

CSCHE 2018

# A novel sustainable design for production of liquid fuels

**Leila Hoseinzade**

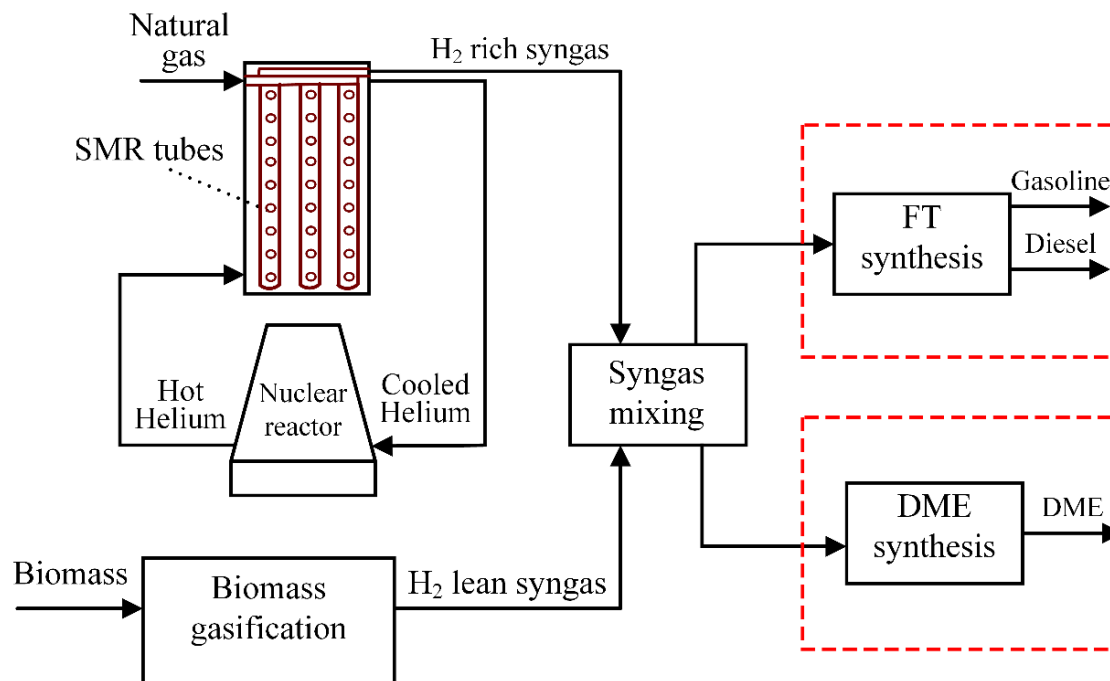
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- Global pressure to reduce greenhouse gas emissions
- Energy security
- Generally high oil prices
- Abundant biomass resources in Ontario province of Canada
- Strong nuclear capabilities and resources in Ontario province of Canada



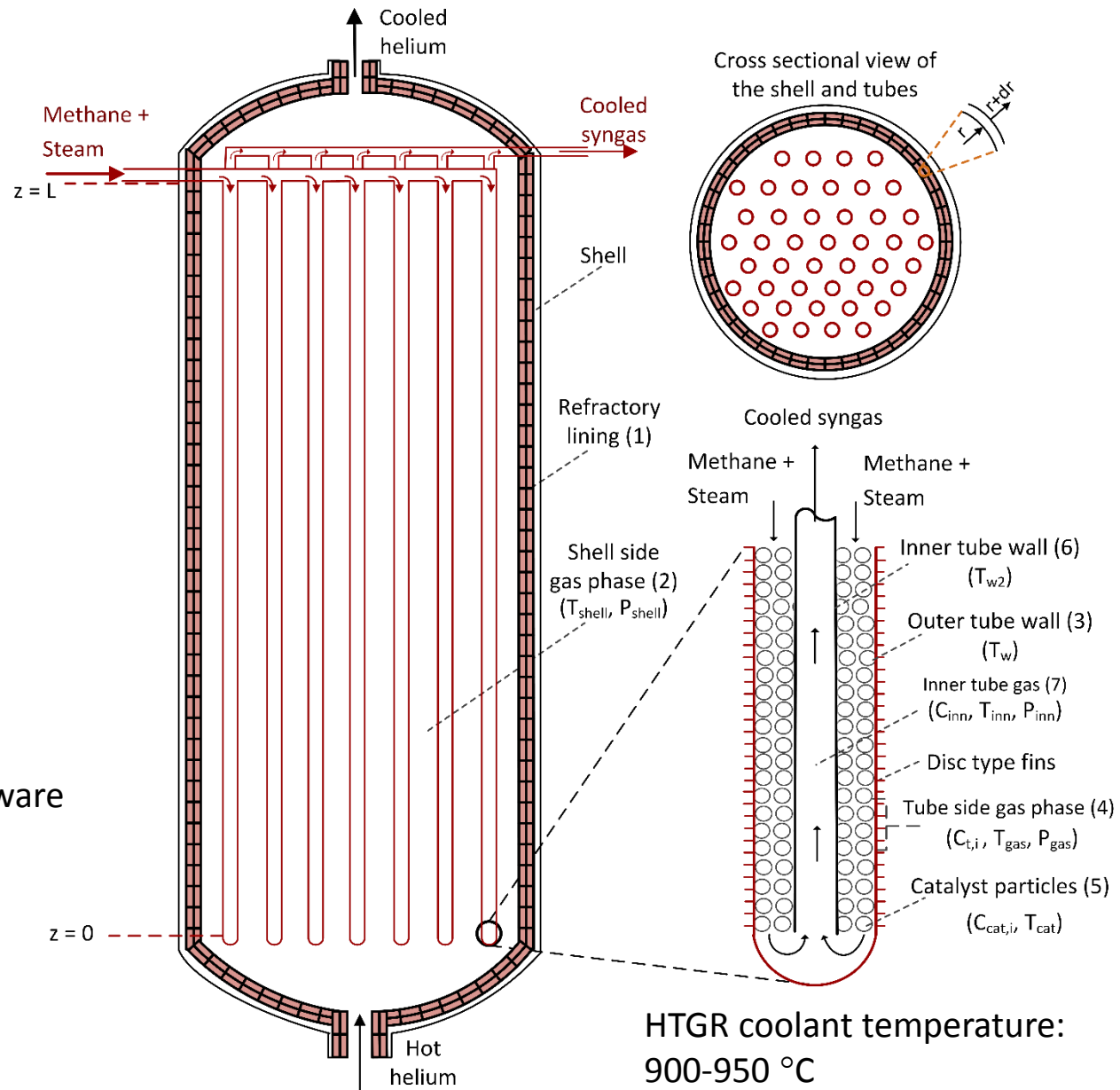
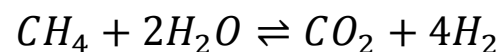
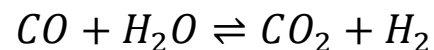
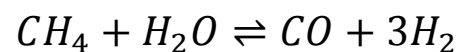
SMR: Steam methane reforming  
FT: Fischer-Tropsch  
DME: Dimethyl ether

# Integrated HTGR/Steam Methane Reforming (SMR) system

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

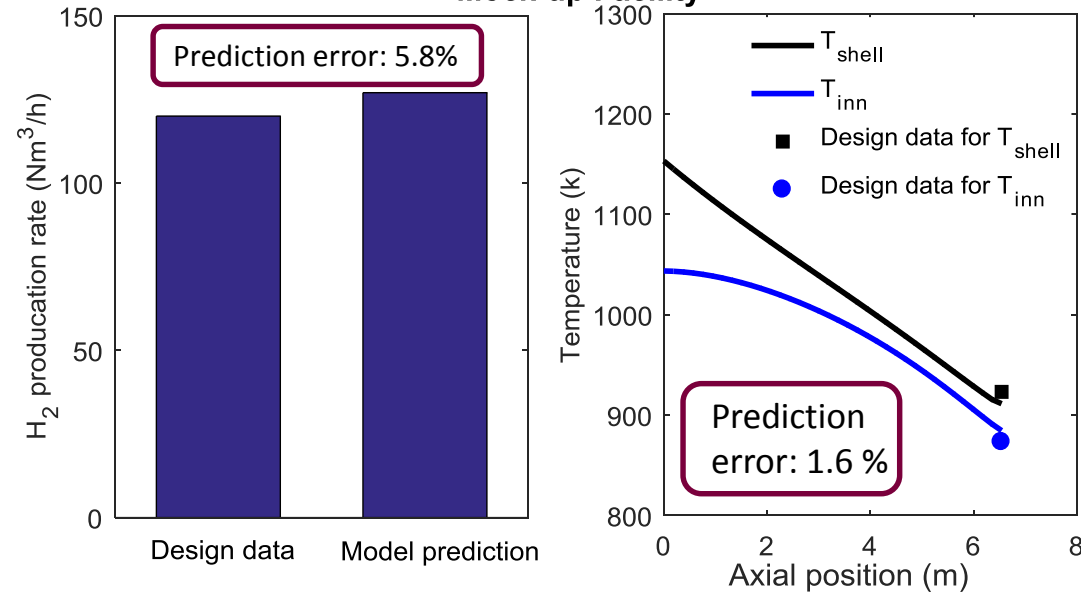
- Is 2 dimensional and dynamic
- Is **multi-scale**, considering:
  - Bulk gas effects
  - Spatial differences within the catalyst particles
- Is based on **first principles**
- Contains seven sub-models
- Is a set of **PDAE**
- Implemented in **gPROMS** software

SMR reactions:

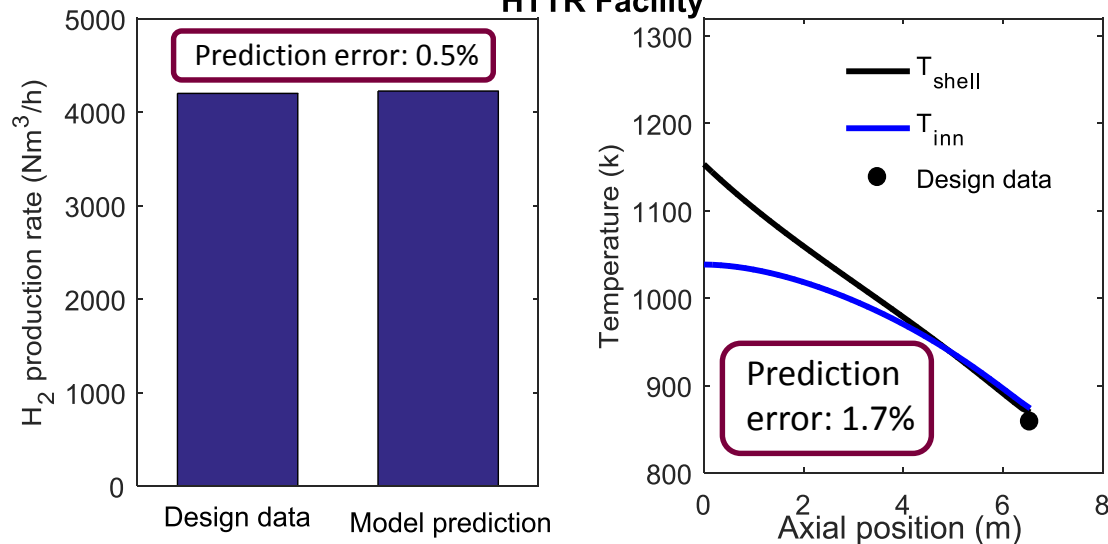


# Model Fitting Using Two Pilot Scale Facility Design Data

**Mock-up Facility**



**HTTR Facility**

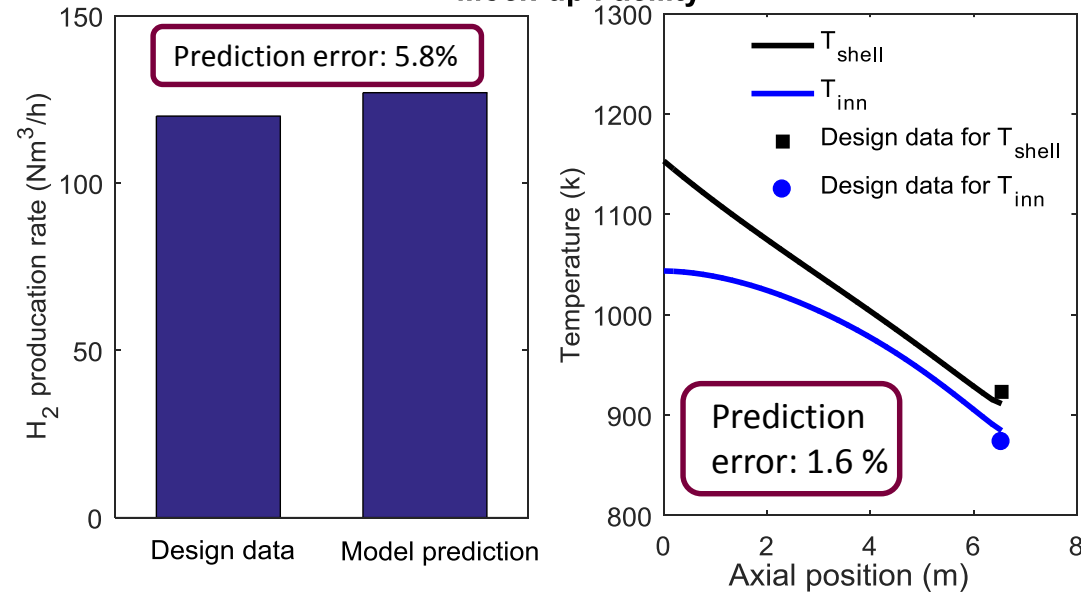


**Design Specifications**

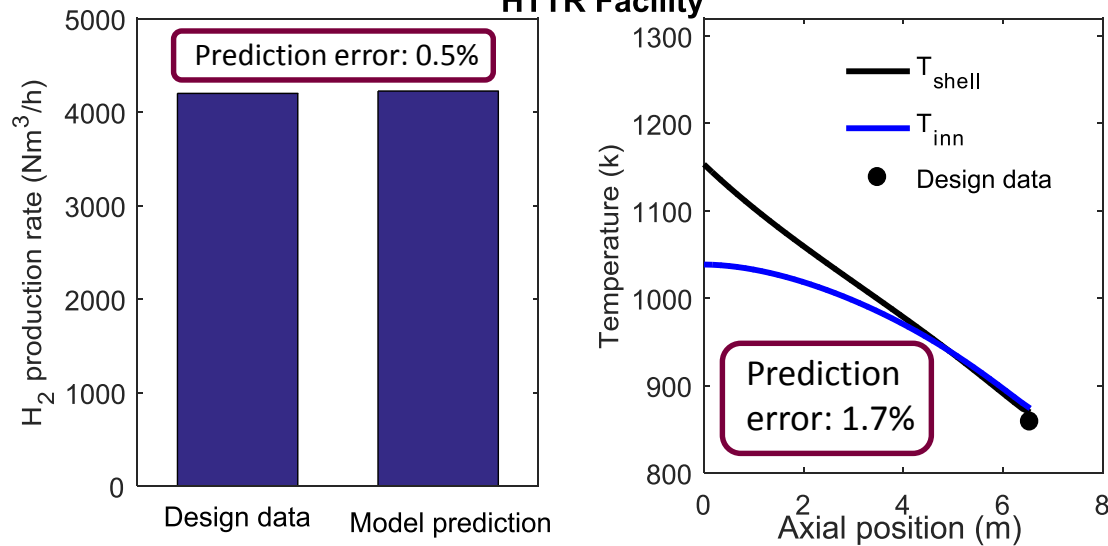
Specification	Mock-up facility	HTTR facility
Process gas conditions		
Inlet P	4.3 MPa	4.5 MPa
Inlet T	450 °C	450 °C
NG feed rate	43.2 kg/h	1296 kg/h
S/C	3.5	3.5
Outlet T	600 °C	580 °C
Helium gas conditions		
Inlet P	4.0 MPa	4.1 MPa
Inlet T	880 °C	880 °C
Feed rate	327.6 kg/h	8748 kg/h
Outlet T	650 °C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

# Model Fitting Using Two Pilot Scale Facility Design Data

**Mock-up Facility**



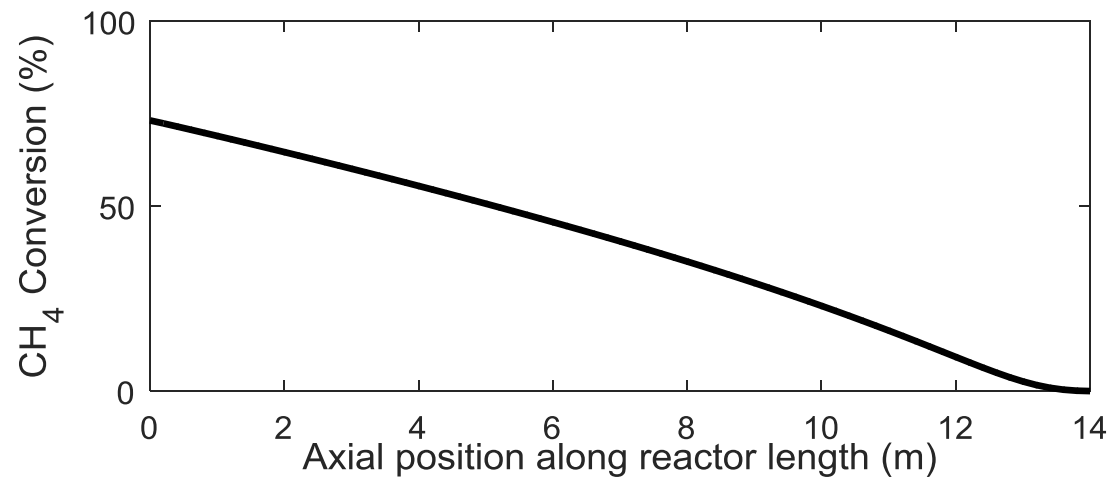
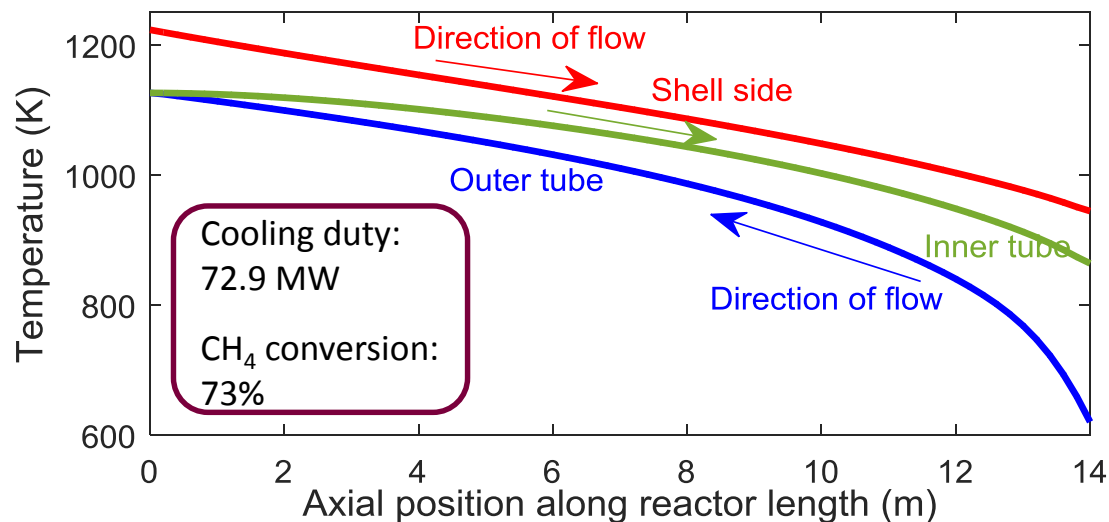
**HTTR Facility**



**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)

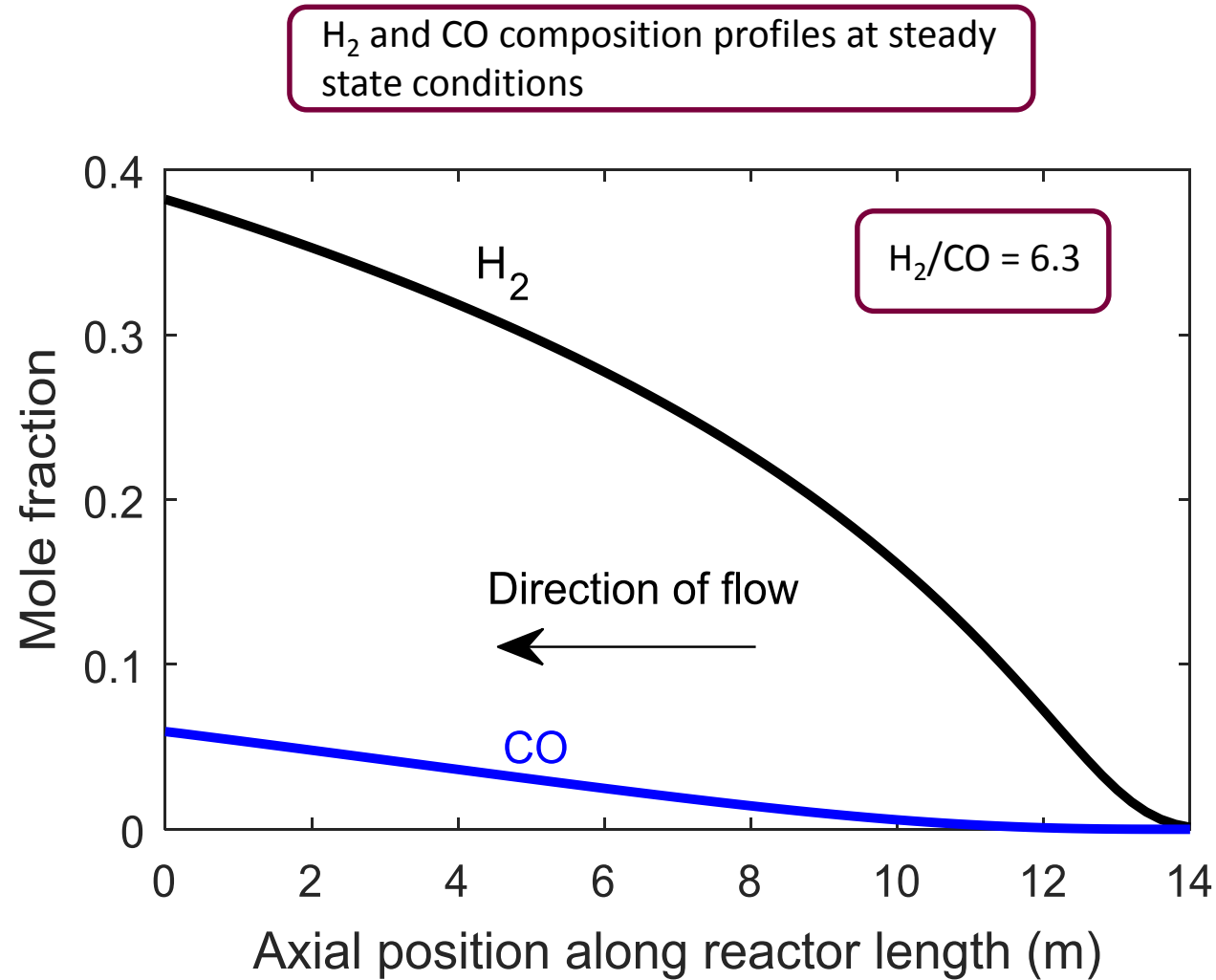
Shell, tube and inner tube temperature and methane conversion profiles at steady state condition



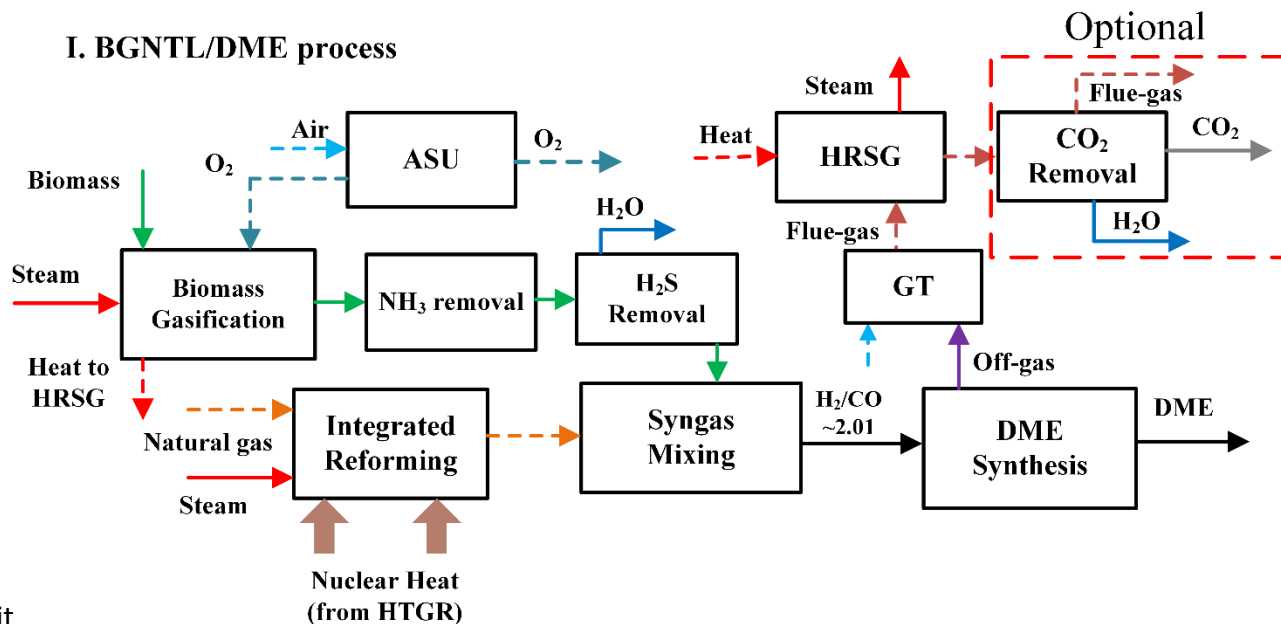
Design Specification

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

- High **steam to carbon** 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
- Can obtain the desired  $H_2/CO$  ratio by:
  - Using mixed reforming process
  - Mixing  $H_2$  rich syngas with biomass gasification-derived syngas



- Natural gas reforming is integrated with nuclear heat
- Biomass is gasified to produce  $H_2$  lean syngas
- Gasification heat is used to generate steam
- Syngas from two routes mixed to obtain desired  $H_2/CO$  ratio
- Off-gas is sent to power generation section



ASU: Air separation unit

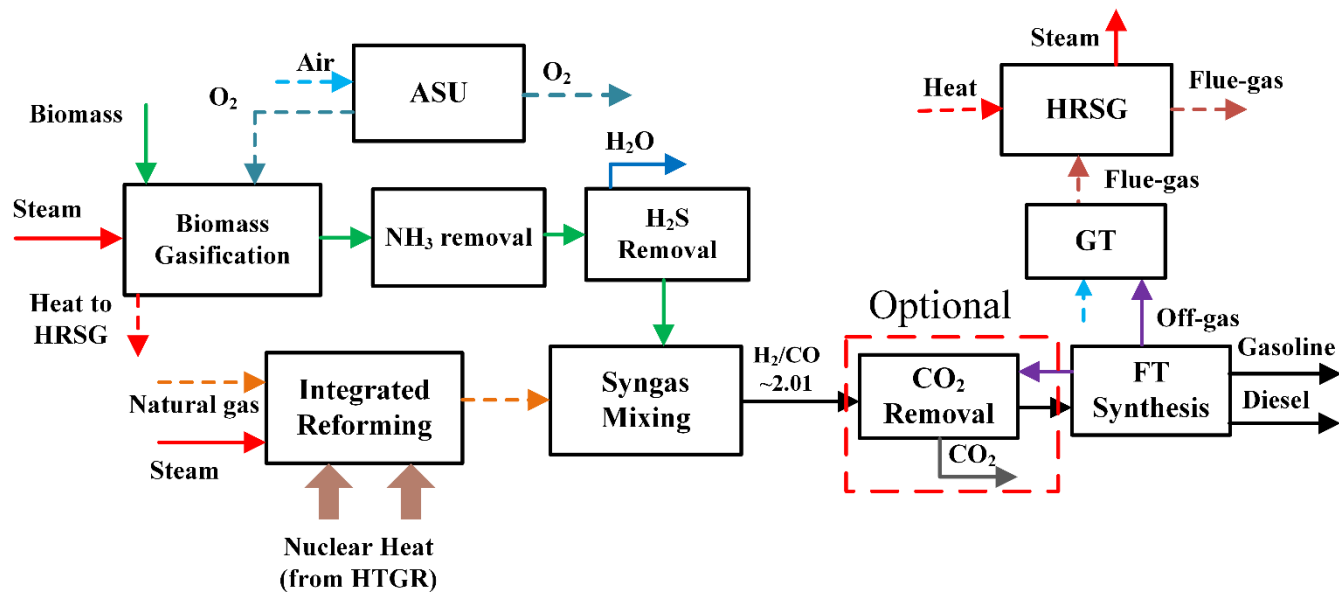
HRSG: Heat recovery steam generator

GT: Gas turbine

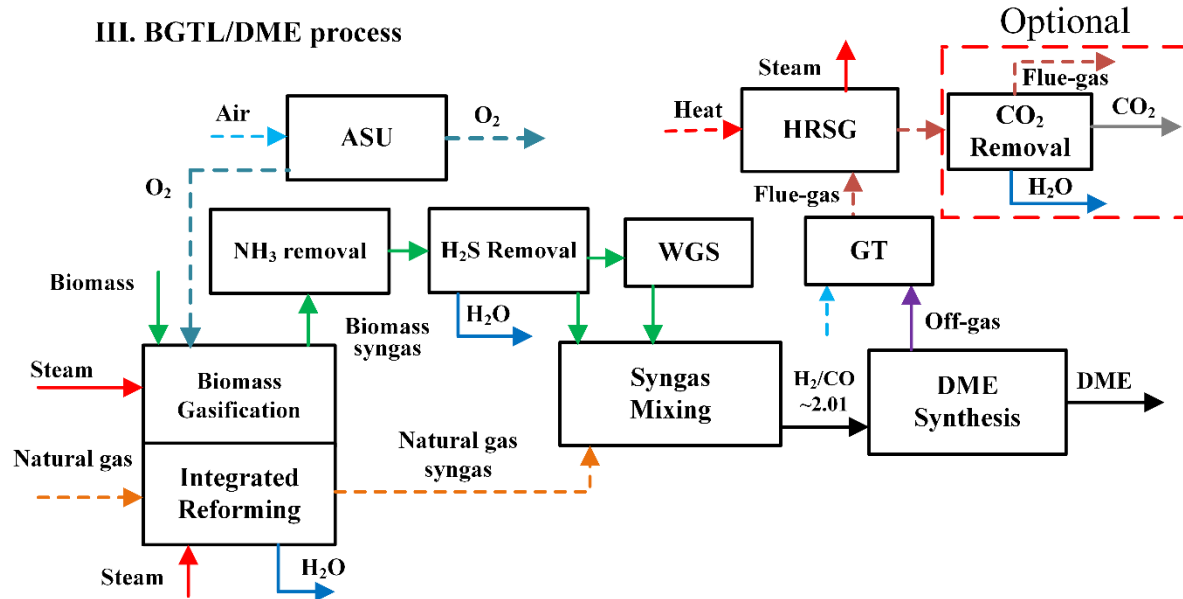


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## II. BGNTL/FT process



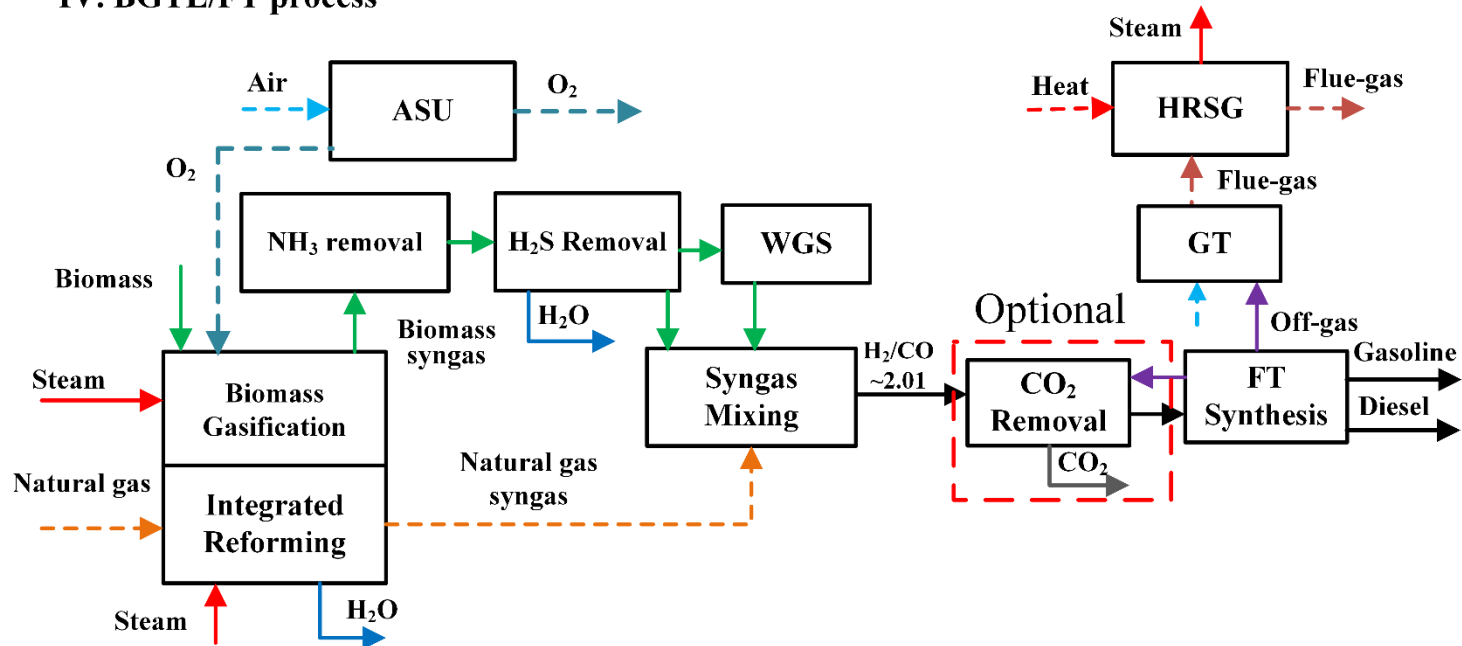
- Biomass gasification is integrated with natural gas reforming
- WGS unit is used to upgrade syngas to desired  $H_2/CO$  ratio for the downstream process
- Off-gas is sent to power generation section



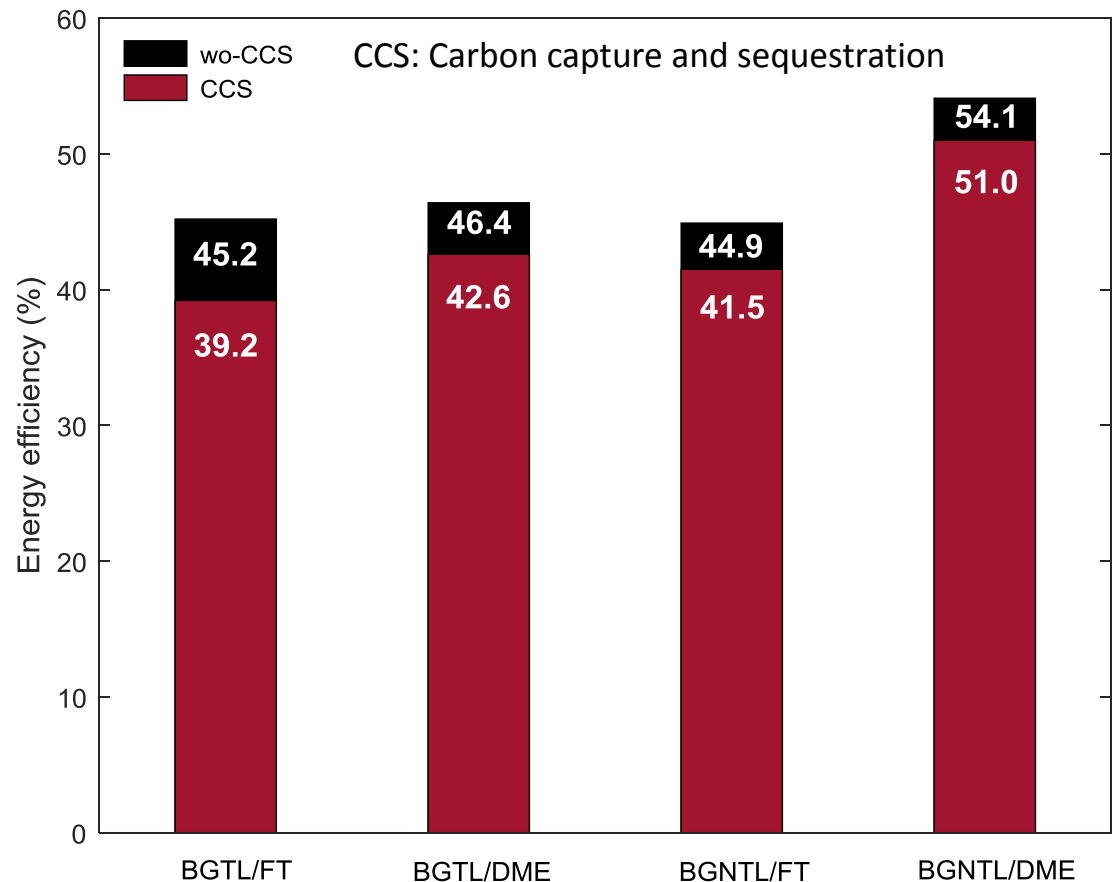
WGS: Water gas shift

- Biomass gasification is integrated with natural gas reforming
- WGS unit is used to upgrade syngas to desired  $H_2/CO$  ratio for the downstream process
- Off-gas is sent to power generation section

## IV. BGTL/FT process

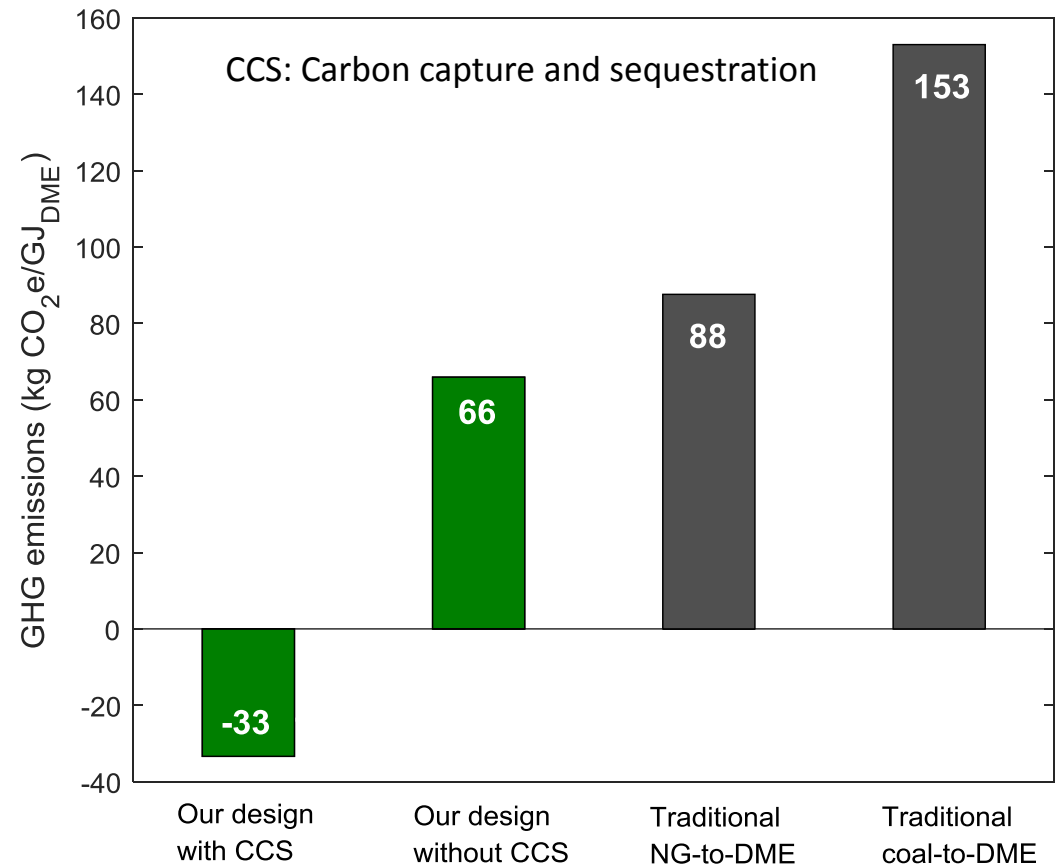


- Biomass, gas and nuclear heat integration leads higher efficiency
- DME production is more efficient than diesel and gasoline production
- Energy efficiency of **54%** can be achieved due to nuclear heat integration



# Economic and environmental impacts of BGTL and BGNTL processes

- Nuclear integrated process is highly **profitable** if it is used for **DME production**
- Minimum selling price of DME is **0.910 CAD/kg** without CCS and **1.16 CAD/kg** when CCS is enabled (current price 1.3 CAD/kg)
- **57% lower** GHG emissions comparing to a traditional coal-to-DME plant in the non-CCS case
- **25% lower** GHG emissions comparing to a traditional NG-to-DME plant in the non-CCS case
- **Net negative GHG emissions** when CCS is enabled



- A dynamic model was developed for the integrated nuclear heat and steam methane reforming system based on first principles.
- The model was validated using reported data in the literature.
- Integrated nuclear heat and steam methane reforming system is efficient for hydrogen rich syngas production.
- Integrated nuclear heat and natural gas reforming process was combined with biomass gasification to reach the desired  $H_2/CO$  ratio for downstream processes.
- The biomass, gas, nuclear heat to liquids process was shown to be highly efficient, profitable and environmentally friendly specifically if it is used for DME production.

## Acknowledgments

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