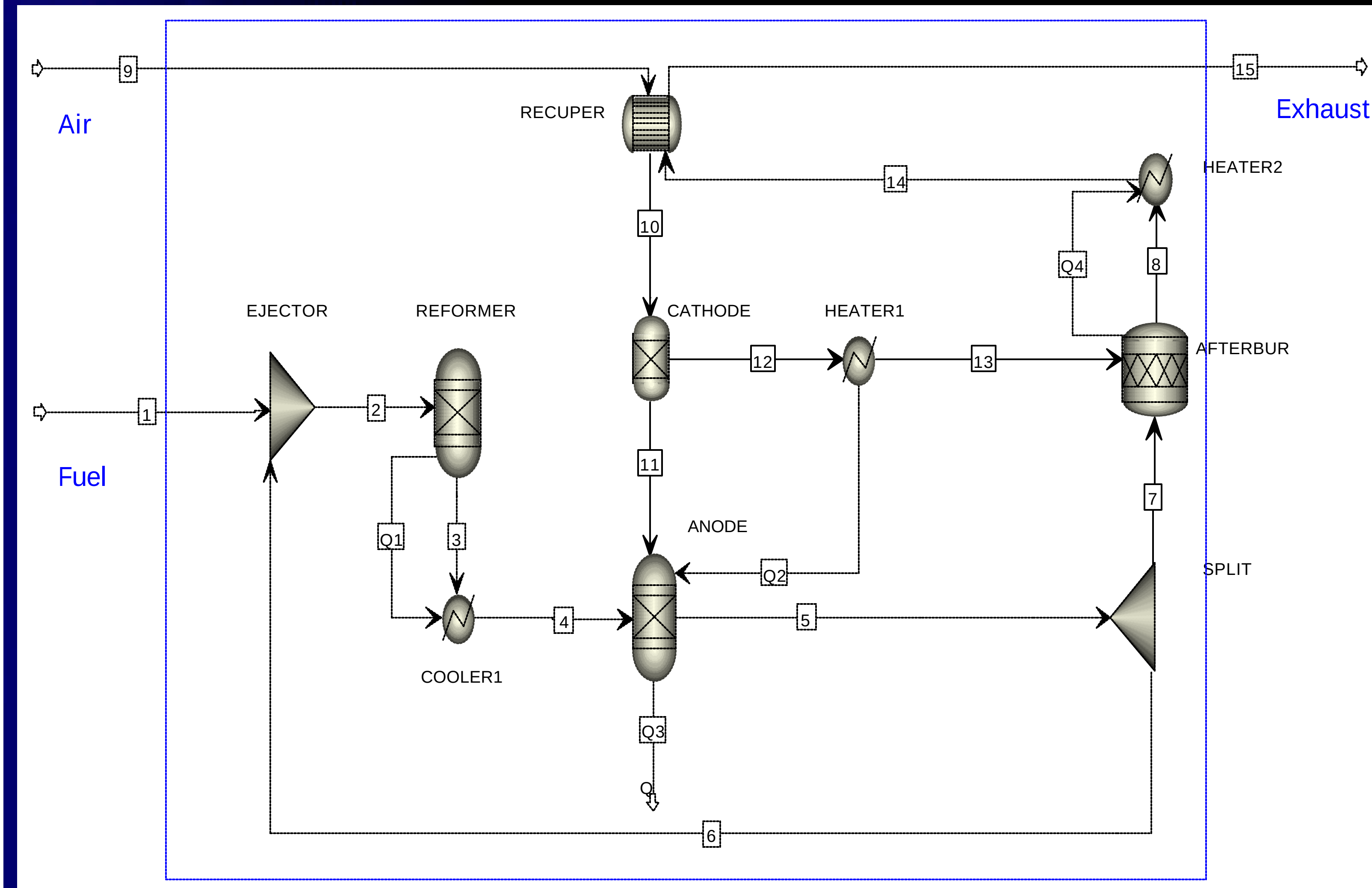


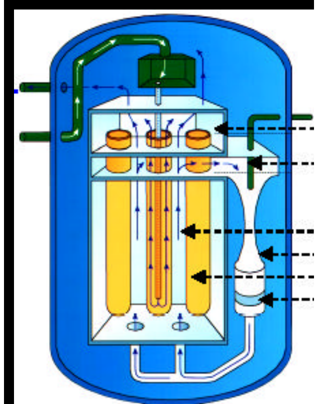
- How to develop a SOFC Model, which can
  - Predict the fuel cell performance accurately
  - Be implemented in Aspen Plus

SOFC Modeling in Aspen Plus: Approach

Common Approach	Our Approach
▪ Develop a complete SOFC stack model in a programming language such as Fortran or C++	▪ Incorporate a series of fuel cell performance curves (expressed by semi-empirical equations) into Aspen Plus
▪ Link it to a commercial simulator (Aspen Plus, Hysis, ProII) as a user-defined model or subroutines.	▪ Develop the rest of SOFC using existing Aspen Plus unit operation models

Aspen Plus SOFC Model





Based on the Siemens-Westinghouse natural gas feed tubular internal reforming SOFC technology

Mechanistic Model - Objectives

- Develop an accurate cell-level model to predict steady-state cell performance and flue gas compositions
- Investigate the influence of cell design, microstructure and operating variables on steady-state cell performance and its flue gas compositions
- Develop the cell performance map based on operation of H_2 and CO mixtures
- Generate parameters for correlations used in the AspenPlus model

Parameters To Be Investigated

- Operating parameters
  - Inlet air and fuel temperature
  - Fuel and air utilization (U_f & U_a)
  - Inlet gas composition
  - Steam-to-carbon ratio
- Material parameters
  - Pore size
  - Porosity
  - Tortuosity factor
  - Composition of electronic/ionic conductors
- Design parameters
  - Cell geometry (length, width, etc.)
  - Electrode thickness
  - Electrolyte thickness

Mechanistic Model - Methodology

- Develop one- and two-dimensional mechanistic model of a single-cell SOFC considering H_2 and CO oxidations.
- Experimental setup and investigation
- Validation of the developed model
- Investigate the influence of cell design, microstructure and operating variables on steady-state cell performance and its flue gas compositions.
- Develop the cell performance map for mixtures of H_2 and CO

Experimental Setup and investigation

- Generate experimentally polarization curves for different situations

Example of proposed experimental plan

Fuel no.	Composition				$\frac{P(CO)}{P(CO)+P(H_2)}$	H_2:CO
	H_2 (%)	H_2O (%)	CO (%)	CO_2 (%)		
F1	80	20	0	0	0	1:0
F2	64.2	16.0	14.9	4.9	0.20	4:1
F3	38.8	9.7	38.8	12.6	0.50	1:1
F4	18.8	4.7	57.8	18.8	0.75	1:3
F5	0	0	75.5	24.5	1	0:1

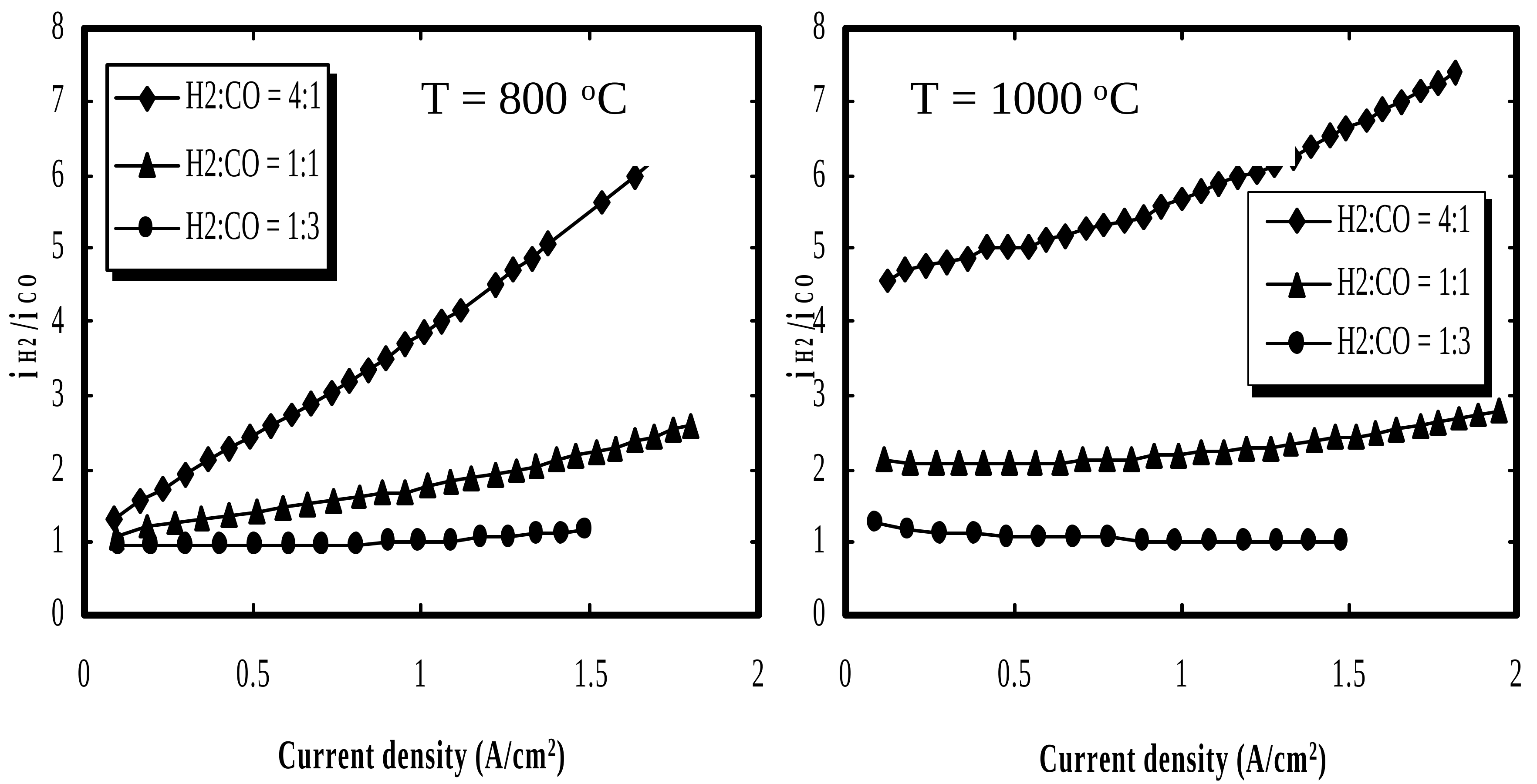
Preliminary Model Results- Model Validation

Relative consumption of H_2 to CO (**mol H_2 / mol CO**) for the same concentration of H_2 and CO

Temp.	UW model	Yasuda *et al.* experiment (1999)
800 °C	1.1-2.6	1.9-2.3
1000 °C	2.0-2.6	2.3-3.1

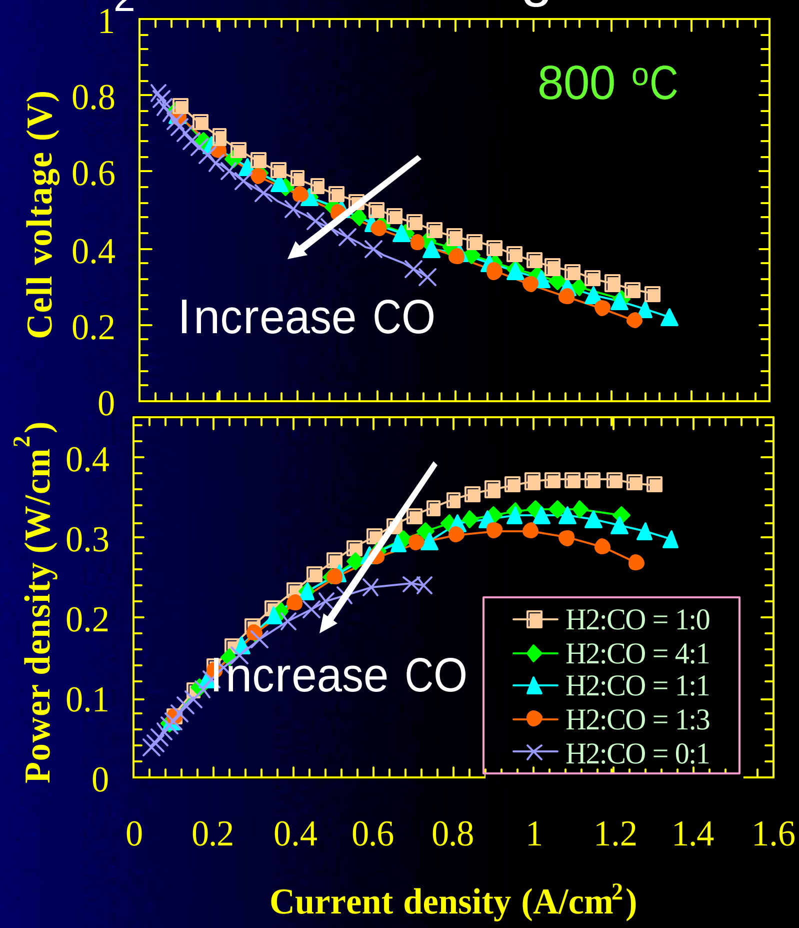
Model agrees with published experimental data

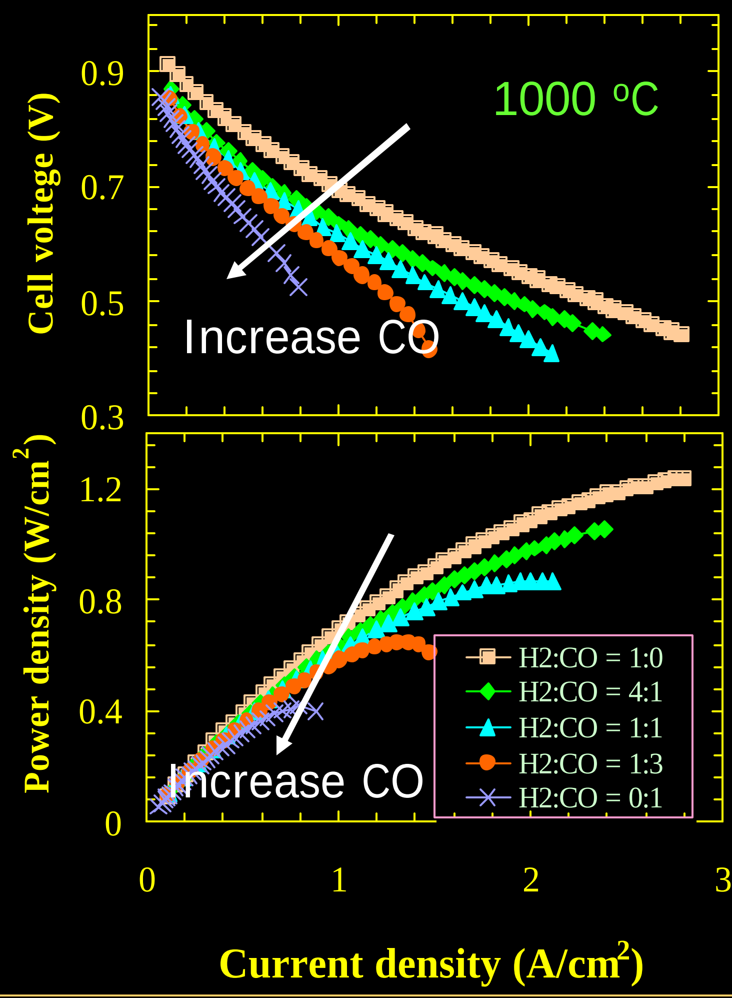
Preliminary Model Results- Effect of gas compositions



Preliminary Model Results-Effect of Gas Compositions

- SOFC performance decreases as CO concentration increases
- H_2:CO should be greater than 1:3

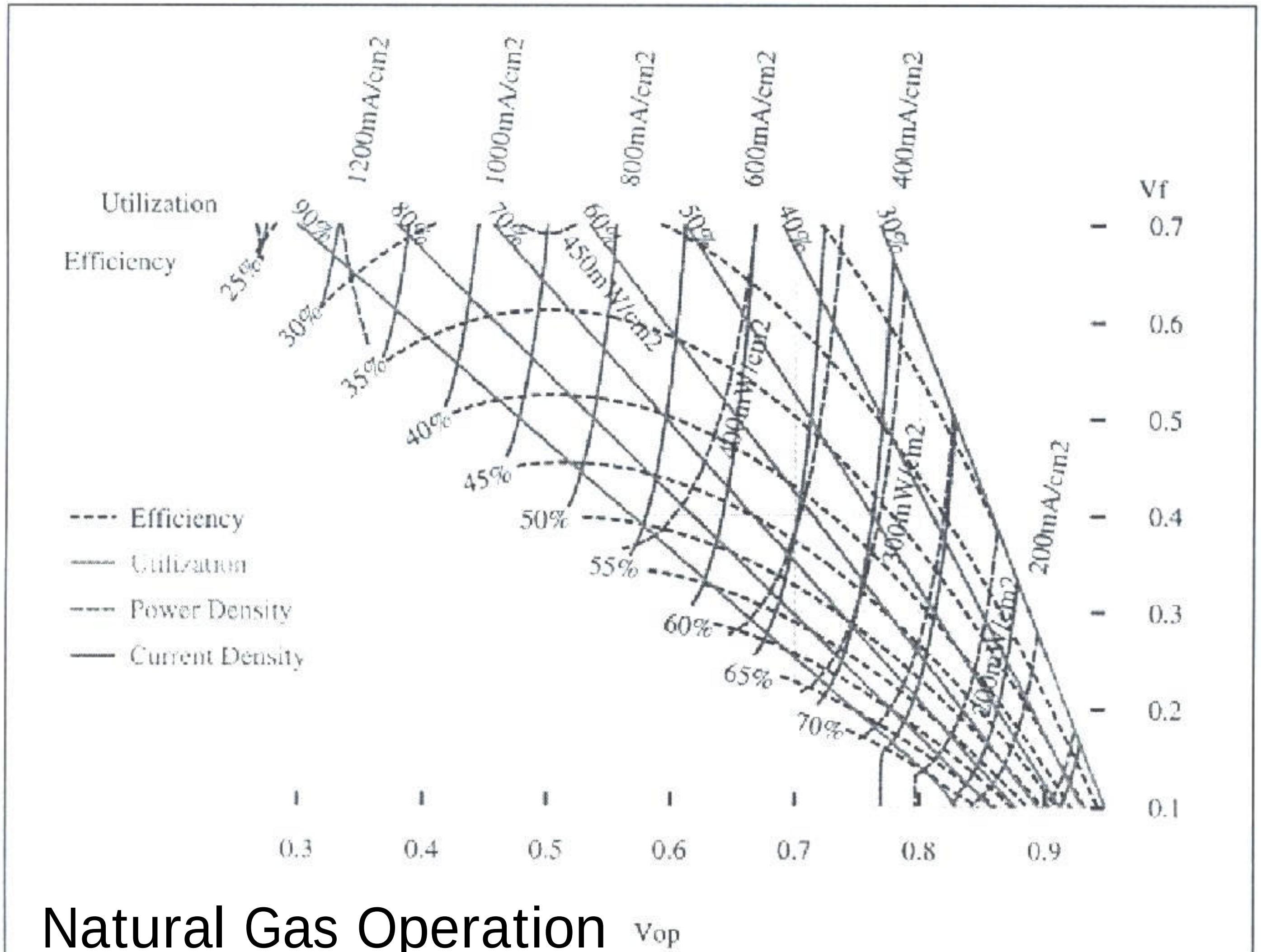




Achievements

- Two technical papers (One accepted, One to be submitted)
  - R. Suwanwarangkul, E. Croiset, M.W. Fowler, P.L. Douglas, E. Entchev and M. Douglas,“Performance Comparison of Fick’s, the Dusty-gas and the Stefan-Maxwell Models to Predict the Concentration Overpotential in a SOFC Anode”, J Power Sources, In press.
  - W. Zhang, E. Croiset , P.L. Douglas, M.W. Fowler, E. Entchev and M. Douglas, “Simulation of a Tubular Solid Oxide Fuel Cell Using AspenPlus Unit Operation Models”, to be submitted by end of April.
- One conference paper
  - R. Suwanwarangkul, E. Croiset, M.W. Fowler, P.L. Douglas, E. Entchev and M. Douglas, “Modeling of Anode-supported SOFCs Operating with H_2 and CO Feed Mixtures”, Proc. Of 8^{th} International Symposium on Solid Oxide Fuel Cells (SOFC-VIII), S.C. Singhal, M. Dokiya (Eds.), 1348-1357 (2003).

Cell Performance Map



Natural Gas Operation

SOFC Performance Map, H2O/CH4 = 2.0, 0.5 ohm-cm2

Design of Experiment

Gas comp.	U_f		U_a		S/C ratio		T_a		T_f	
	High	Low	High	Low	High	Low	High	Low	High	Low
F1	v	v	v	v			v	v	v	v
F2	v	v			v	v				
F3	v	v			v	v				
F4	v	v			v	v				
F5	v	v	v	v			v	v	v	v

- Each experiment must be performed 3 times.
- Interest experimental data:
  – Cell power
  – Exit gas compositions
  – Fuel and air flowrate
  – Exit fuel and air temperature