CSCHE 2017

Modeling and Simulation of Integrated Methane Reforming and Nuclear Heat systems

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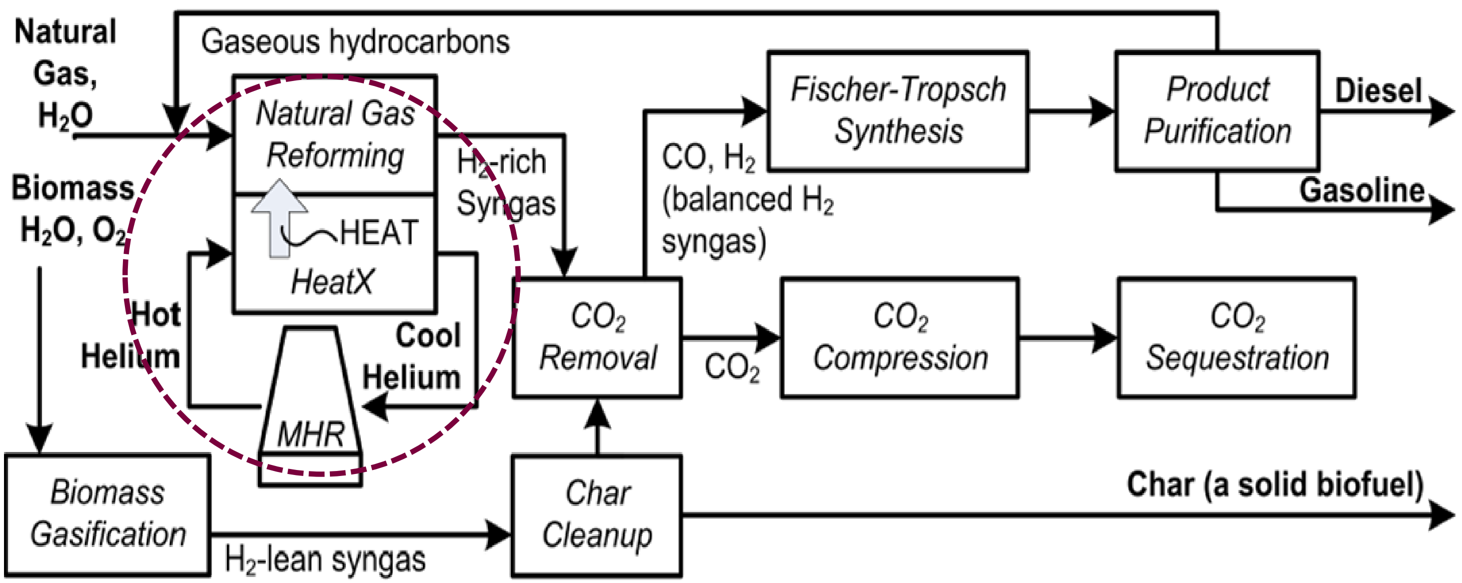
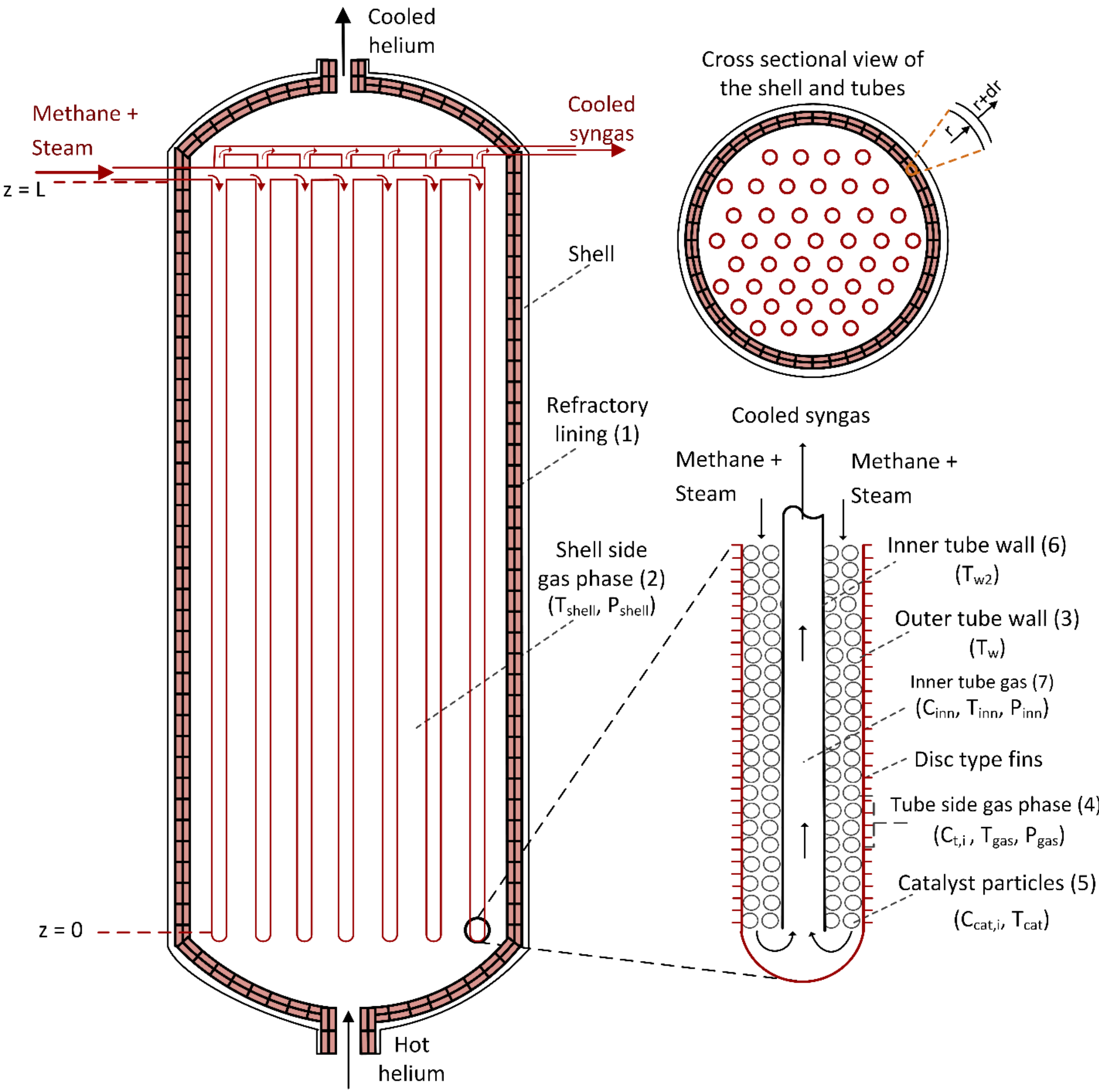
Introduction

- Global pressure to reduce GHG emissions
- High demand for the liquid fuels
- Biomass is a sustainable feedstock and abundant in Ontario
- Advantages of nuclear heat integration:
  - High efficiency
  - Zero CO_2 emissions
- Steam Methane Reforming (SMR) process is highly energy intensive
- Integrated nuclear heat/SMR process requires a detailed analysis



Integrated HTGR/Steam Methane Reforming (SMR) system



Model of the integrated High Temperature Gas-cooled Reactor (HTGR)/SMR system:

- Is 2 dimensional and dynamic
- Is multi-scale, considering:
  - Bulk gas effects
  - Spatial differences within the catalyst particles
- Is based on first principles
- Contains seven sub-models
- Is a set of PDAE
- Implemented in gPROMS software package

SMR reactions:

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

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

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

HTGR coolant temperature: 900-950 °C

Model Fitting Using Two Pilot Scale Facility Design Data

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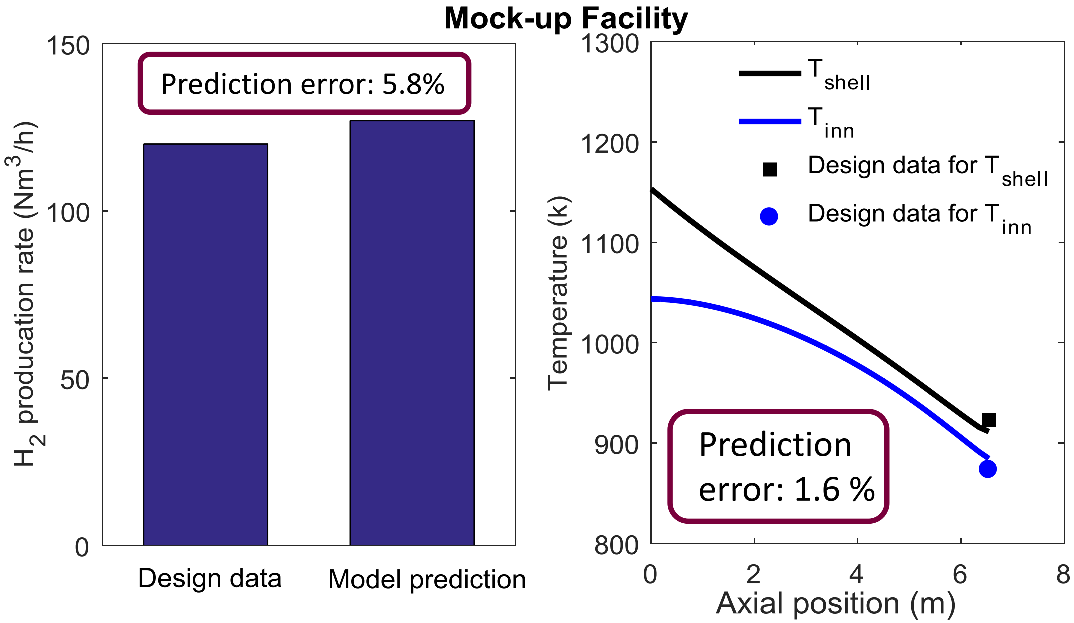
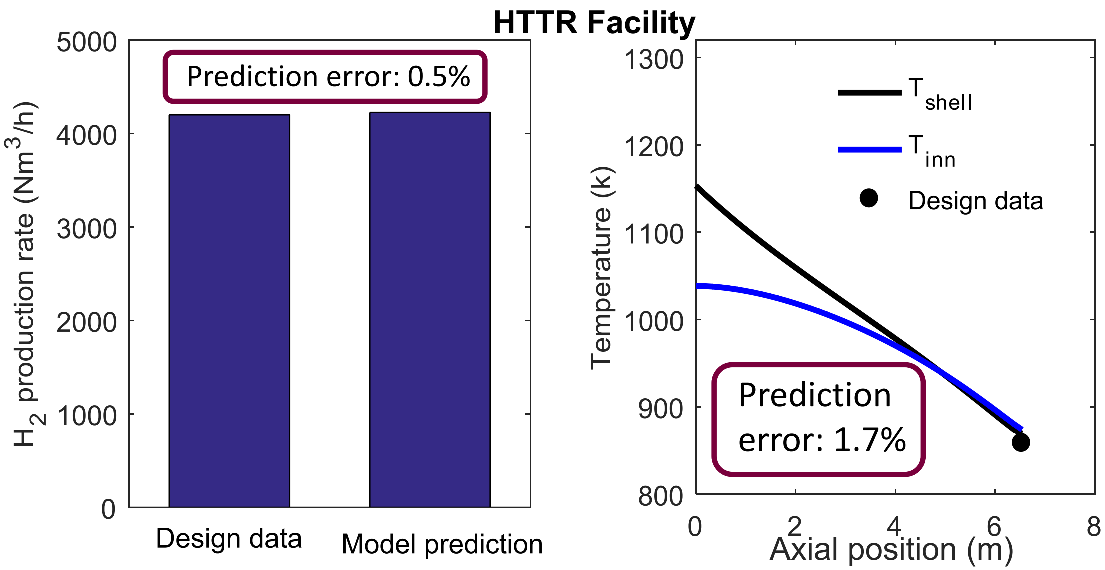




Design Specifications

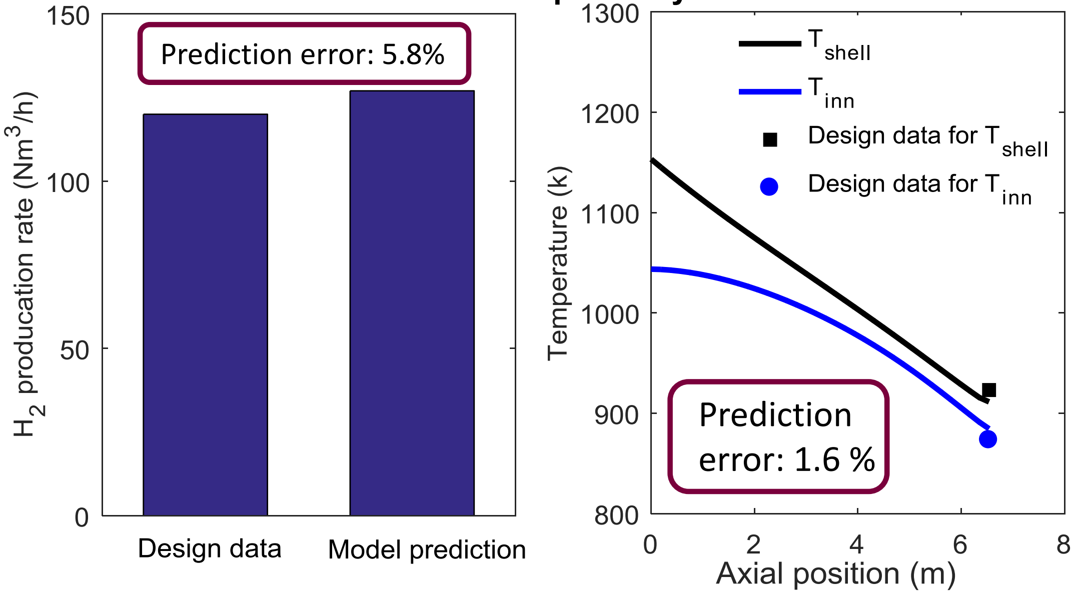
Specification	Mock-up facility	HTTR facility
Process gas conditions		
Inlet P	4.3 MPa	4.5 MPa
Inlet T	450 °C	450 °C
NG feed rate	43.2 kg/h	1296 kg/h
S/C	3.5	3.5
Outlet T	600 °C	580 °C
Helium gas conditions		
Inlet P	4.0 MPa	4.1 MPa
Inlet T	880 °C	880 °C
Feed rate	327.6 kg/h	8748 kg/h
Outlet T	650 °C	580 °C
Hydrogen product	120 Nm^3/h	4200 Nm^3/h
Heat transfer duty	420 kW	10 MW

Design data sources: 1. Inagaki, Y., et al. *No. IAEA-TECDOC--1210*. 2001. 2. Yan, XL. et al. CRC Press ,2016.

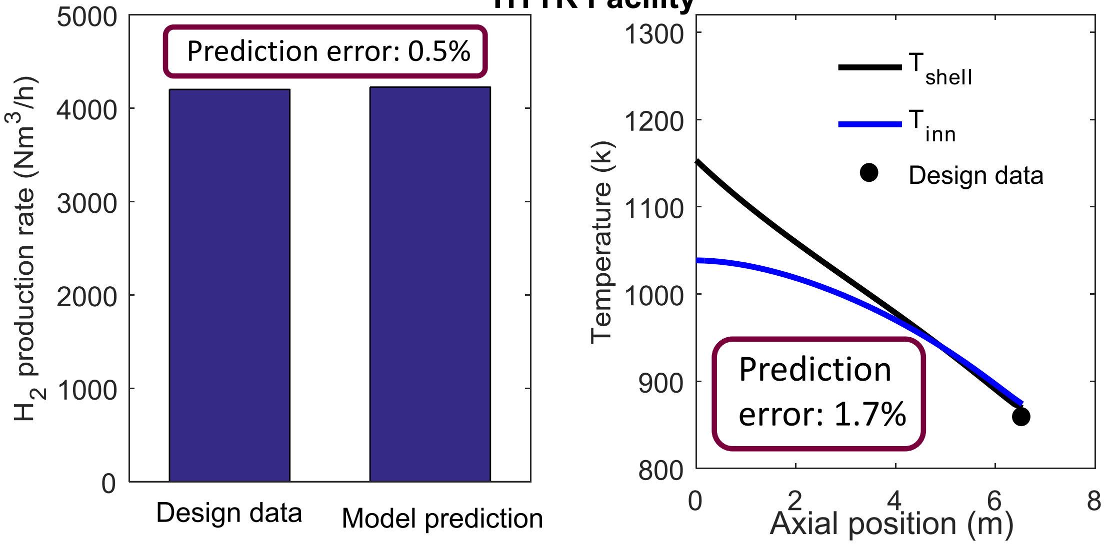
Model Fitting Using Two Pilot Scale Facility Design Data

McMaster University

Mock-up Facility



HTTR Facility



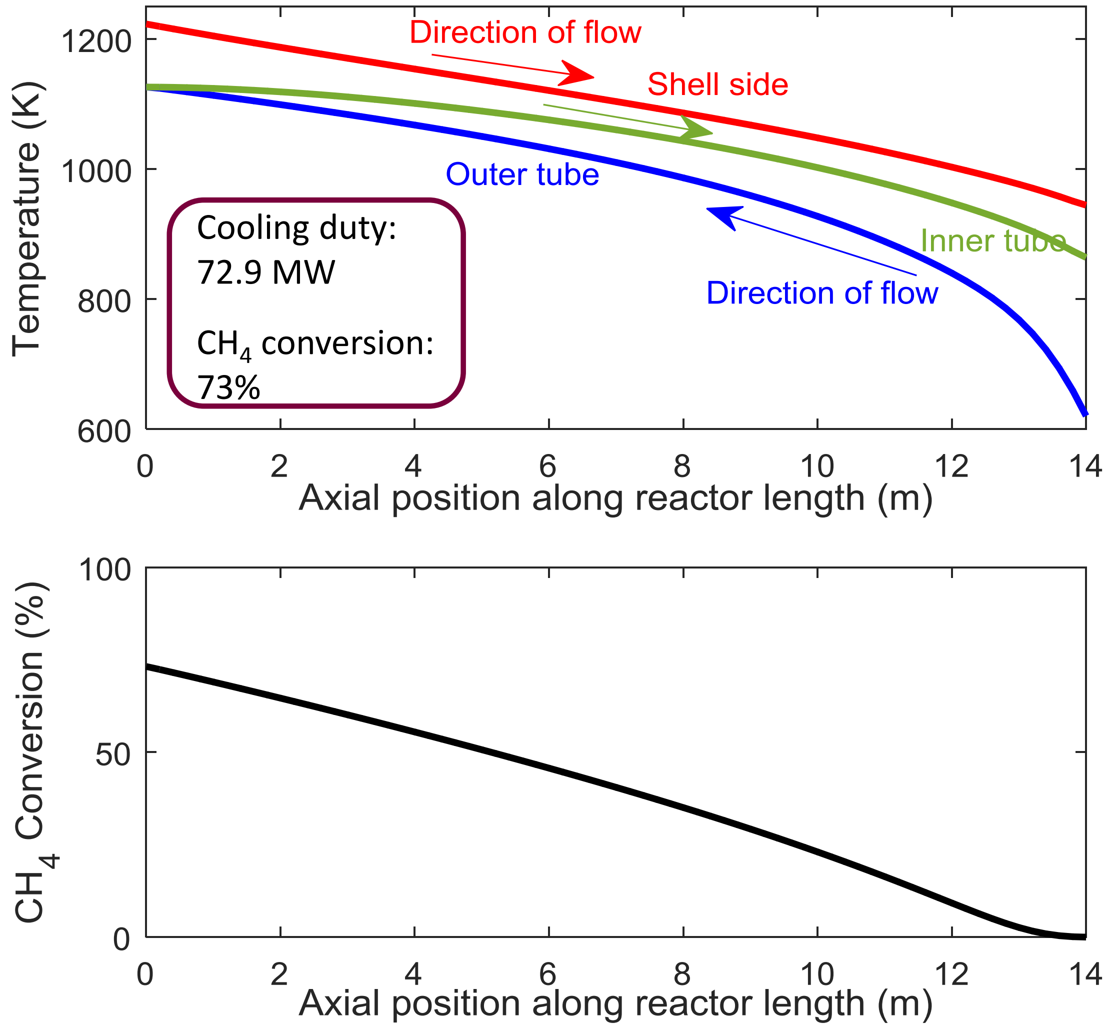
Design Parameters

Parameter	Mock-up	HTTR
Number of tubes	1	30
Catalyst type	Ni-alumina	Ni-alumina
Tube materials	Incoloy 800H	Incoloy 800 H
Tube length	6.54 (m)	6.54 (m)
Tube thickness	1 (cm)	1 (cm)
Tube inner diameter	12.8 (cm)	12.8 (cm)
Inner tube diameter	5.72 (cm)	5.72 (cm)
Catalyst particle diameter	1.2 (cm)	1.2 (cm)
Refractory inner diameter	16.2 (cm)	86 (cm)

Design data sources: 1. Inagaki, Y., et al. *No. IAEA-TECDOC--1210*. 2001. 2. Yan, XL. et al. CRC Press ,2016.

Large Scale Design Results

Shell, tube and inner tube temperature and methane conversion profiles at steady state condition



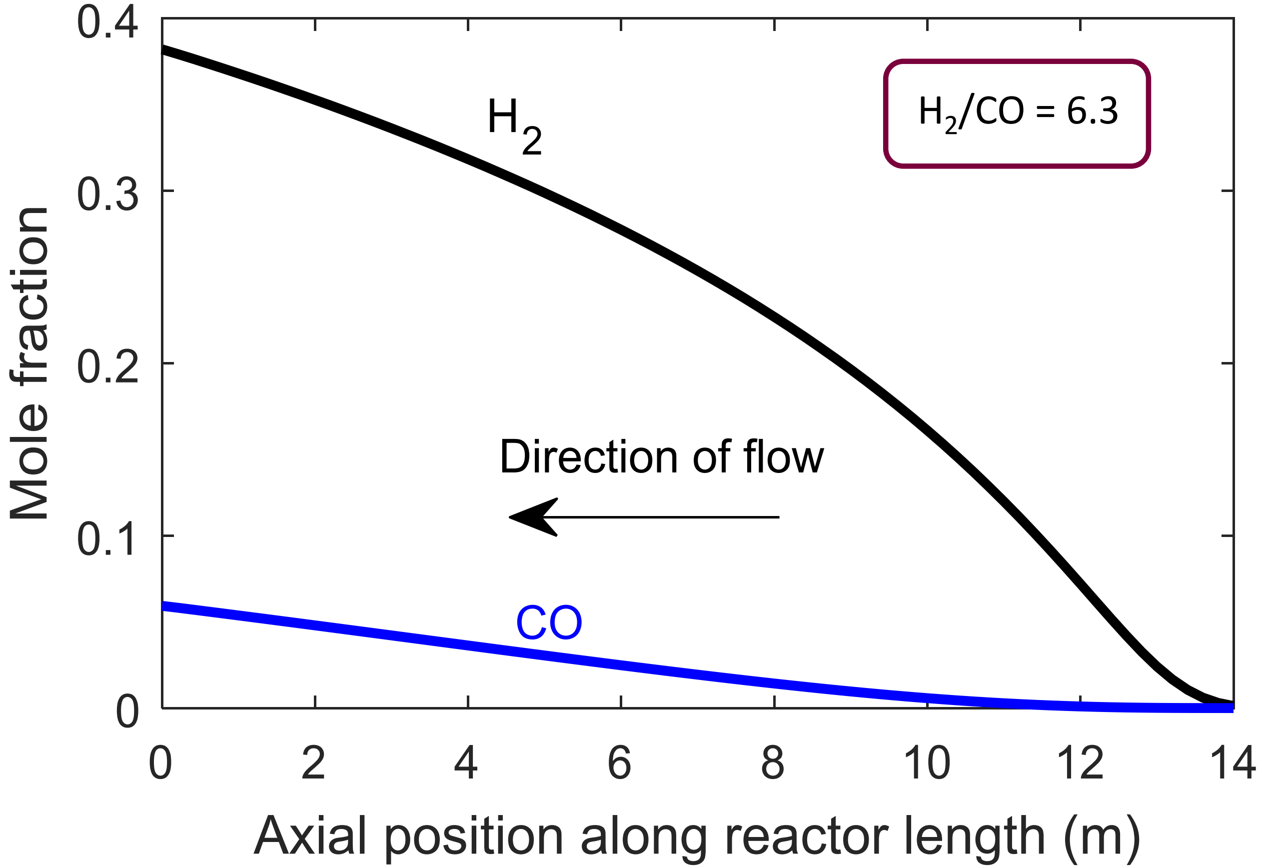
Design Specification

Specification	Large scale design
Number of tubes	199
Tube outer diameter	12 (cm)
Tube thickness	1 (cm)
Tube length	14 (m)
Tube materials	Incoloy 617
Process gas conditions	
Inlet P	5.6 MPa
Inlet T	347 °C
Feed rate	34.8 kg/s
S/C	4
Helium gas conditions	
Inlet P	4.987 MPa
Inlet T	950 °C
Feed rate	50.3 kg/s

Design specification source: Yan, XL. et al. *Nuclear hydrogen production handbook*. CRC Press, 2016.

Large Scale Design Results

H_2 and CO composition profiles at steady state conditions



- High S/C ratio in the feed is required for higher methane conversion
- It causes high H_2/CO ratios in the product
- The desired H_2/CO ratio for Fischer-Tropsch (FT) applications is 2
- If used for FT process, CO and H_2 separation and remixing in a proper ratio is necessary

Means

- HTGR/SMR integration is efficient for H_2 production
- Extra separation cost for FT applications is required

A Redesign for Syngas Production for FT Applications

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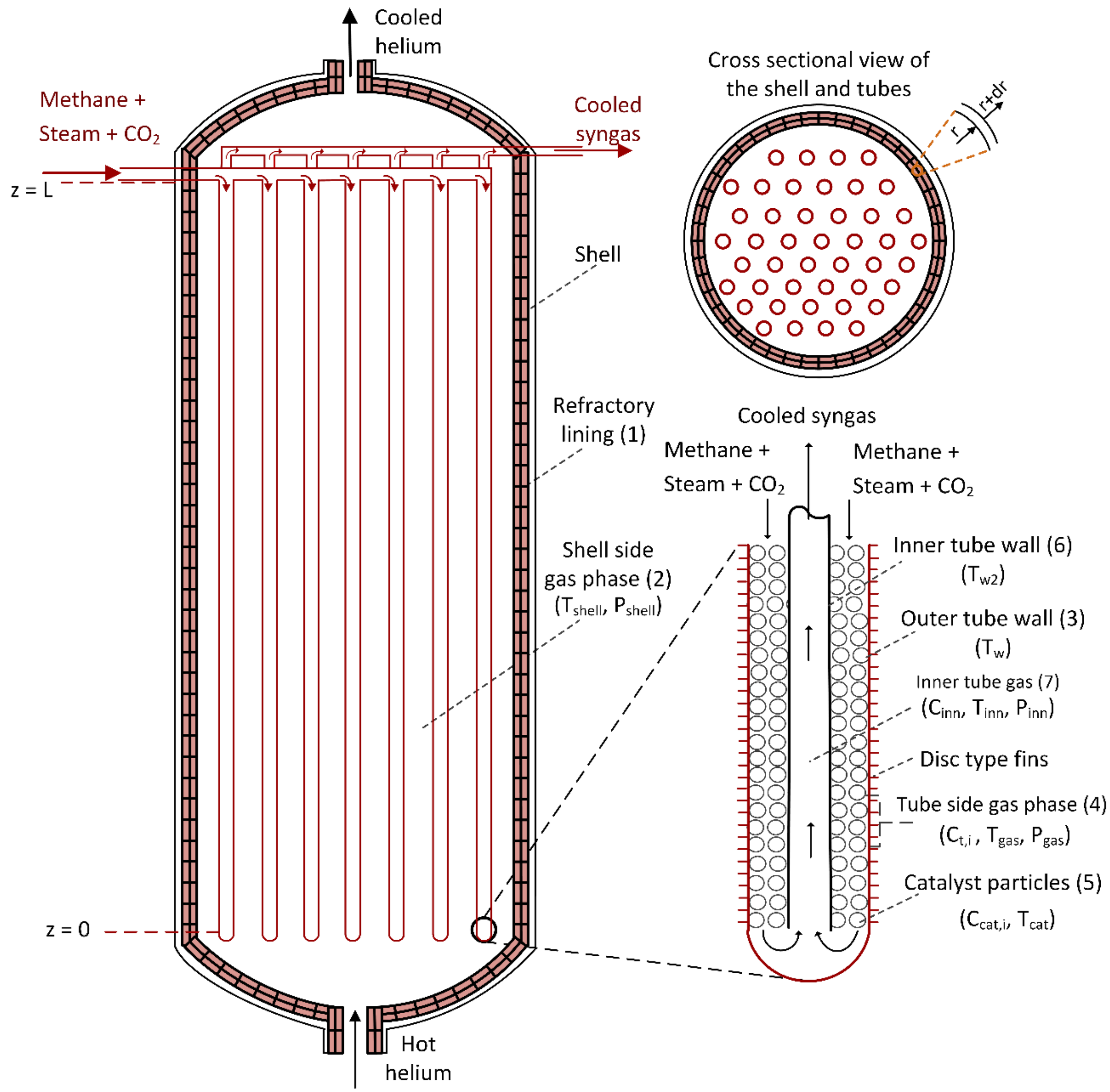
Integrated HTGR/Mixed Reforming of Methane (MRM) system



Advantages of MRM over SMR:

- There is potential to reduce CO_2 emissions
- Proper H_2/CO ratios for FT synthesis can be achieved

Mixed reforming reactions:

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

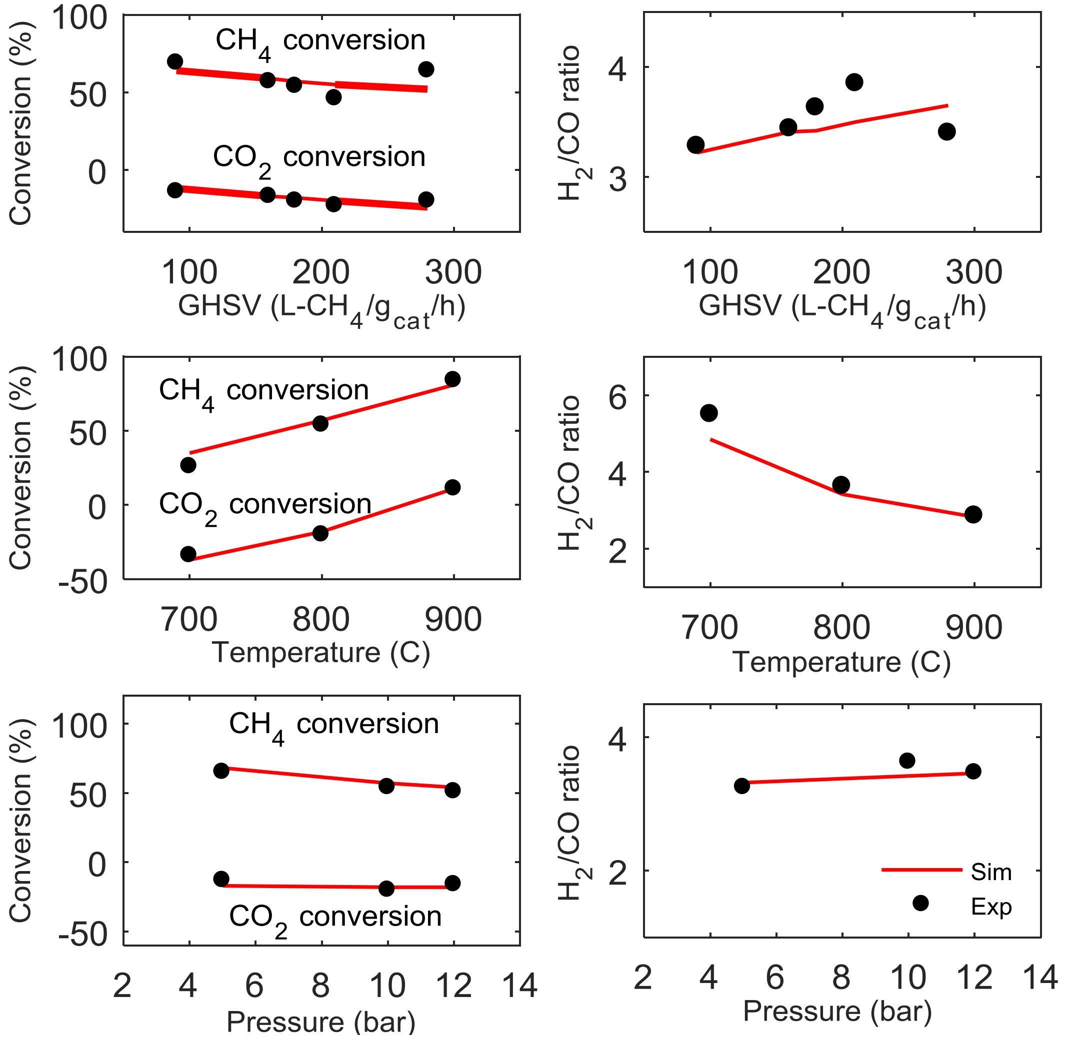
$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

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

$$CH_4 + CO_2 \rightleftharpoons 2CO + 2H_2$$

Model Validation

MRM model validation using lab scale data sets at non-equilibrium condition



- Shell side model was validated for the HTGR/SMR system
- No experimental data on the HTGR/MRM exists
- Some lab scale experimental data are available for the MRM process

Average absolute error of prediction for:

- CO_2 conversion: 2%
- CH_4 conversion: 4.35%
- H_2/CO ratio: 0.183

Experimental data source: Park, N., et al. *Fuel* 115 (2014): 357-365.

Model Validation

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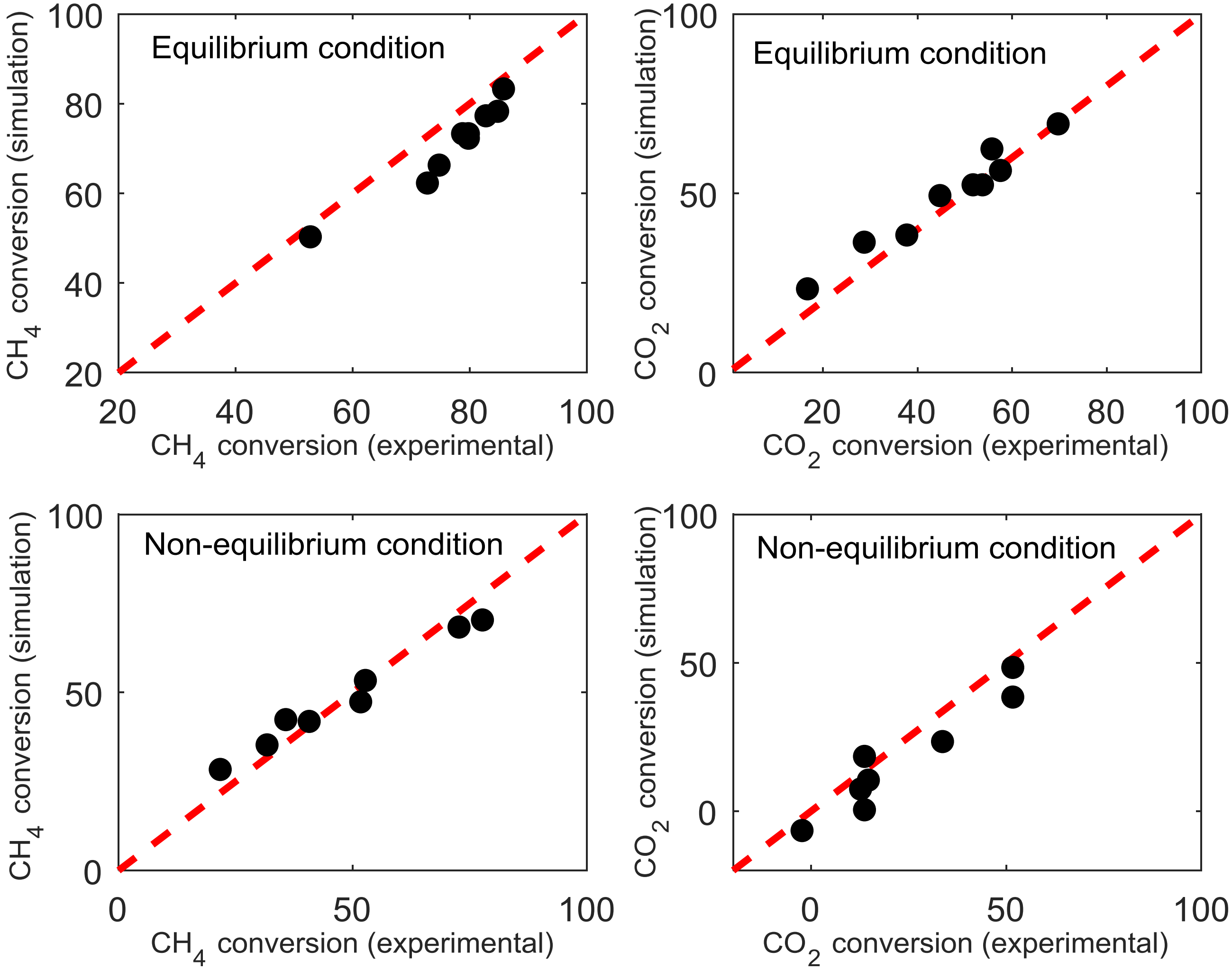
Parity plot for MRM model validation using lab scale data sets at equilibrium/non-equilibrium conditions



Operating condition range for the data set:

- Temperature: 700-900°C
- Pressure: 0.25-1.0 Mpa
- GHSV: 2500-400,000 mL-CH_4/g_{cat} h

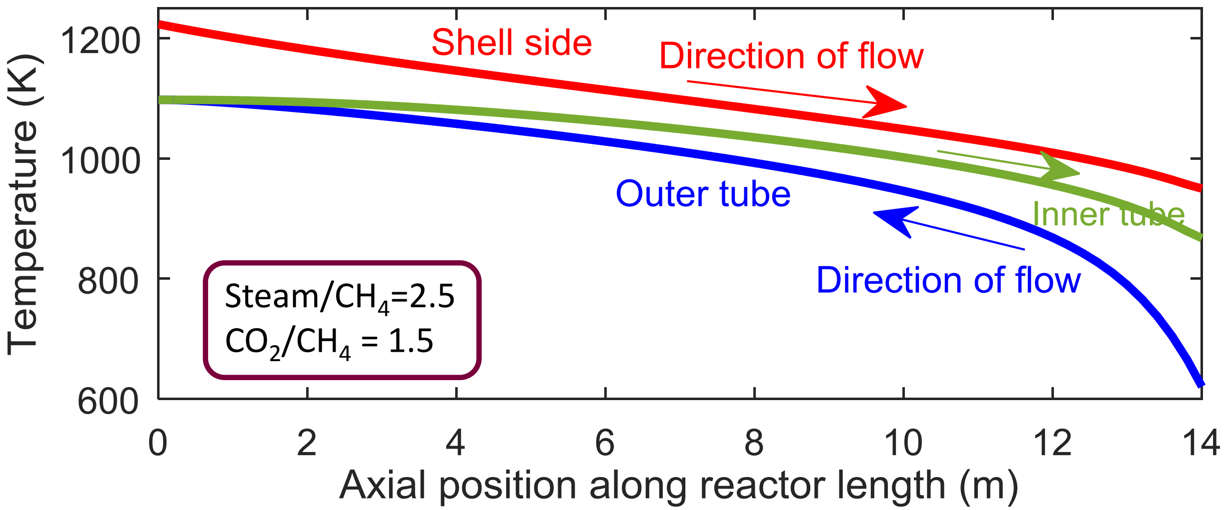
Average absolute error of prediction for:

- CH_4 conversion/ Equilibrium: 6%
- CO_2 conversion/ Equilibrium: 3%
- CH_4 conversion/ non-equilibrium: 7.8%
- CO_2 conversion/ non-equilibrium : 4%

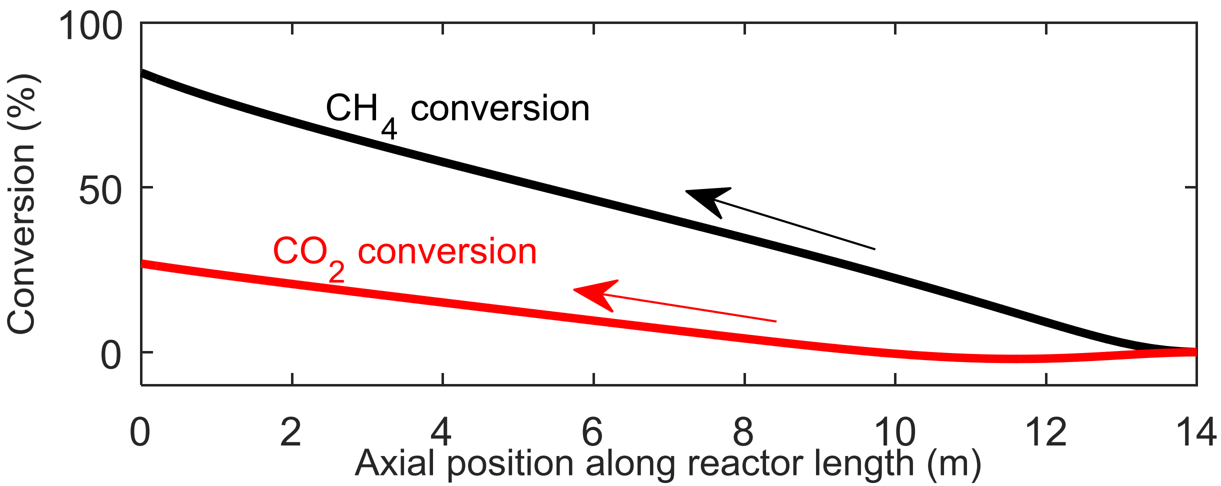
Experimental data source: Jun H. J., et al. *Nat. Gas Chem.* 20 (2011): 9-17.

Results of the Redesign for Syngas Production

Shell, tube and inner tube temperature and CH_4 & CO_2 conversion profiles at steady state condition

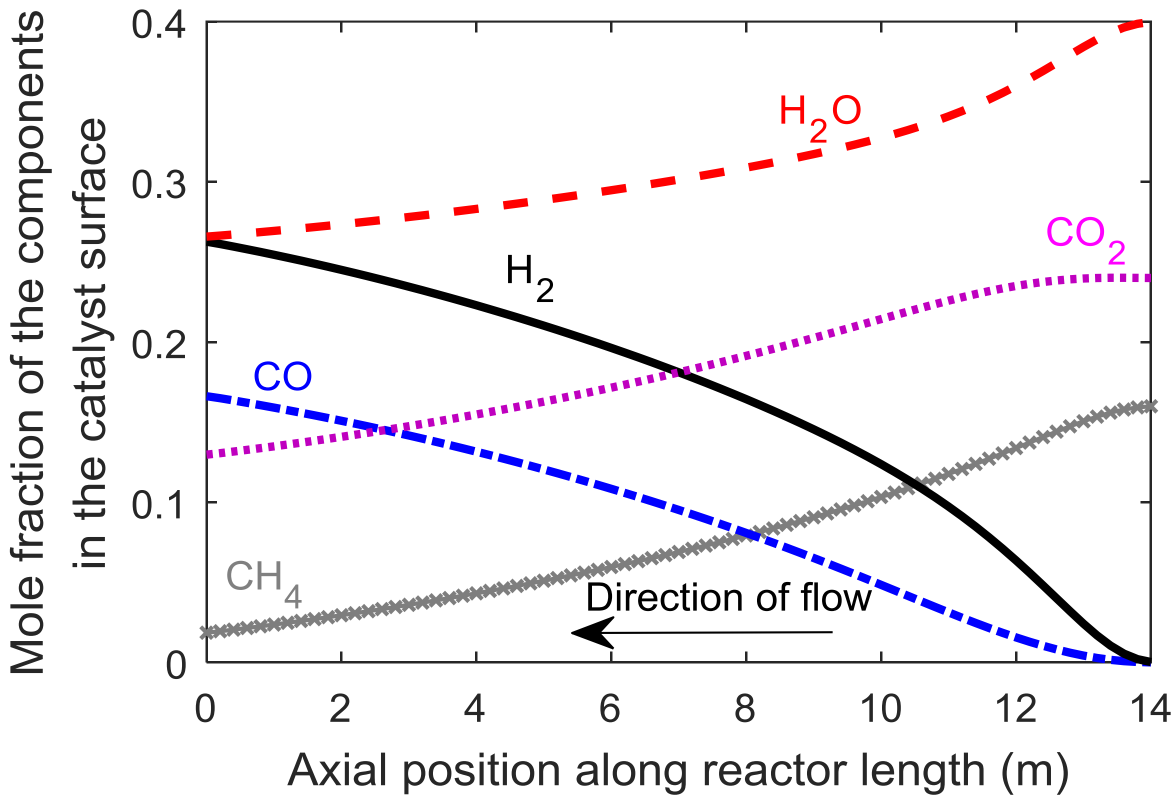


Cooling duty=72 MW
CH_4 conversion=85%
CO_2 conversion=27%



Results of the Redesign for Syngas Production

composition profiles of different component at steady state conditions



- With the given feed ratios, a H_2/CO ratio of 1.7 was achieved
- Desired syngas ratio for the FT applications can be achieved using MRM process
- Also, 27% of CO_2 is consumed and converted to valuable products

Conclusions

- A dynamic model was developed for the integrated HTGR/methane reforming system based on first principles.
- The model was validated using reported design/experimental data.
- Integrated HTGR/SMR is an efficient process for hydrogen production.
- Desired H_2/CO ratios and lower CO_2 emissions can be achieved by redesigning the HTGR/SMR system.
- A Life cycle analysis is required to determine the environmental impacts of HTGR/SMR and its redesign.
- The presented model is useful to address the challenges in the applications of integrated HTGR/MRM and HTGR/SMR systems.

Acknowledgments

- Ontario Ministry of Innovation - Early Researcher Award
- McMaster Advanced Control Consortium