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Direct Synthesis of Dimethyl Ether from Solar Thermochemical Syngas

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Project Background

- Dimethyl ether (DME) is a promising alternative diesel fuel as it eliminates particulate emissions and contains no carbon-carbon bonds[1]
- Designed process is an add on to another process designed by researchers at Pacific Northwest National Laboratories (PNNL) which converts 70% of solar energy to chemical energy that can then be stored and reused
- Our process uses a single-step microreactor with catalysts to make DME from chemical product made by process from PNNL

1. "Alternative Fuels Data Center: Dimethyl Ether." *Energy.Gov*, 2013, afdc.energy.gov/fuels/emerging_dme.html. Accessed 30 May 2020.

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Objectives

- Profitably make and sell DME as a more sustainable alternative fuel using syngas produced using solar energy
- Reduce carbon emissions and waste in process as much as possible
- Purify reaction side products methanol and hydrogen for additional sales to help make process economically feasible

H_2Product		
Purity Required for Sale	>99.97	mol%
MeOH and DME Products		
Purity Required for Sale	>99.8	mol%

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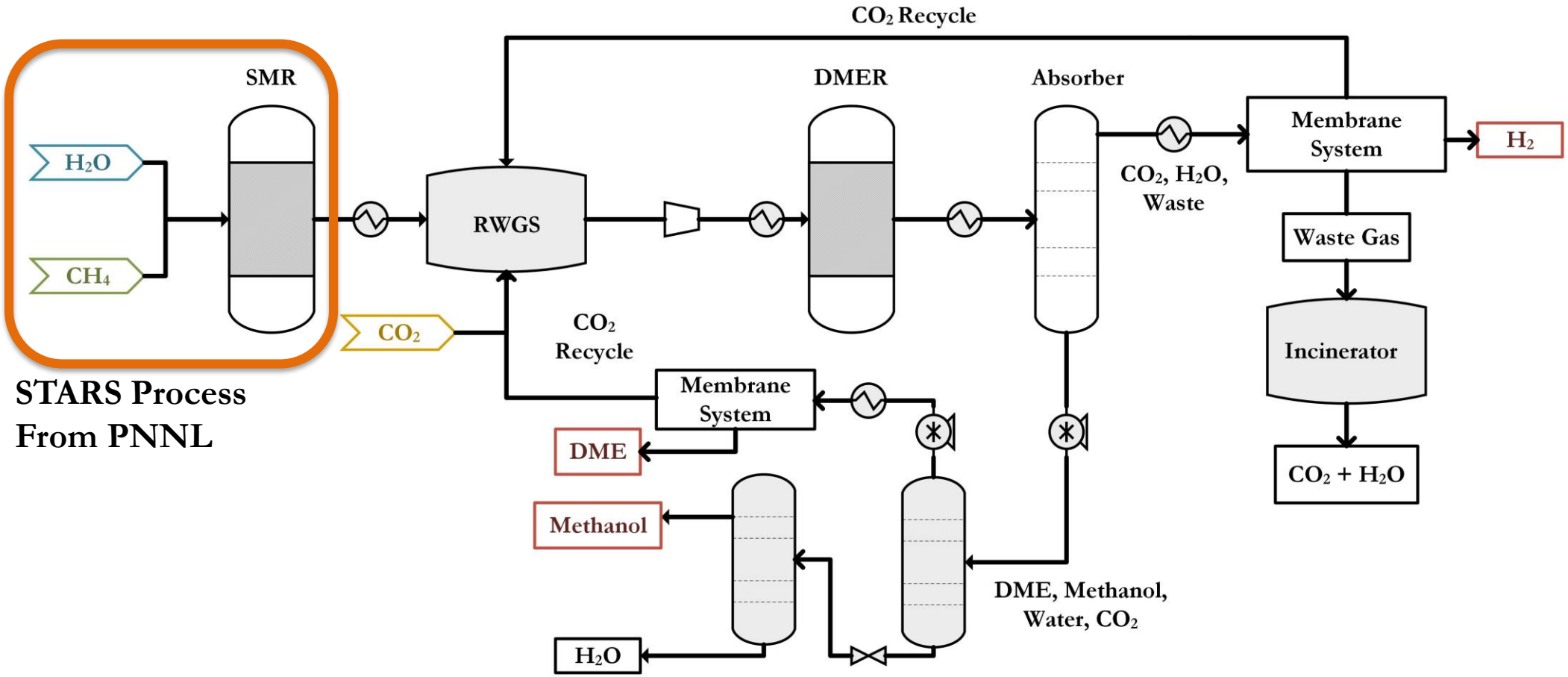
Process Overview



STARS Process
From PNNL

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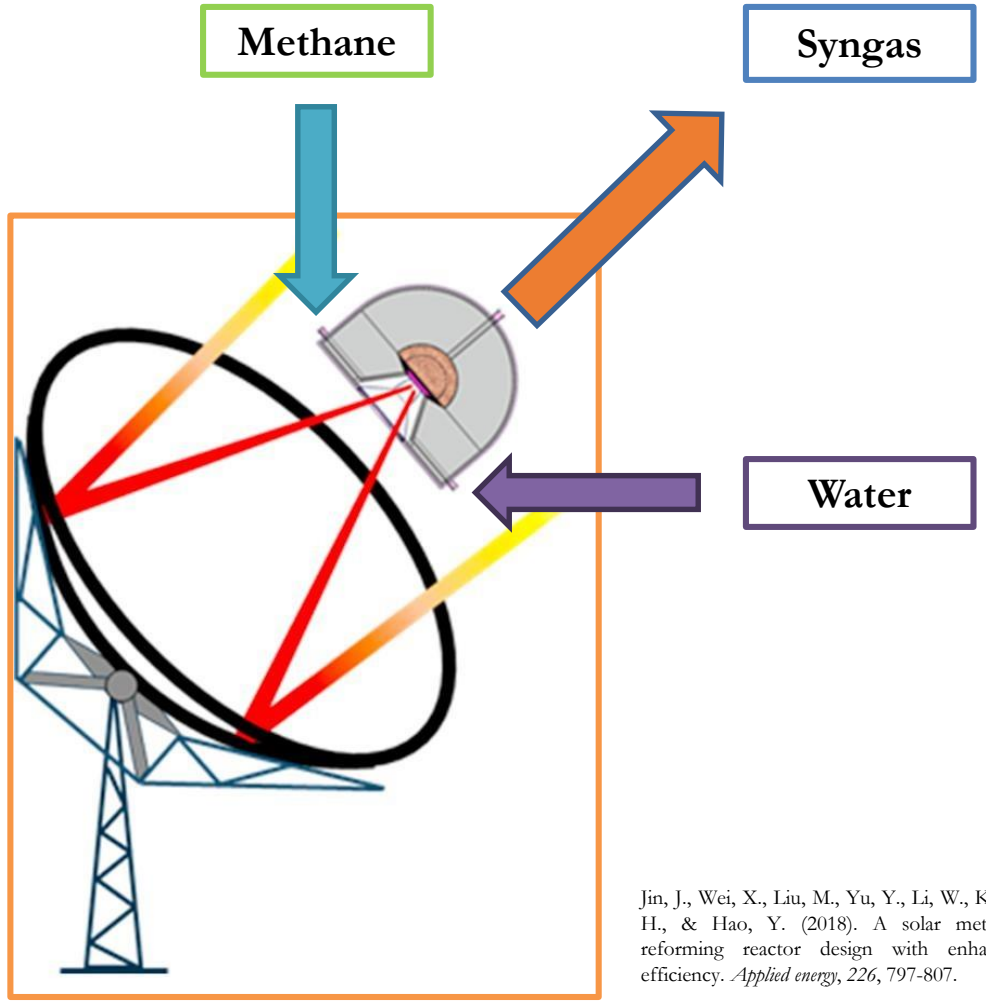
STARS Process

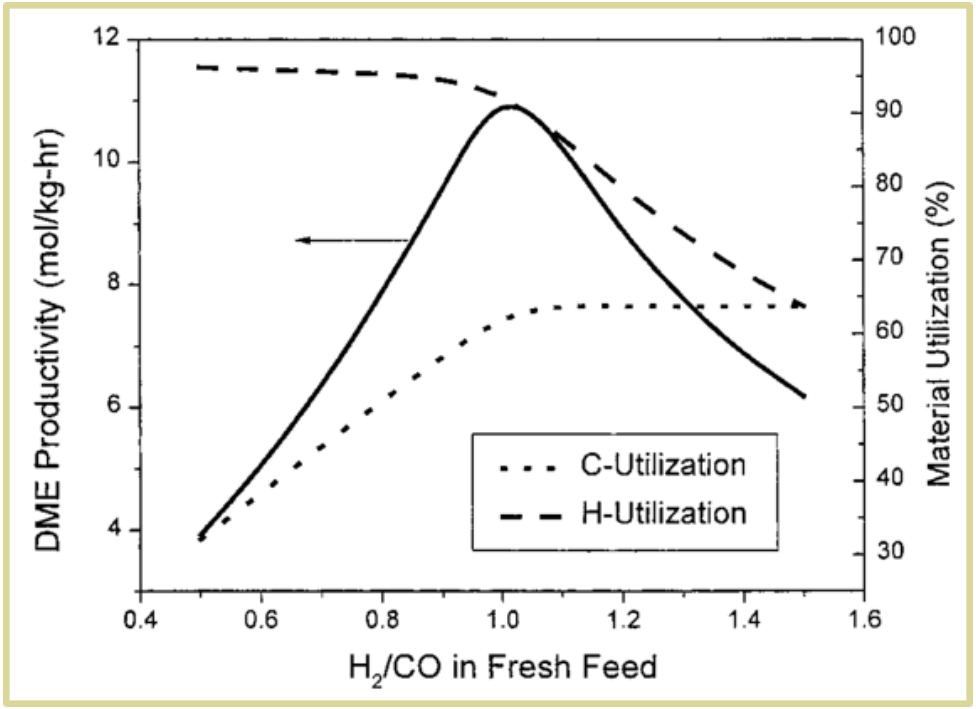


Jin, J., Wei, X., Liu, M., Yu, Y., Li, W., Kong, H., & Hao, Y. (2018). A solar methane reforming reactor design with enhanced efficiency. *Applied energy*, *226*, 797-807.

- STARS was designed by researchers at PNNL
- Makes syngas from methane using solar energy for required reaction
- Syngas is a mixture of carbon monoxide (CO) and hydrogen (H_2) gas that can be made into DME using another reaction

Reverse Water Gas Shift Reaction

- Different ratios of H_2:CO in syngas are more efficient for DME production
  - Syngas comes out of initial process at 4.5:1 ratio of H_2:CO
- Reverse Water Gas Shift can be used to change ratio to more something more optimal for DME production (<1.5:1)



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Dimethyl Ether Reactor

- Found that 1:1 ratio of H_2:CO has the greatest productivity of DME in catalytic microreactor
- Temperature of reactor limited by operating conditions of catalysts needed for reaction

Syngas Ratio	1 : 1 H_2:CO	2 : 1 H_2:CO	4.5 : 1 H_2:CO
CO_2feed required [kmol/hr]	1.0	0.305	0.0
DMER Temp [°C]	220	220	220
DME yield [kg/hr]	3.59	3.24	2.95

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Separating Products

Absorber	Gas Membrane Systems	Distillation Columns
Cold water under high pressures absorb methanol and dimethyl ether from gas stream exiting DME reactor Species not absorbed into liquid water sent to gas membrane system for further separation	Preferentially absorb certain chemical species based on the membranes structure Allow separations on gas streams that typically require large energy inputs and more expensive equipment	Methanol and DME in liquid water stream from absorber go to distillation system Different boiling points of the three species allow separation by boiling and then condensing back to liquid state

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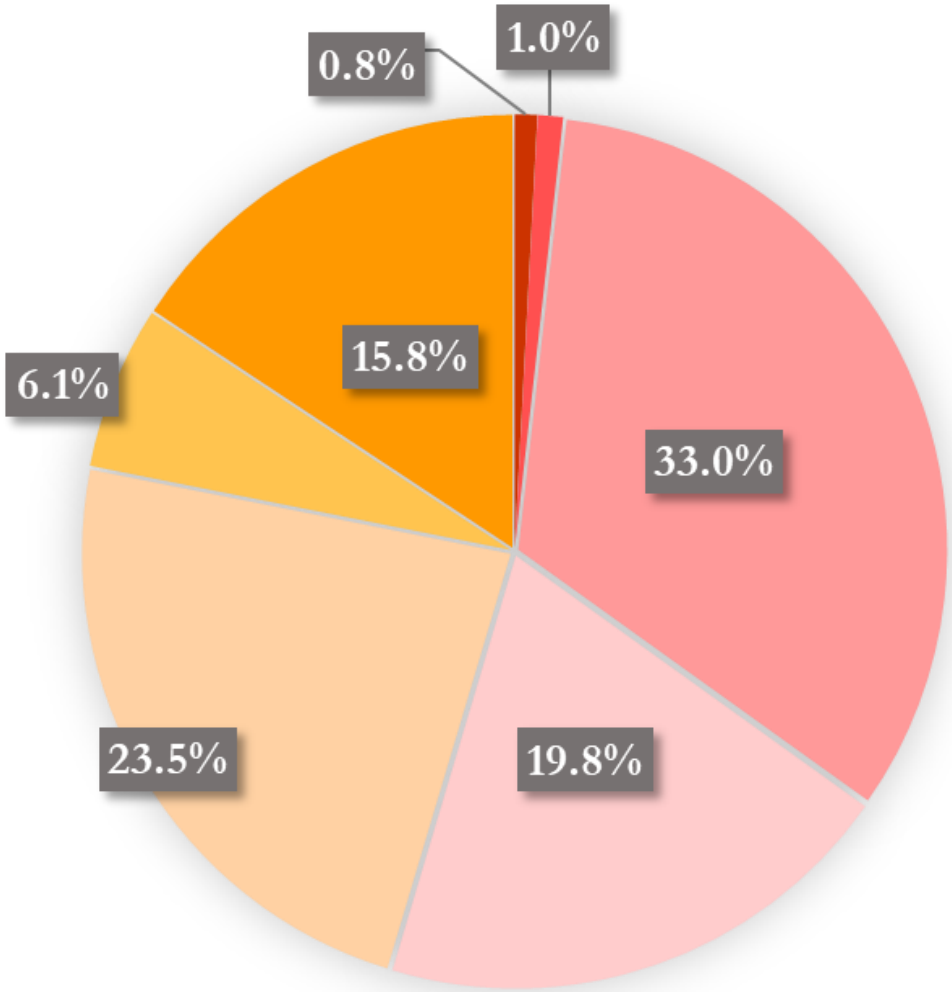
Economics

w/ 15% Profit Margin

	Our Price	Market Price*
DME	$43/kg	$408/kg Sigma Aldritch
H_2	$13/kg	$13/kg CAFCP
MeOH	$10/kg	$10/kg Alibaba



*** 99% pure DME on Alibaba = $15 /kg**

Green Chemistry

Metric	E-Factor	Atom Efficiency
Goal	1-5	50%
Actual	2.5	47%

- **E-Factor** is a **ratio of the waste to the product** (the higher the value, the more waste produced)
- **Atom efficiency** (economy) is the how **much of the reactants' atoms are incorporated into the final products**

- The plant **does not use any solvents** (solvents are the major contributors to toxicity)
- **Reuse of waste water** streams as **heating/cooling** streams in other parts of the process for heat integration

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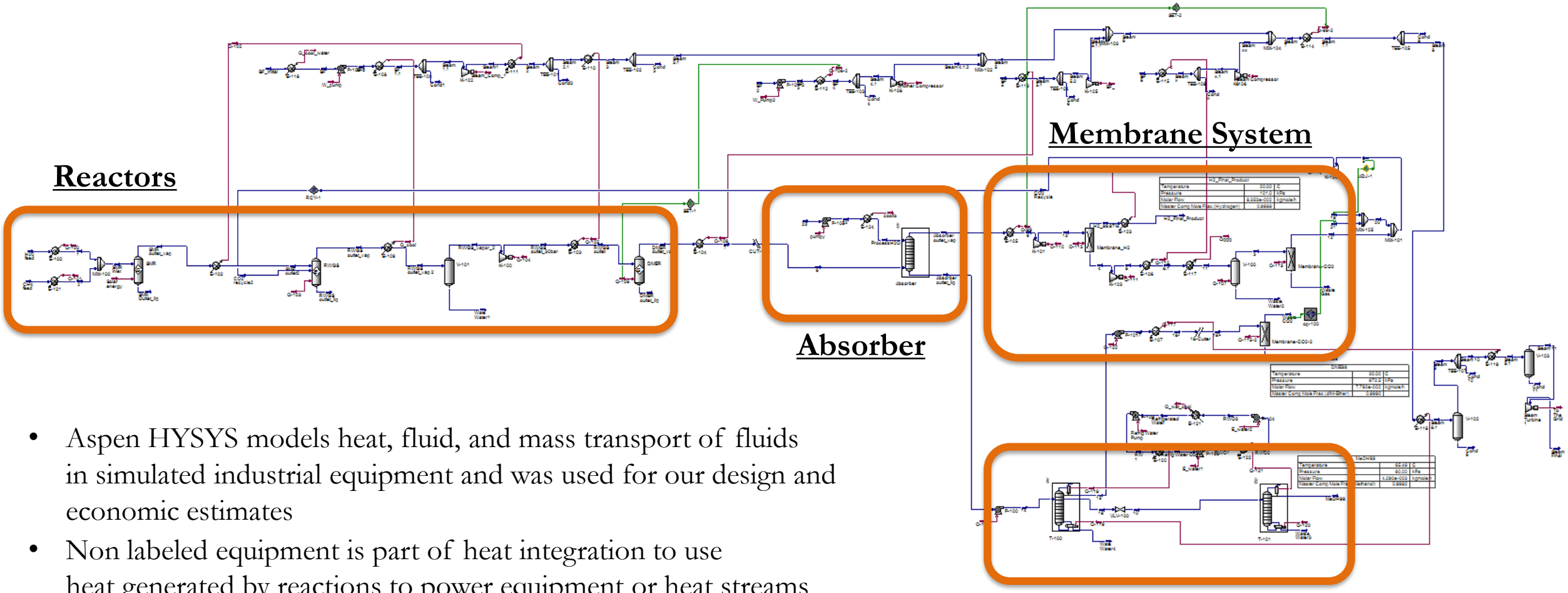
HYSYS Simulation



- Aspen HYSYS models heat, fluid, and mass transport of fluids in simulated industrial equipment and was used for our design and economic estimates
- Non labeled equipment is part of heat integration to use heat generated by reactions to power equipment or heat streams

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HYSYS Simulation Tables

DME Reactor Outlet		
Temperature	220.0	C
Pressure	3000	kPa
Master Comp Mass Flow (diM-Ether)	3.5974	kg/h
Master Comp Mass Flow (Methanol)	0.1384	kg/h
Master Comp Mass Flow (Hydrogen)	0.1681	kg/h
Master Comp Mass Flow (CO)	3.3818	kg/h
Master Comp Mass Flow (CO2)	40.7317	kg/h
Master Comp Mass Flow (H2O)	0.0739	kg/h

Product Recovery Percent	
diM-Ether	0.9923
Methanol	0.9956
Hydrogen	0.9998

DME Final Product		
Temperature	30.00	C
Pressure	669.3	kPa
Mass Flow	3.576	kg/h
Master Comp Mole Frac (diM-Ether)	0.9990	

Methanol Side Product		
Temperature	65.46	C
Pressure	90.00	kPa
Mass Flow	0.1373	kg/h
Master Comp Mole Frac (Methanol)	0.9982	

H2 Side Product		
Temperature	20.00	C
Pressure	101.0	kPa
Mass Flow	0.1685	kg/h
Master Comp Mole Frac (Hydrogen)	0.9999	