2.60/2.62 lecture 21
Energy system modeling and examples

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Intended learning outcomes

- After this lecture, students are capable to
- Identify energy systems
- Explain the reason to carry out system analysis of energy systems
- Describe the basic functionality of Aspen Plus^{TM}
- Perform a system analysis using Aspen Plus^{TM} with the help of manual

Outline

- Advanced energy systems: innovation and characterization

- System analysis: what we can learn from it?

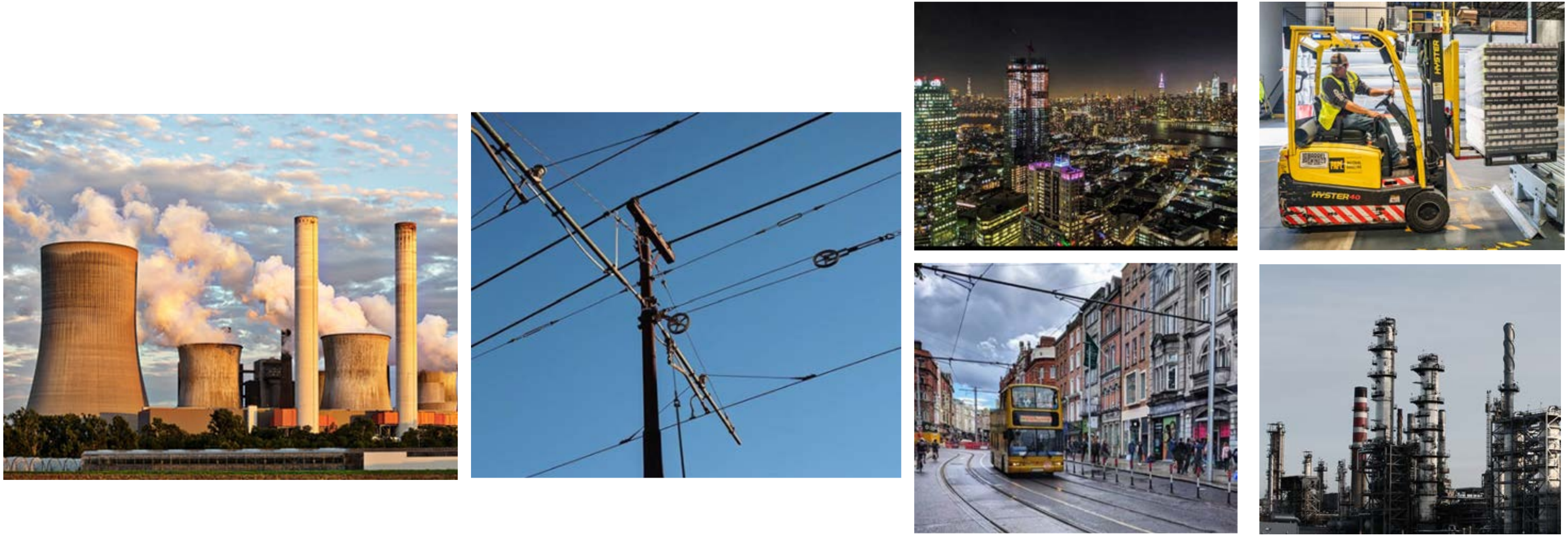
- Aspen Plus^{TM} overview

- Examples
  - 1. A novel IGCC-CC power plant integrated with an oxygen permeable membrane for hydrogen production and carbon capture (CC)
  - 2. Dynamic modeling of a flexible Power-to-X plant for energy storage and hydrogen production

What is an energy system?

- The energy system comprises all the components related to the production, conversion, delivery, and use of energy

---- Intergovernmental Panel on Climate Change [1]



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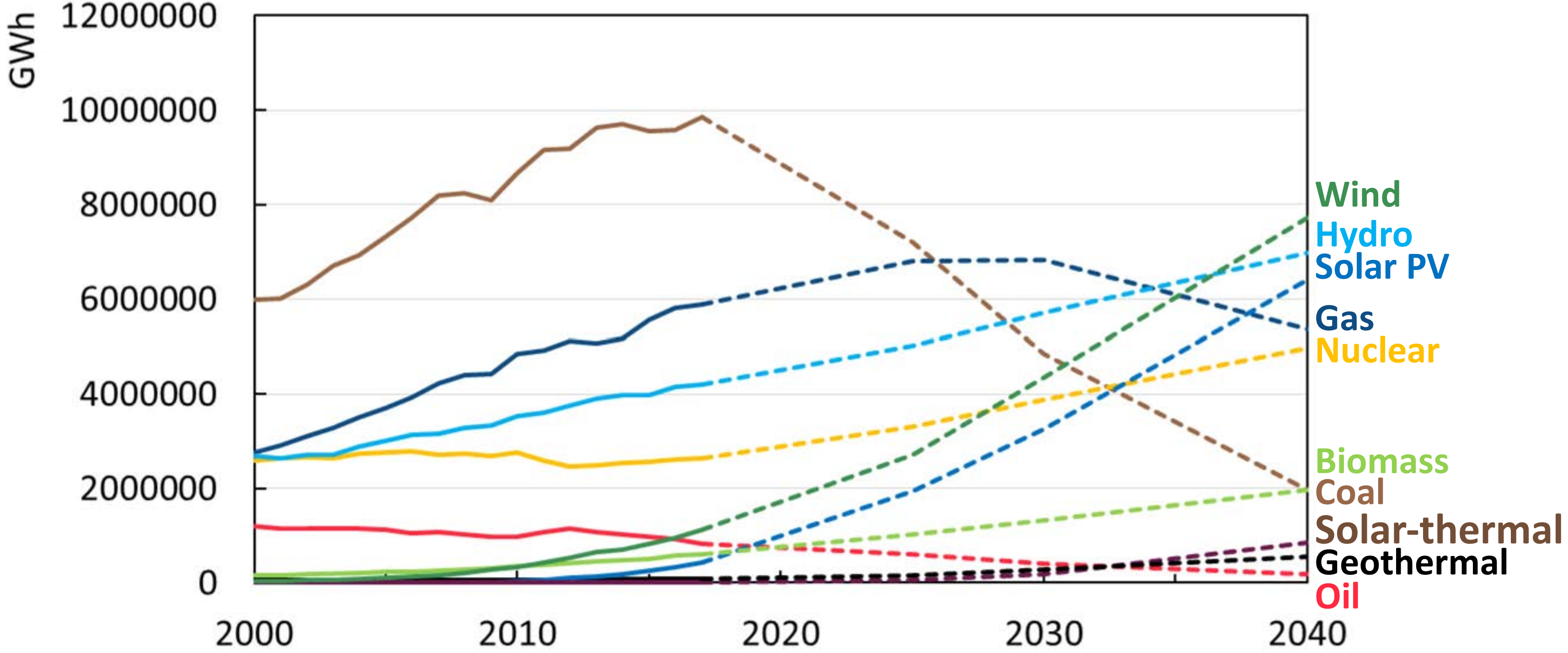
[1] IPCC, Climate change 2014, mitigation of climate change, P1261

Energy production: electricity production as an example

- Global electricity production by source and projection based on sustainable development



Sources: IEA website (up to 2017), IEA world energy outlook 2018, P529

Energy transport – electricity transmission congestion

- Electricity transmission has its own constraints -- thermal, voltage and stability limits designed to ensure reliability
- Congestion occurs when lack of transmission line capacity to deliver electricity reliably
- This can impact
  - Electricity price at peak demand
  - Transmission of the cheap renewable electricity
- Solutions:
  - Grid planning
  - Energy storage

An example: LMP separation in Texas[1]

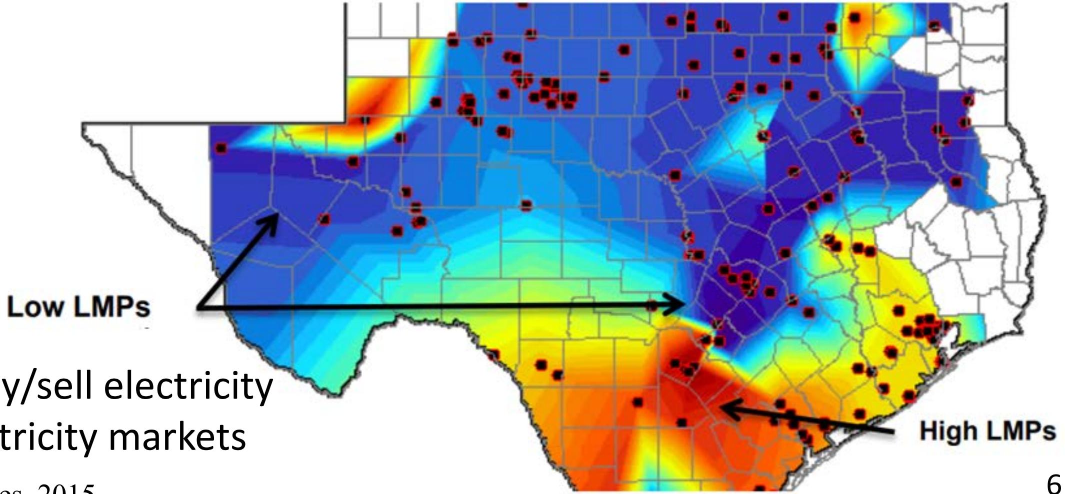


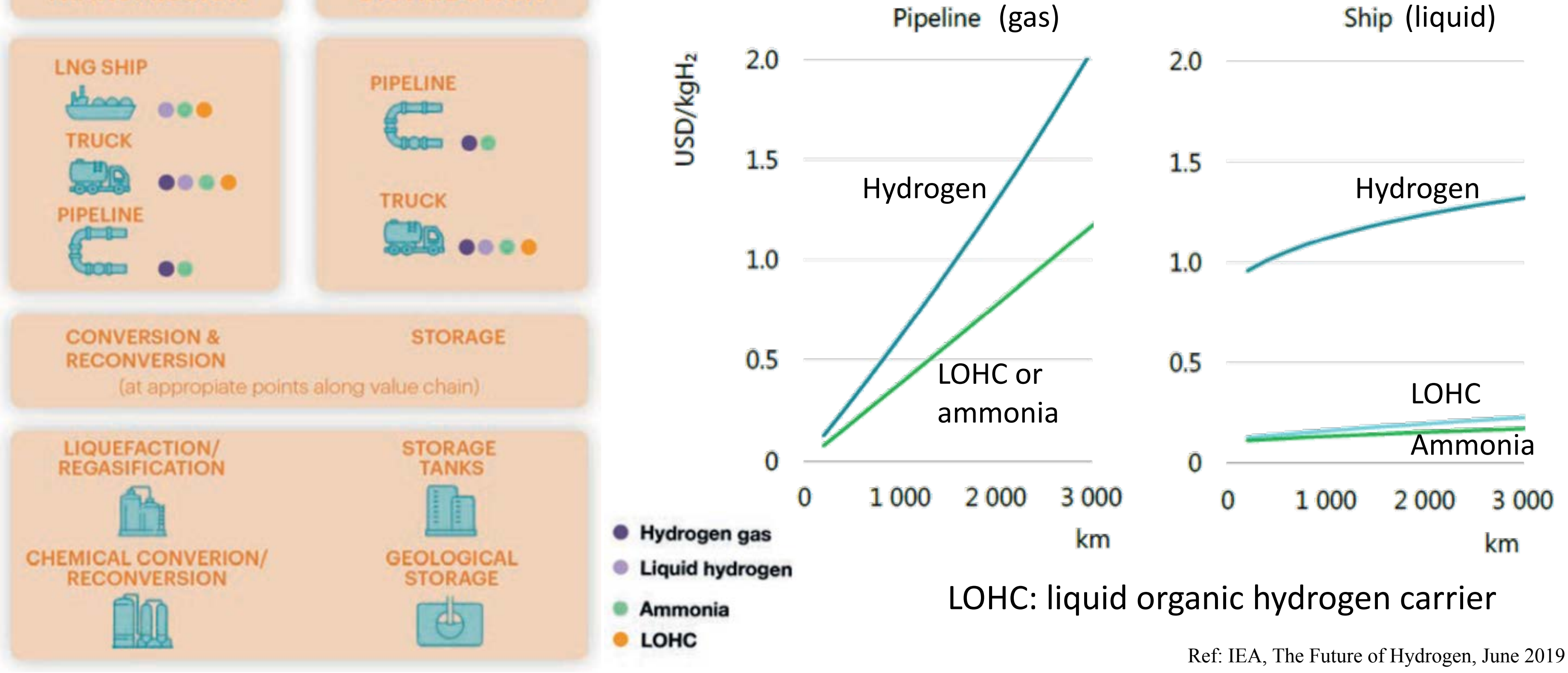
Image courtesy of NREL, DOE.

LMP: locational marginal pricing, cost to buy/sell electricity at different locations within wholesale electricity markets

[1] NREL, 'Renewables-Friendly' Grid Development Strategies, 2015

Energy transport – hydrogen transmission and distribution

Cost of hydrogen storage and transmission

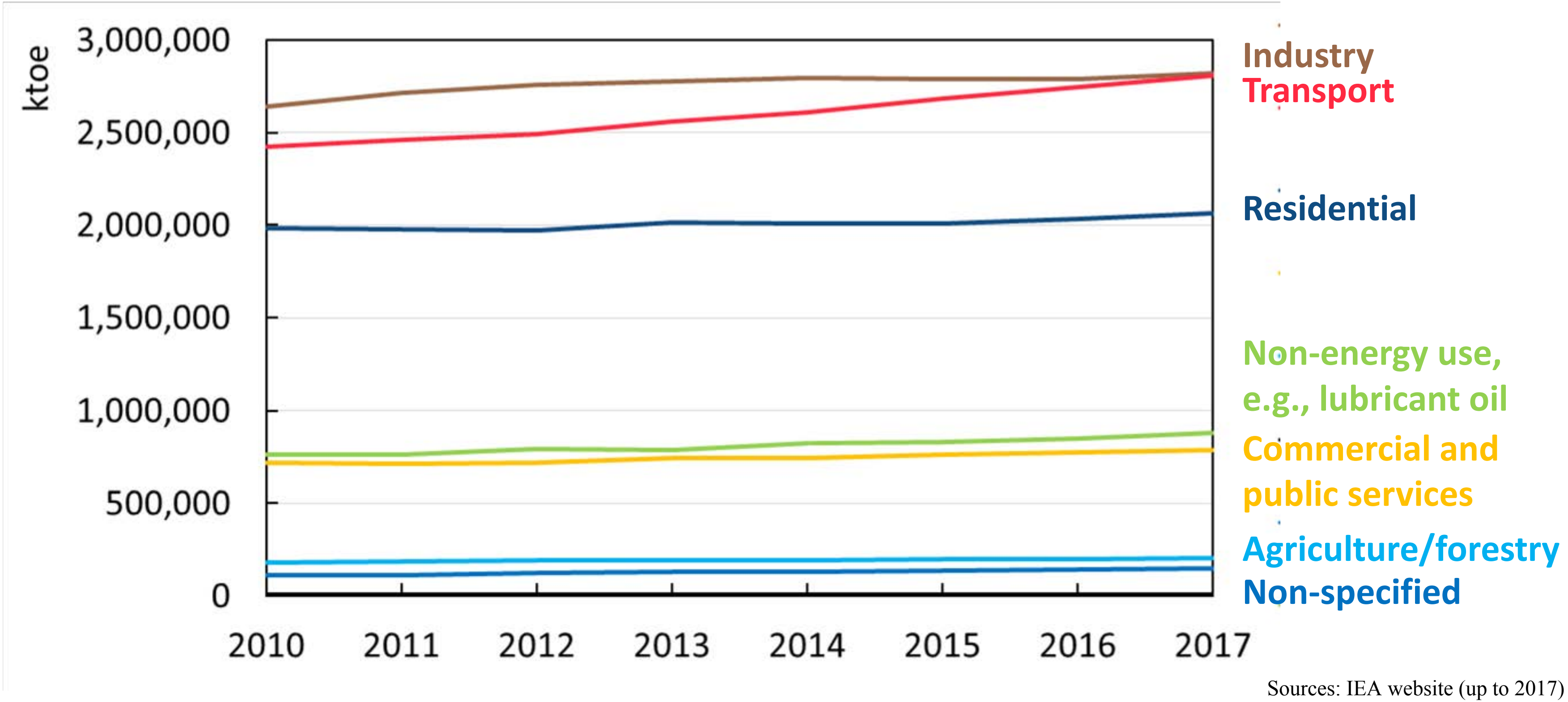


LOHC: liquid organic hydrogen carrier

Ref: IEA, The Future of Hydrogen, June 2019

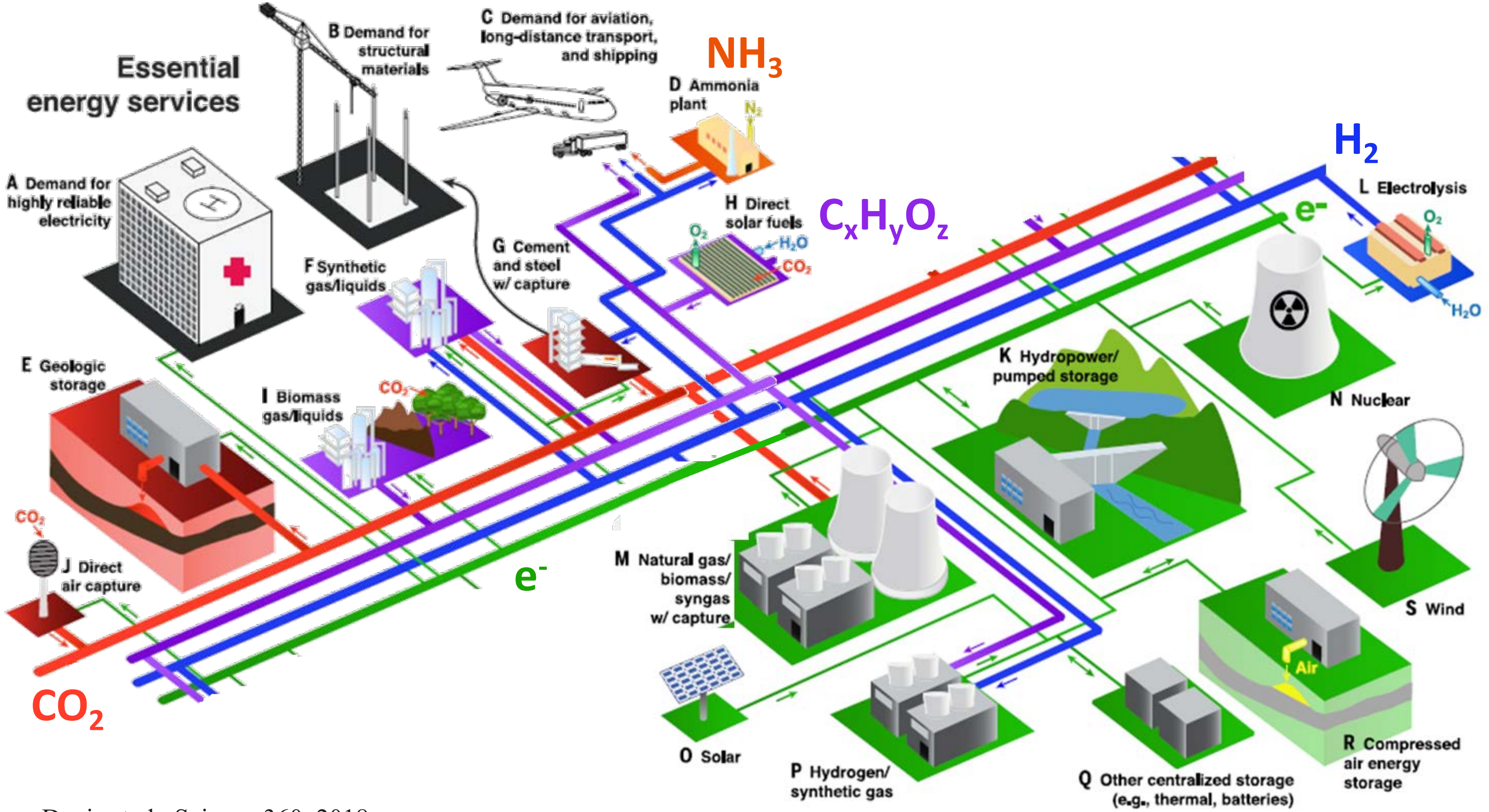
Energy consumption

- Global total energy consumption by sector



Sources: IEA website (up to 2017)

Net-zero emission integrated systems



Modified from Davis et al., Science 360, 2018

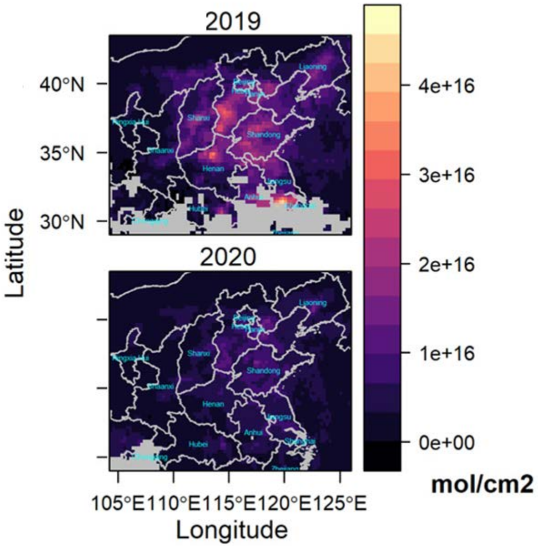
What do we talk about when we talk about energy systems?

- Energy efficiency: energy consumption and production
- Emissions: GHG, pollutants, waste heat, etc.
- Economics: money flow, etc.
- Societal impacts: health, risks, public perception, etc.
- ….

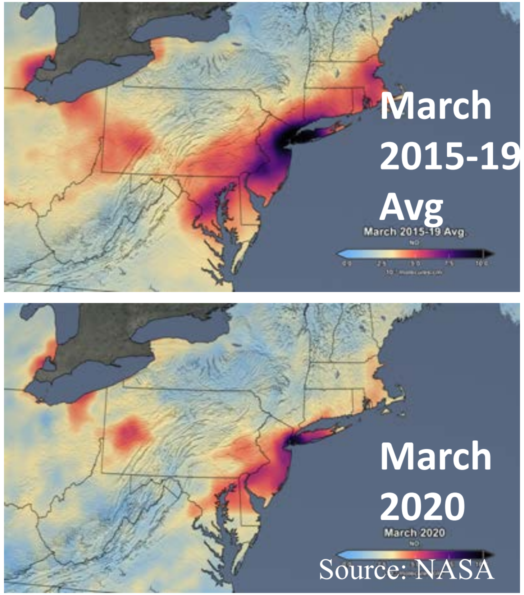
Energy systems and COVID-19: system perspective during analysis

- Pollution drops due to the lockdown of cities, decline in industry production and electricity demand
- But meanwhile, people suffers from health problems, job losses, etc.

NO_2 levels in part of China (a week after Chinese New Year)



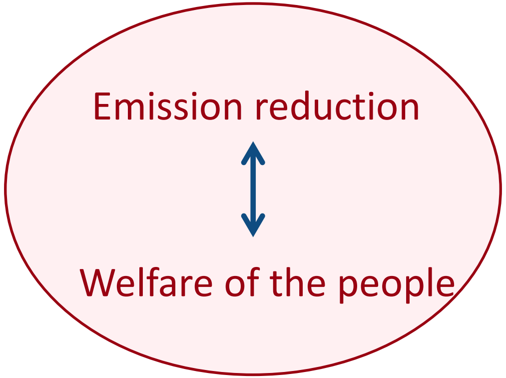
NO_2 levels in Northeast US in March



Source: NASA

Image courtesy of NASA.

System point of view



Emission reduction

↕

Welfare of the people

Energy consumption will ramp up after COVID-19, but in what manners?

- Fossil fuels?
  - Short term incentive due to low prices

Oil plunges 39% to 21-year low as sinking demand spurs uncertainty around storage

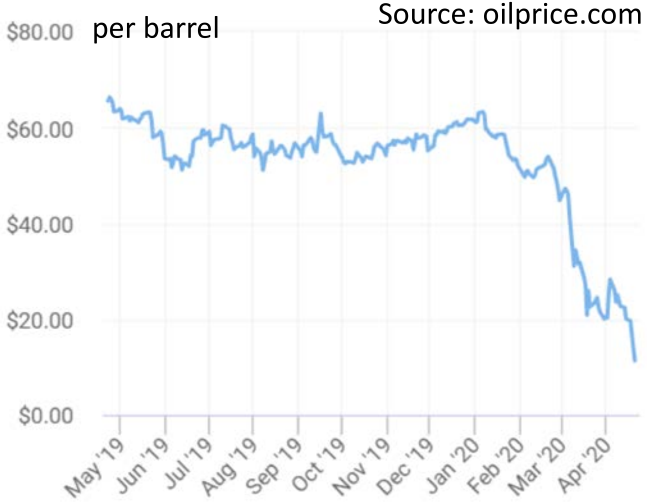
Saloni Sardana
Apr. 20, 2020, 05:39 AM

- Renewables?

> “Once COVID-19 has been defeated, attracting investments and re-establishing the manufacturing and supply chains for wind and solar power will take much longer than turning up production at oil wells and restarting thermal power plant units.” – *Nature Energy*

- Policies, supply chains, investments, manufacturing capabilities

West Texas intermediate (WTI) price



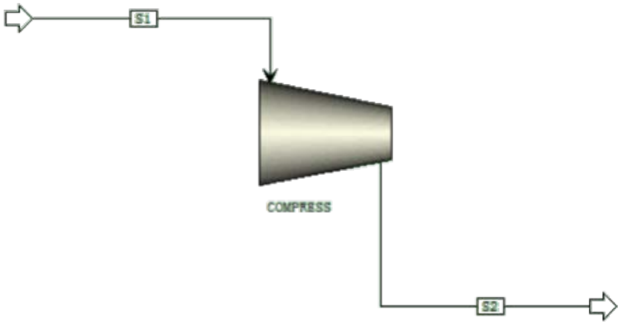
Ref: Recovering fast and slow. *Nat Energy* **5,** 273 (2020).

What do we talk about when we talk about energy systems?

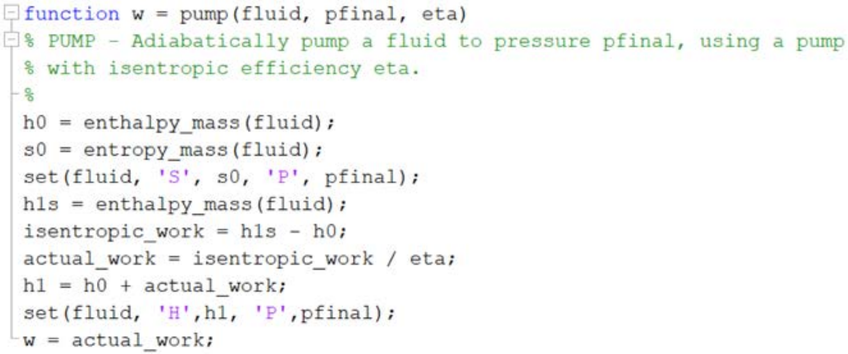
- Energy efficiency: energy consumption and production
- Emissions: GHG, pollutants, waste heat, etc.
- Economics: money flow, etc.
- Societal impacts: health, risks, public perception, etc.
- ….
- **It is useful to obtain these information of the complex energy systems (integrated mechanical, chemical and electrical components) using some modeling softwares**

Some modeling softwares

- With interactive graphical user interfaces (Drag-and-connect)
  - Aspen Plus
  - Thermoflow
  - gPROMS



- Mainly coding
  - EES
  - Matlab
  - Cantera



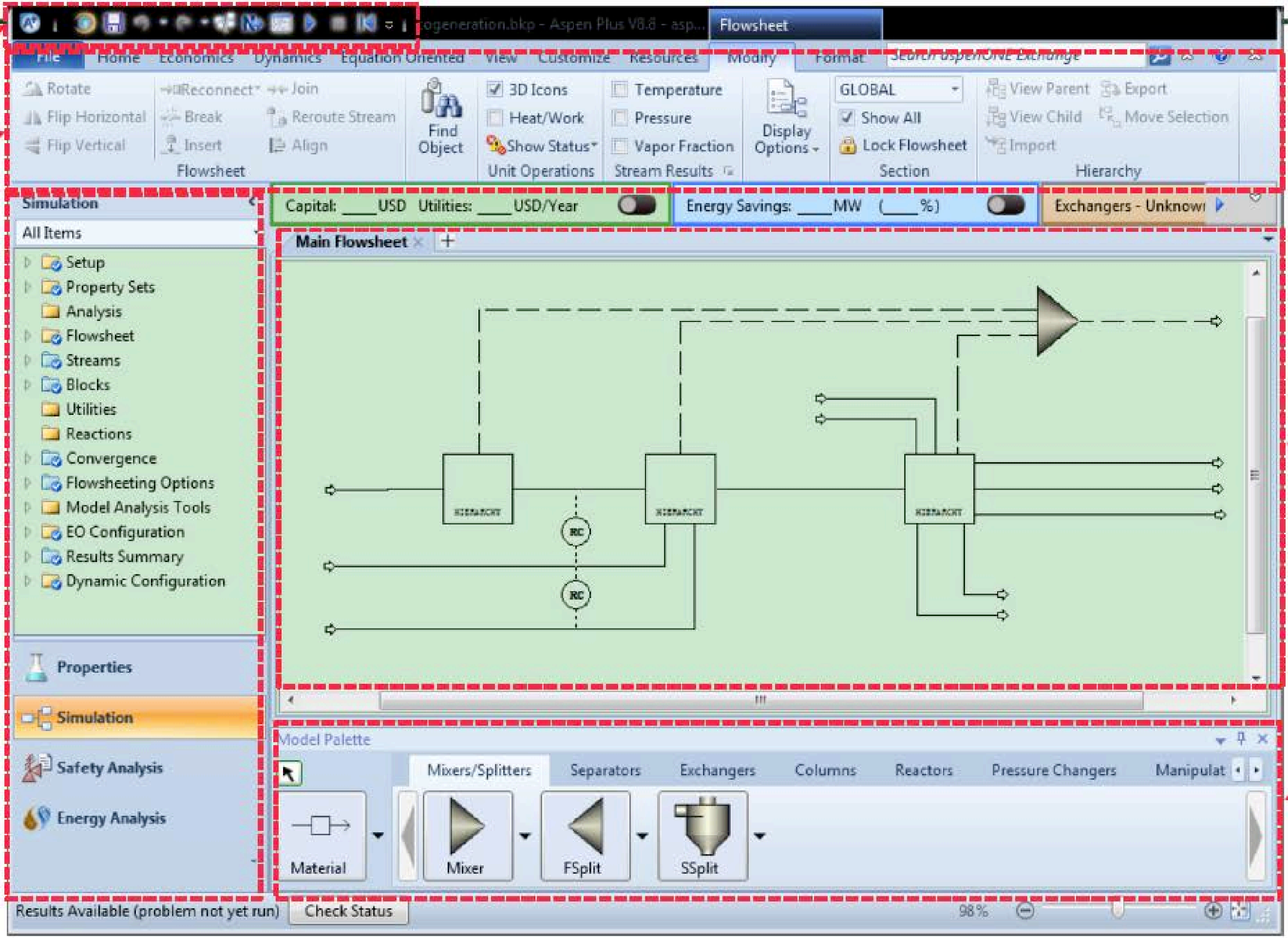
```
function w = pump(fluid, pfinal, eta)
% PUMP - Adiabatically pump a fluid to pressure pfinal, using a pump
% with isentropic efficiency eta.
%
h0 = enthalpy_mass(fluid);
s0 = entropy_mass(fluid);
set(fluid, 'S', s0, 'P', pfinal);
h1s = enthalpy_mass(fluid);
isentropic_work = h1s - h0;
actual_work = isentropic_work / eta;
h1 = h0 + actual_work;
set(fluid, 'H',h1, 'P',pfinal);
w = actual_work;
```

A tool for energy analysis: Aspen Plus^{TM}

- A process simulation tool
  - Heat Exchanges
  - Reactors
  - Pressure Changers (Valves, Pumps, Compressors, etc.)
  - Distillation Columns
  - Absorption Columns
  - Extractors
  - Flash systems
  - Separators & Mixers
  - Solid Operations (Crushing, sieving, filtration, etc…)
  - User models (unique for you!)
- Given a process design and an appropriate selection of thermodynamic models, it uses mathematical models to predict the performance of the process

Extracted from: chemicalengineeringguy.com

User interface



Short-cut

Ribbon

Simulation configuration

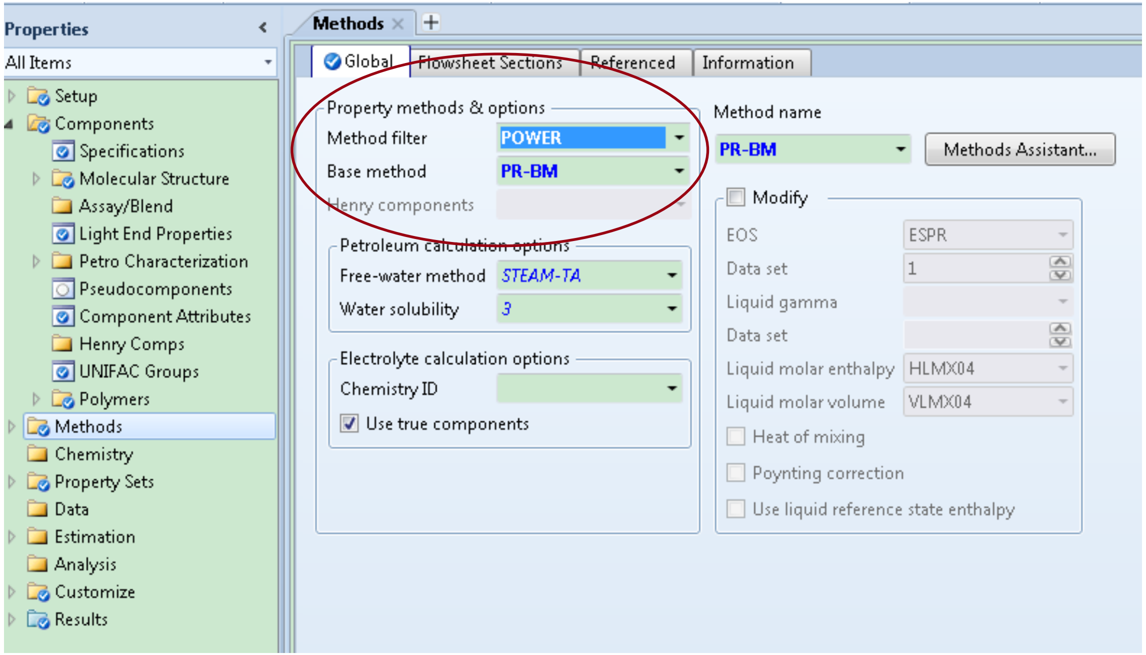
Process flowsheet

Process components

General steps for process modeling using Aspen Plus^{TM}

- 1. Define chemical components in the process and select the appropriate thermodynamics model
- 2. Build the process by dragging and connecting components from the palette
- 3. Define the input of the process and the components' parameters
- 4. If there are some constraints in the flowsheet, e.g., temperature, flow rate, and component performance, input them into the flowsheeting options.
- 5. Run the simulation!

Thermodynamics method is important for evaluating the physical properties



Property methods & options

Method filter: POWER

Base method: PR-BM

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: PR-BM

☐ Modify

EOS: ESPR

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX04

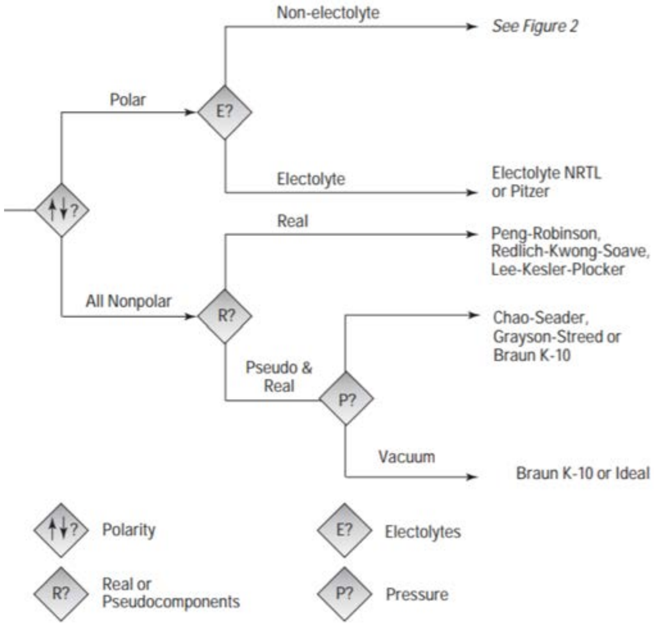
Liquid molar volume: VLMX04

☐ Heat of mixing

☐ Poynting correction

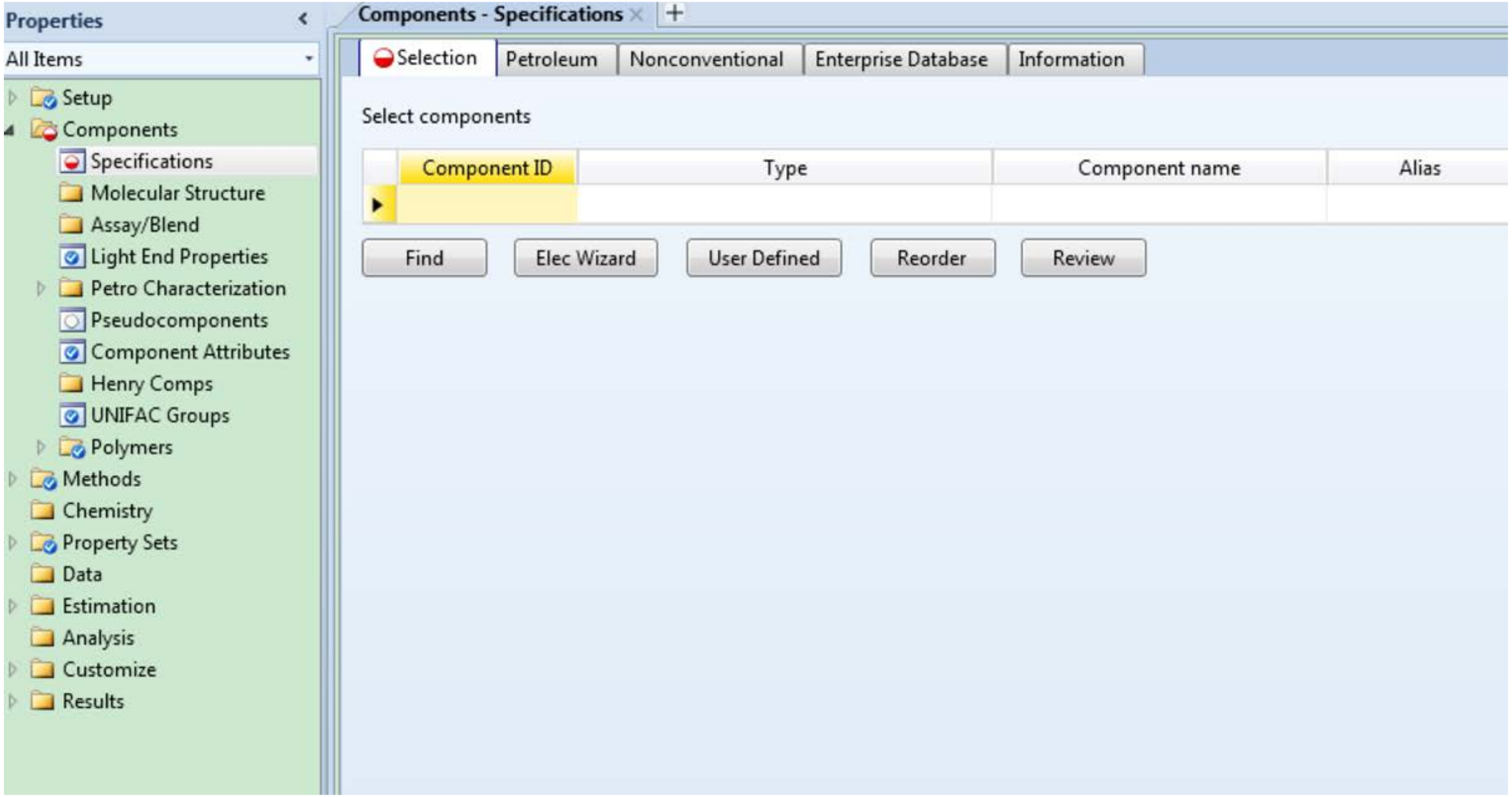
☐ Use liquid reference state enthalpy

Flow chart for method selection

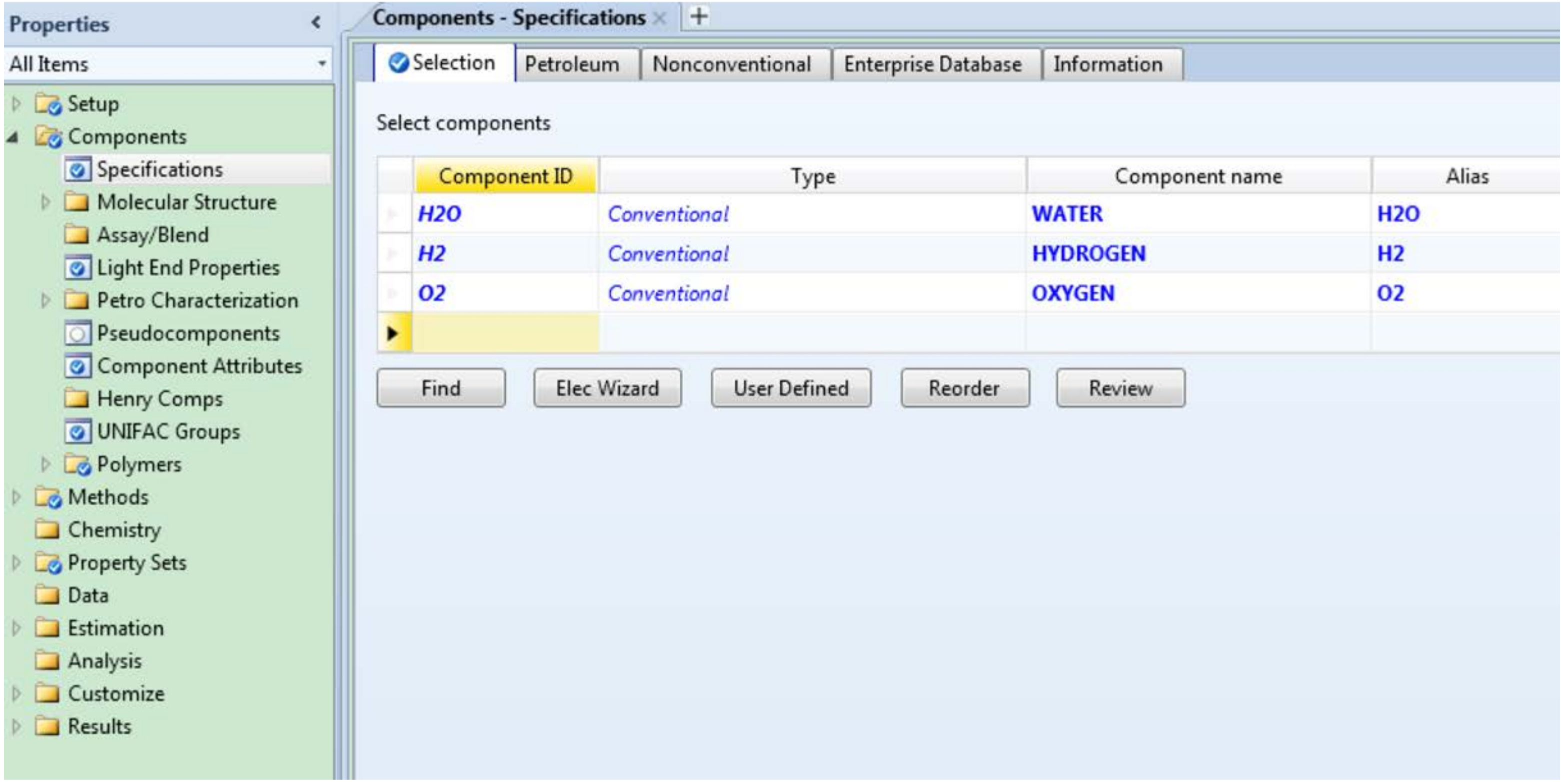


Ref: Don’t Gamble With Physical Properties For Simulations, Eric C. Carlson, Aspen Technology, Inc

First, select components and thermodynamics properties



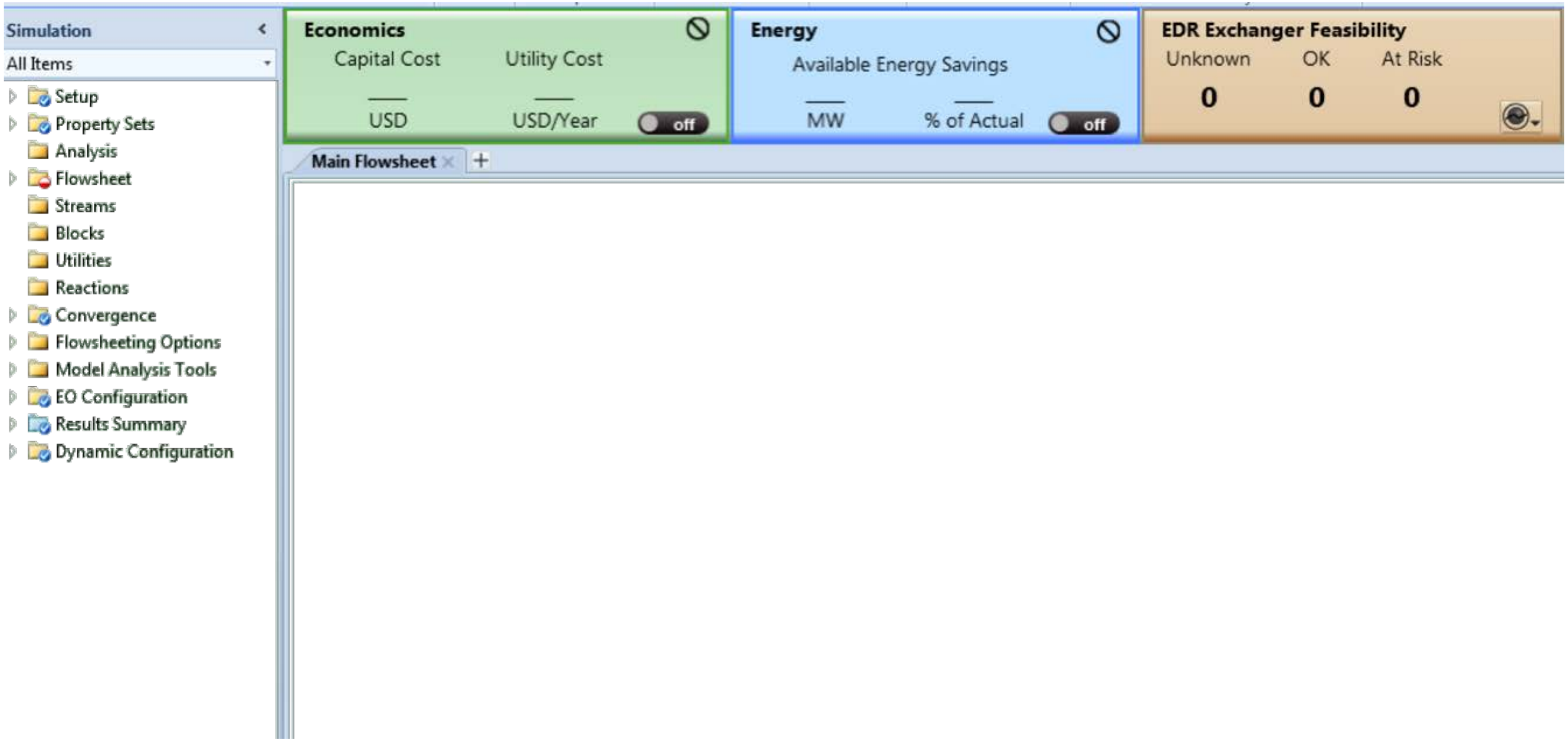
First, select components and thermodynamics properties



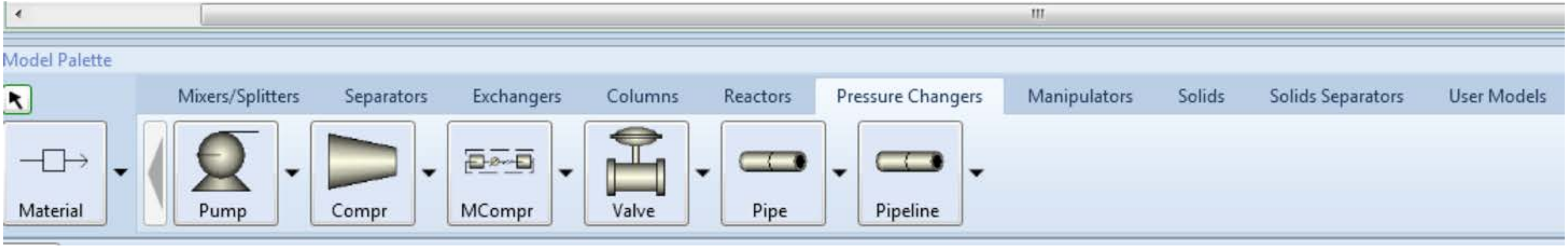
Select components

Component ID	Type	Component name	Alias
H2O	Conventional	WATER	H2O
H2	Conventional	HYDROGEN	H2
O2	Conventional	OXYGEN	O2

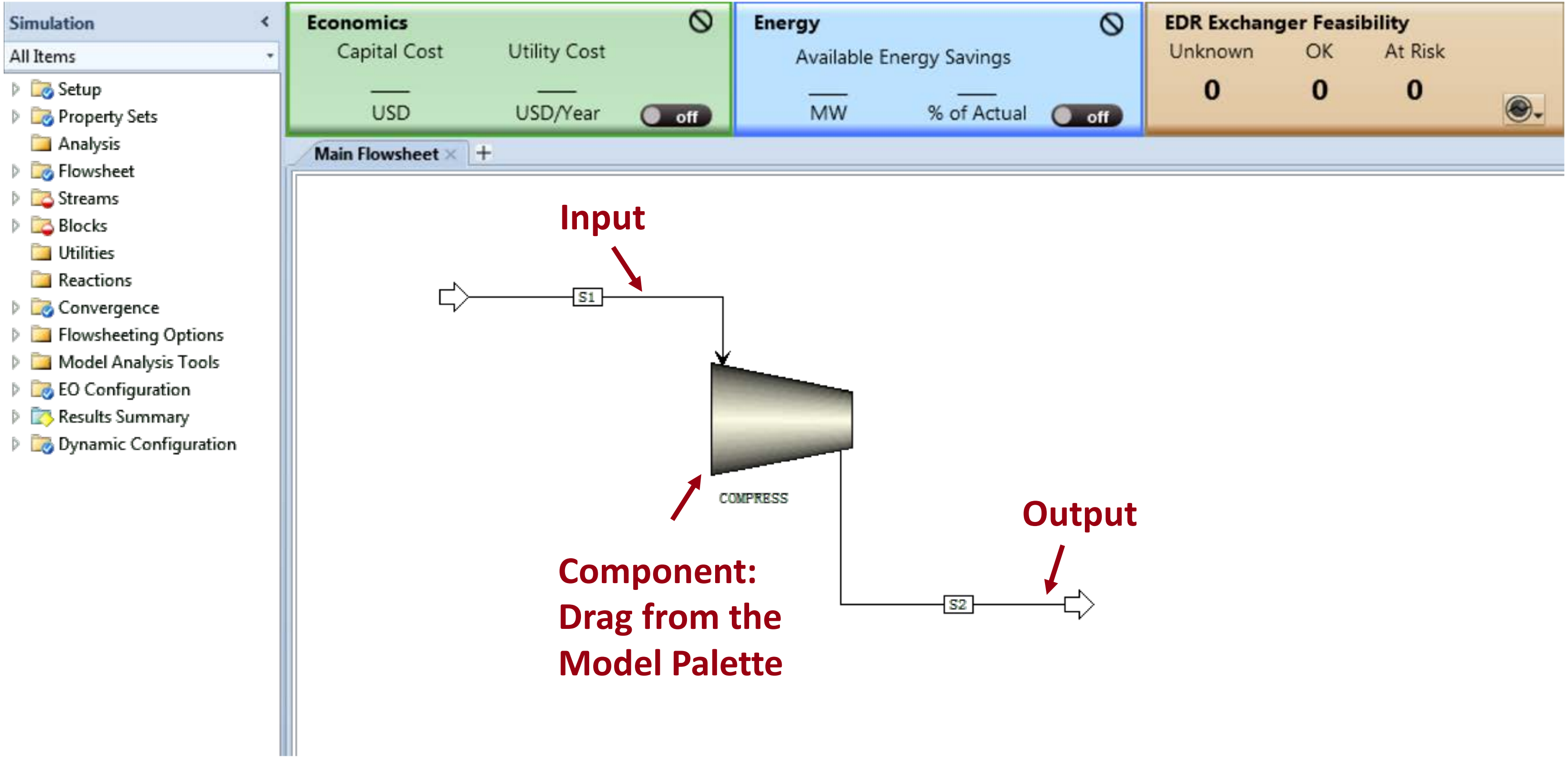
Then, draw the process flowsheet



The process components can be added into the process



Then, connect the components

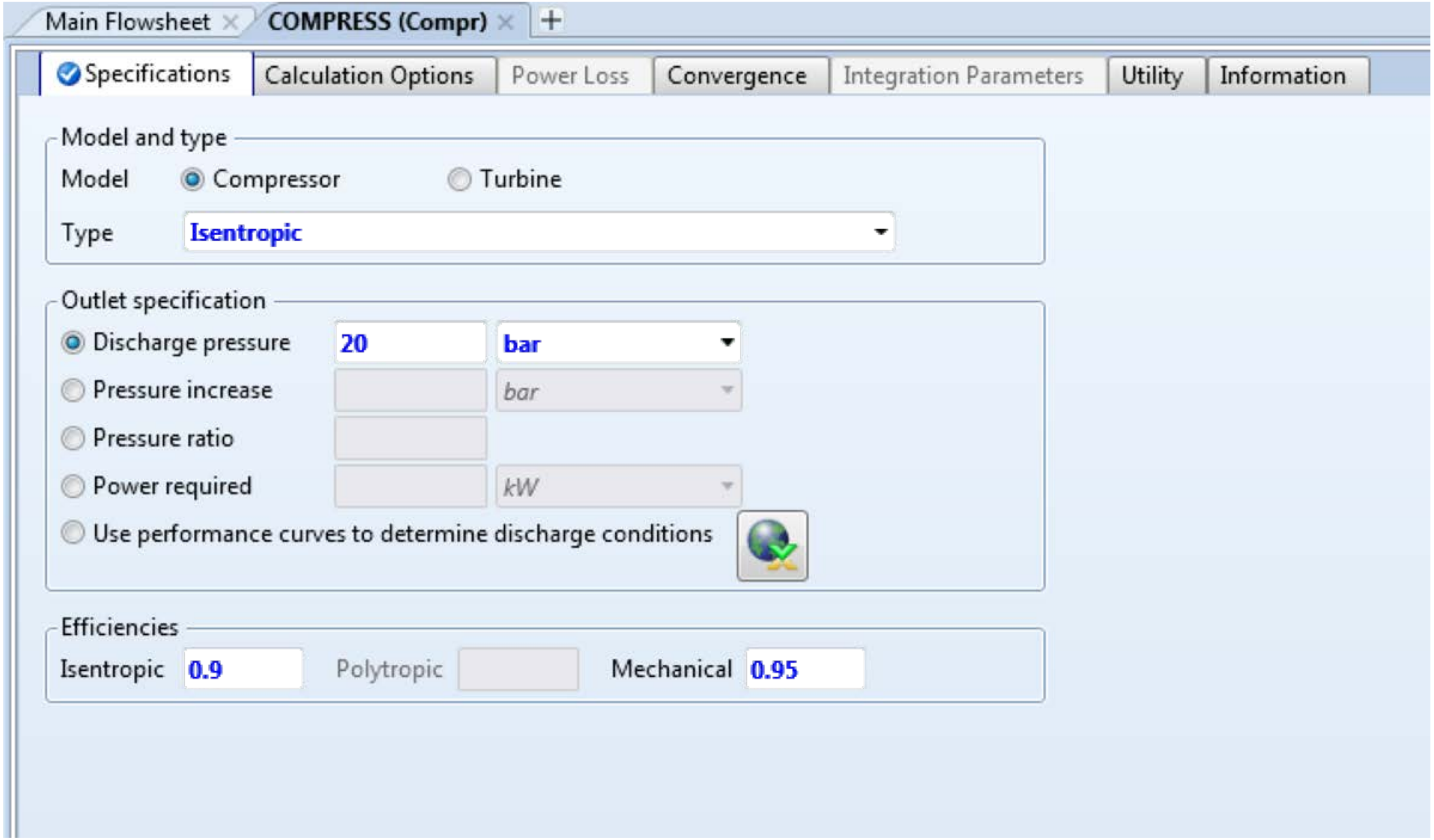


Input

Component: Drag from the Model Palette

Output

By double clicking the component, you can look at its settings



Model and type

Model ● Compressor ○ Turbine

Type: Isentropic

Outlet specification

● Discharge pressure: 20 bar

○ Pressure increase: bar

○ Pressure ratio

○ Power required: kW

○ Use performance curves to determine discharge conditions

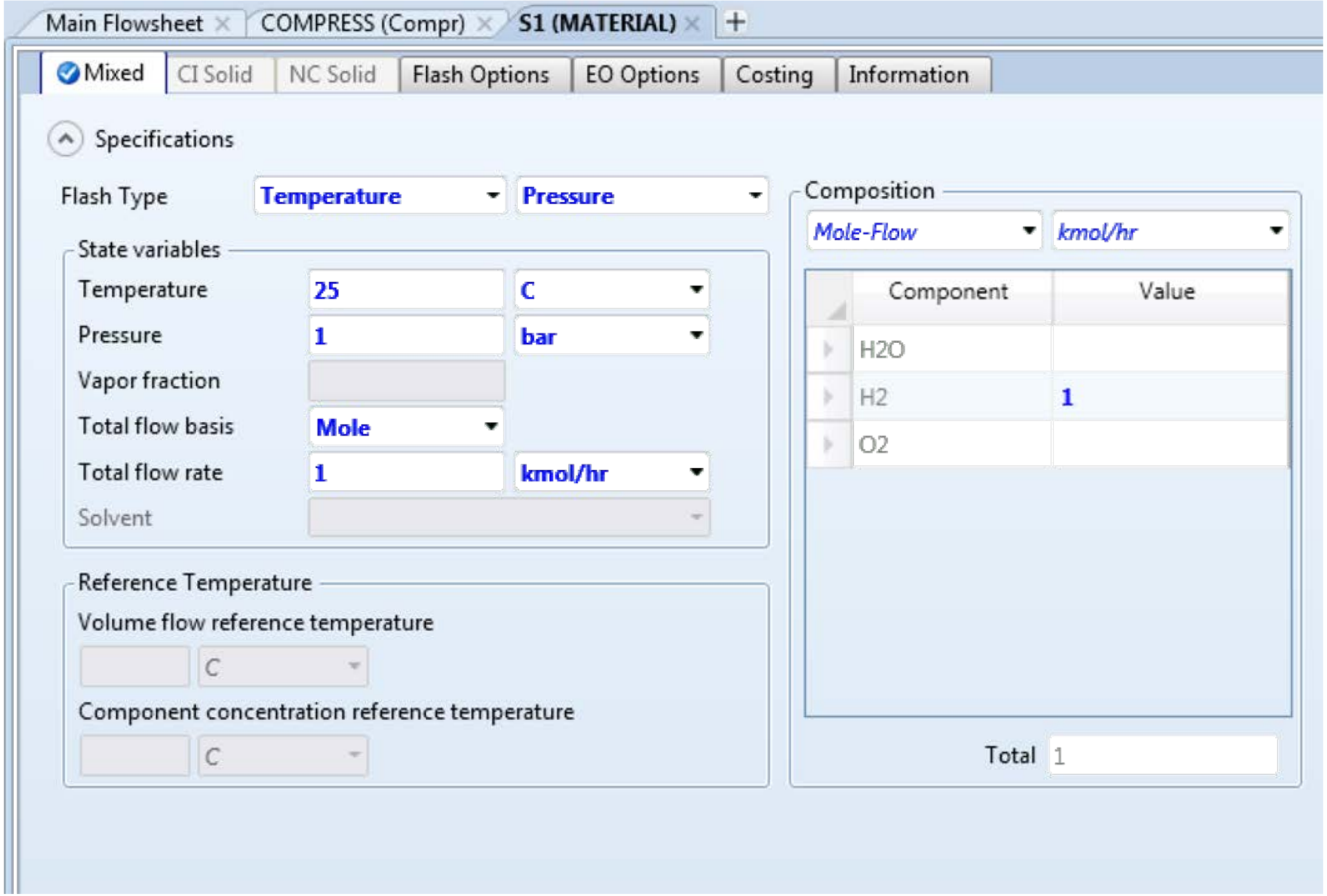
Efficiencies

Isentropic: 0.9

Polytropic:

Mechanical: 0.95

Define the inlet



Flash Type: Temperature, Pressure

State variables
Temperature: 25 C
Pressure: 1 bar
Vapor fraction:
Total flow basis: Mole
Total flow rate: 1 kmol/hr
Solvent:

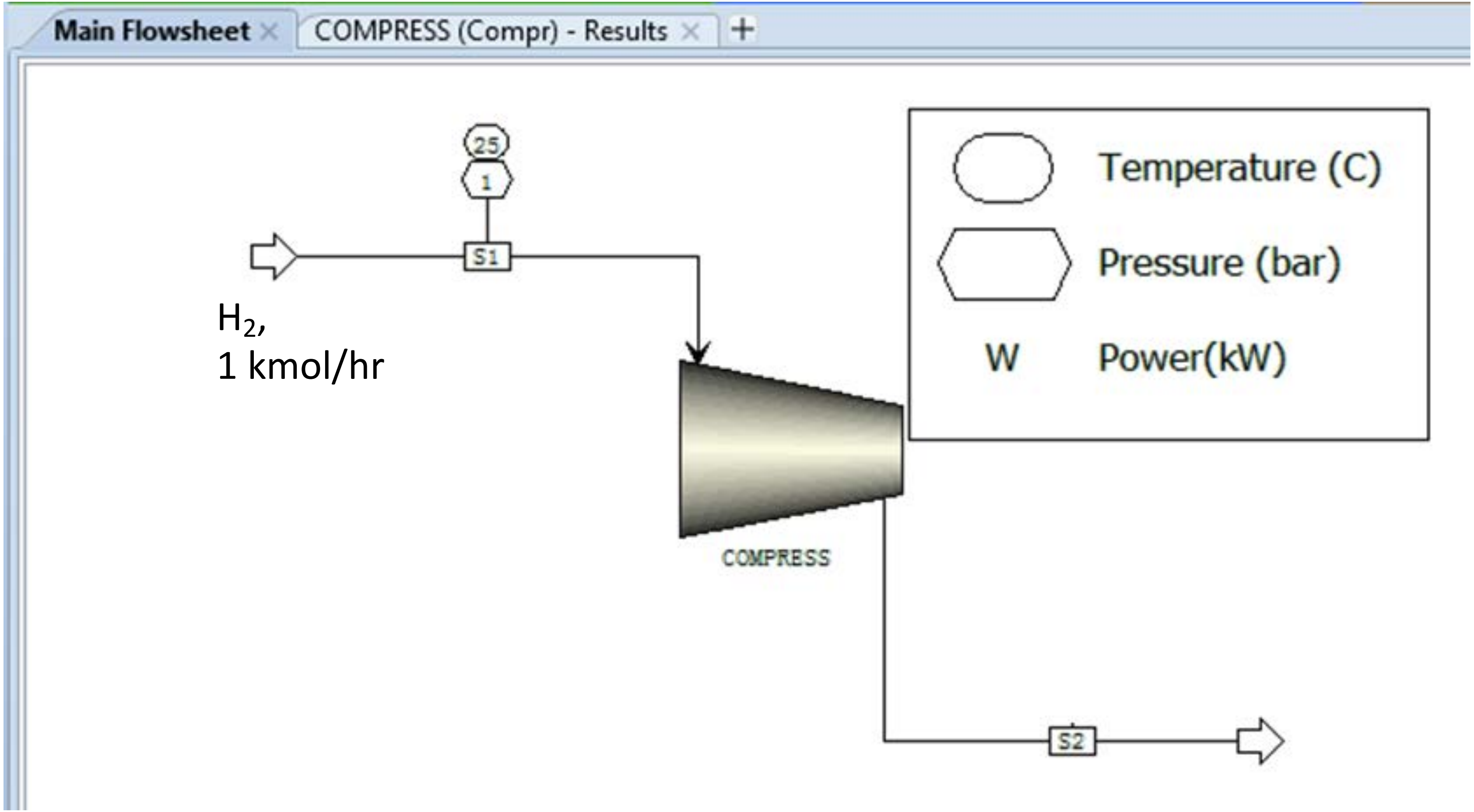
Reference Temperature
Volume flow reference temperature: C
Component concentration reference temperature: C

Composition: Mole-Flow, kmol/hr

Component	Value
H2O	
H2	1
O2	

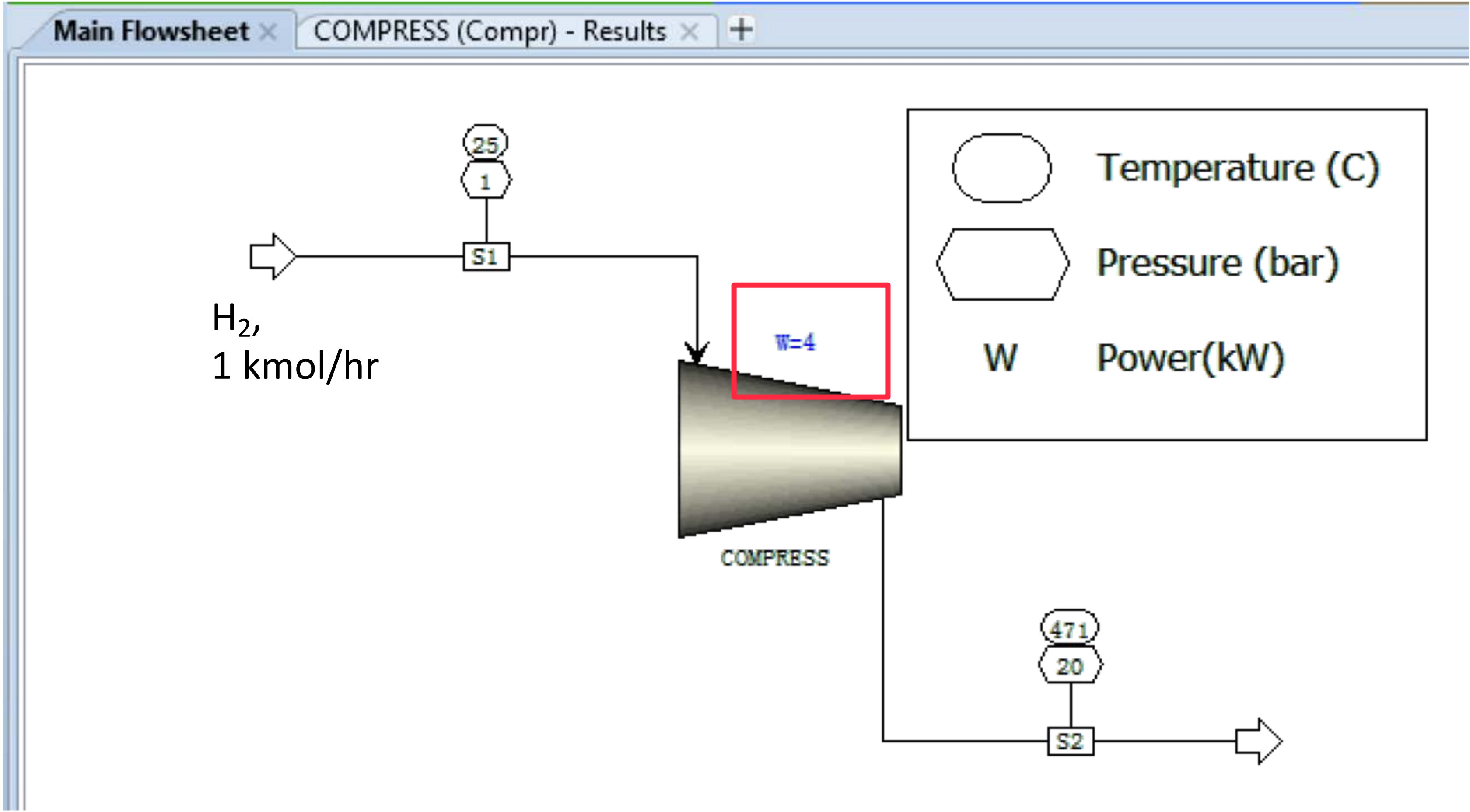
Total: 1

Click run



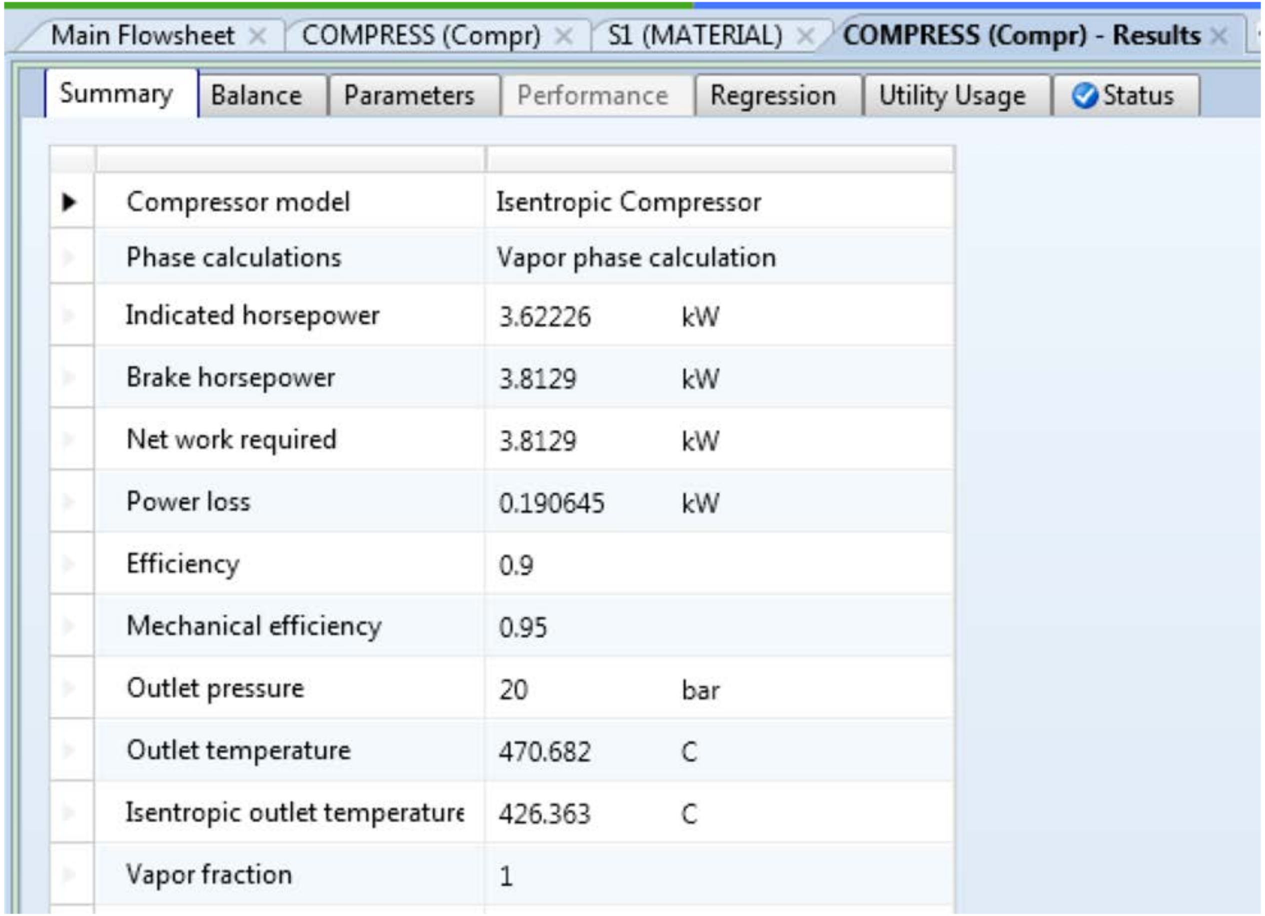
H_2,
1 kmol/hr

Results for the hydrogen pressure



H_2,
1 kmol/hr

More details results can be found by right clicking the component



Compressor model	Isentropic Compressor	
Phase calculations	Vapor phase calculation	
Indicated horsepower	3.62226	kW
Brake horsepower	3.8129	kW
Net work required	3.8129	kW
Power loss	0.190645	kW
Efficiency	0.9	
Mechanical efficiency	0.95	
Outlet pressure	20	bar
Outlet temperature	470.682	C
Isentropic outlet temperature	426.363	C
Vapor fraction	1	

Some examples

- 1. Thermodynamic efficiency of a novel IGCC-CC power plant integrated with an oxygen permeable membrane for hydrogen production and carbon capture (CC)

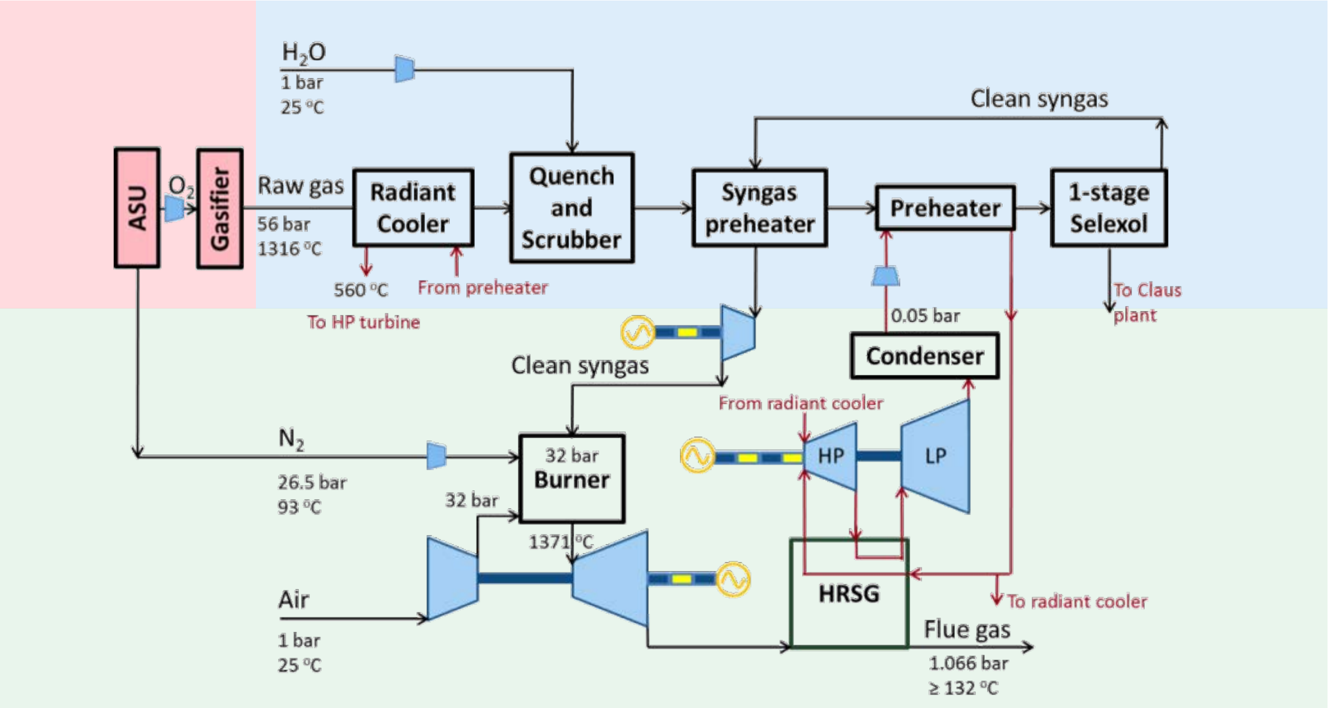
(XY Wu, et al., Journal of Advanced Manufacturing and Processing, 2020, under review)

- 2. Dynamic modeling of a flexible Power-to-X plant

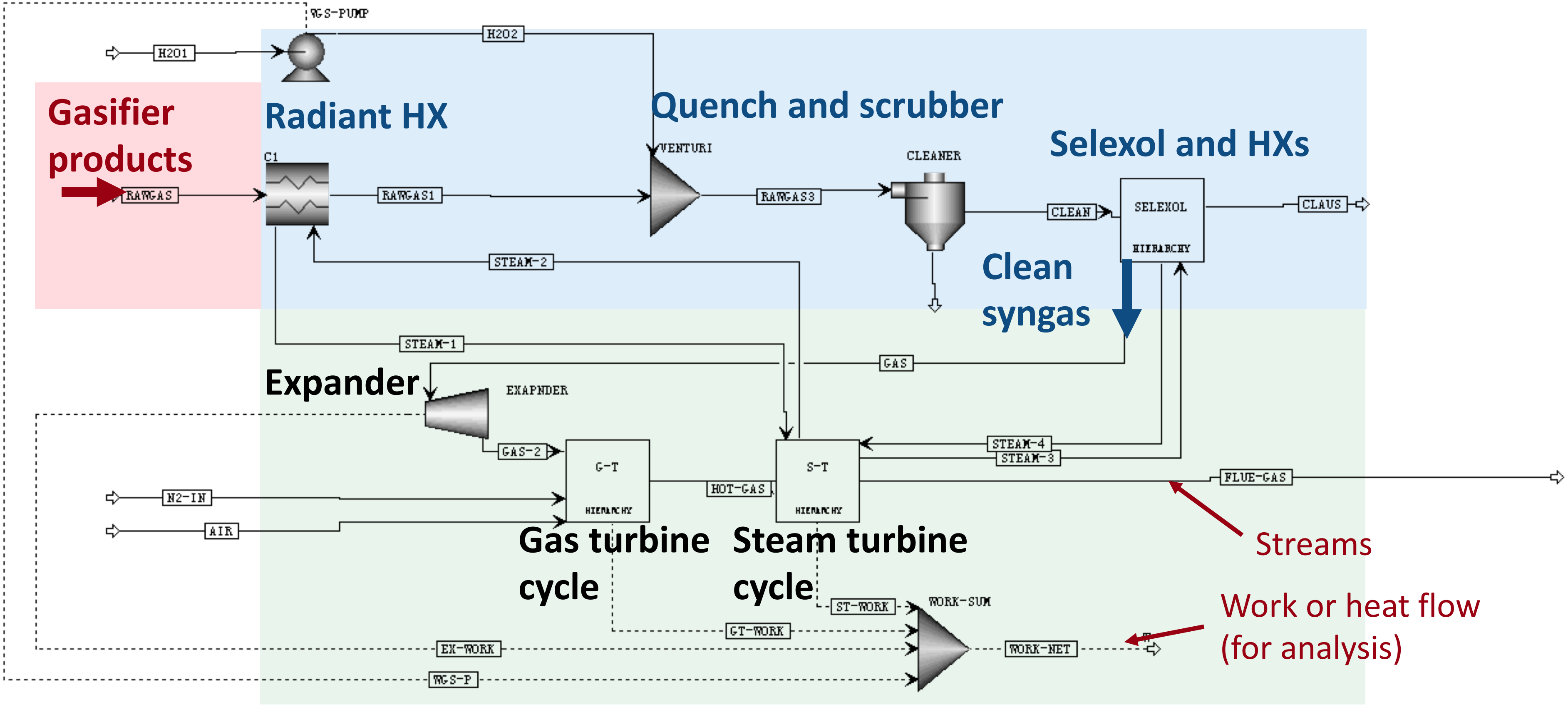
(G Buffo, et al., Journal of Energy Storage, 2020, 29, 101314)

Example 1: Energy efficiency analysis (IGCC-CC)

- Conventional Integrated Gasification Combined Cycle (IGCC) plant includes **gasifier**, **syngas cleaning systems**, and a **combined cycle**



Layout of the Aspen model



Gasifier products

Radiant HX

Quench and scrubber

Selexol and HXs

Clean syngas

Expander

Gas turbine cycle

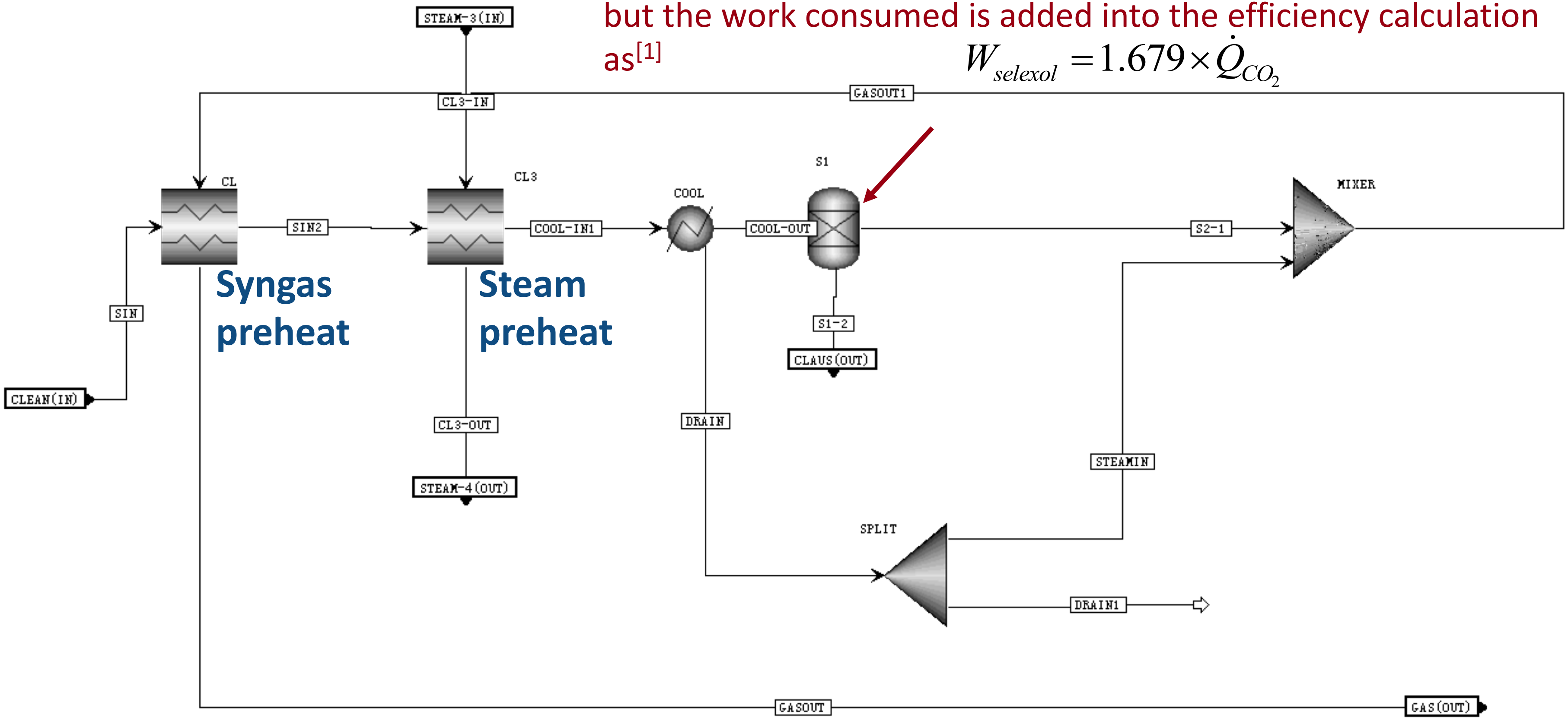
Steam turbine cycle

Streams

Work or heat flow (for analysis)

Selexol reactor

The Selexol process is modeled as a separator in Aspen model, but the work consumed is added into the efficiency calculation as[1] $W_{selexol} = 1.679 \times \dot{Q}_{CO_2}$

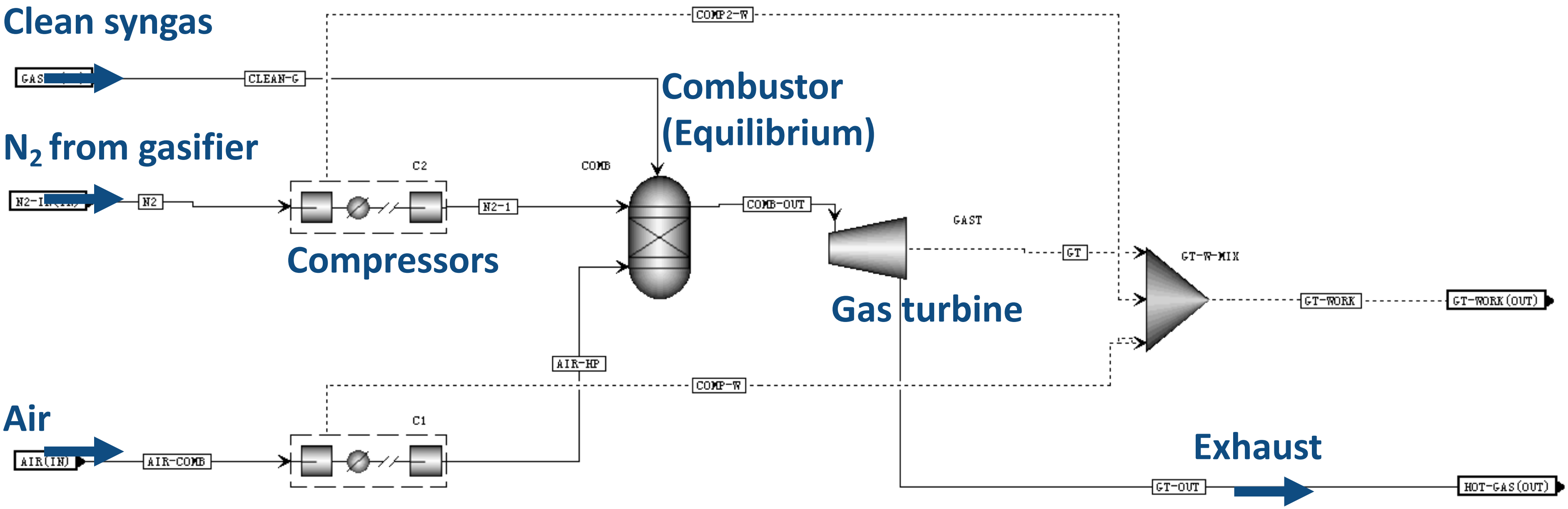


Syngas preheat

Steam preheat

[1] Kyle A, et al., Cost and performance of PC and IGCC plants for a range of carbon dioxide capture, DOE, 2013

Gas turbine cycle



Clean syngas

N_2 from gasifier

Compressors

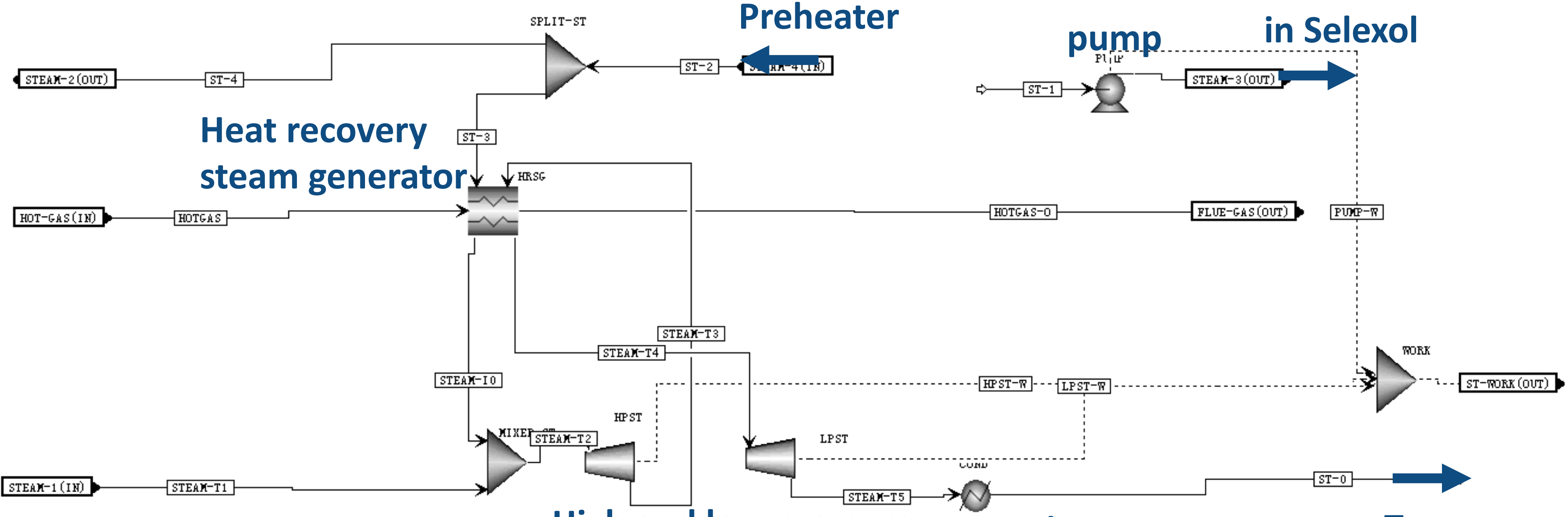
Combustor (Equilibrium)

Gas turbine

Air

Exhaust

Steam turbine cycle



From Preheater

pump

To Preheater in Selexol

Heat recovery steam generator

High and low pressure gas turbines

condenser

To pump

The close-loop is open in order to make the system converge faster

- The condition in the downstream of the condenser is known, which is fed into the pump
- The flow rate of the working fluid is determined by the inlet of the HPST

Validate the base IGCC model with literature

- The first law efficiency is defined:

$$\eta = \frac{W_{net}}{HHV_{coal}}$$

- The net work output of the cycle is calculated as

$$W_{net} = W_{GT} + W_{ST} + W_{EXP} - \sum W_{pump} + \sum W_{CO_2} + \sum W_{O_2} + W_{Selexel} + W_{aux-gasifier} + W_{BOP} + W_{transformer}$$

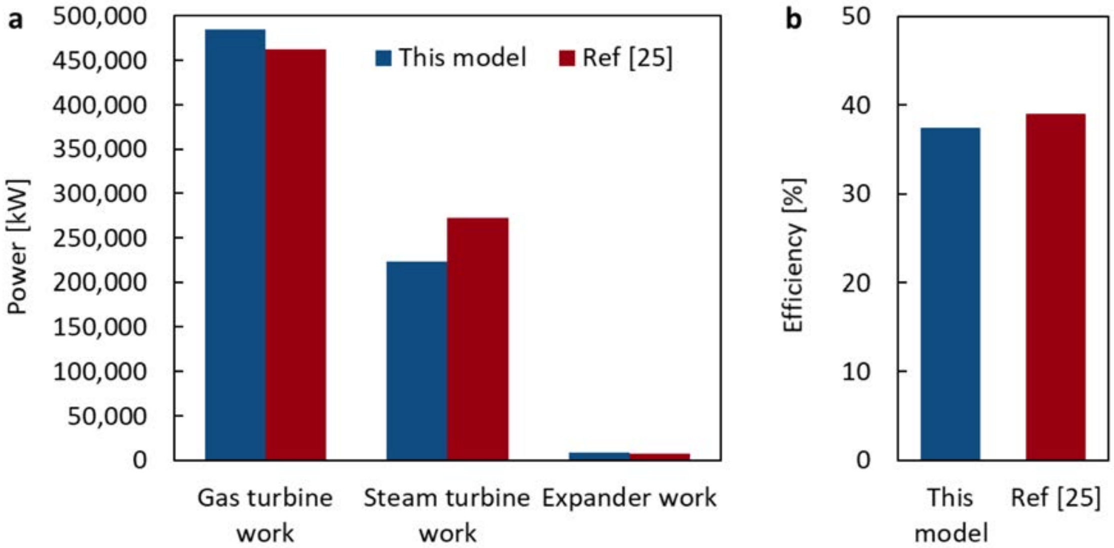


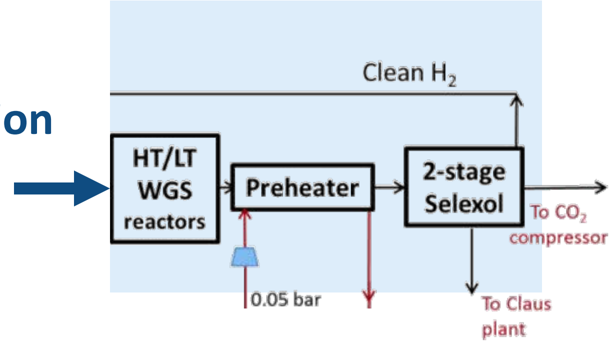
Image courtesy of DOE.

[1] Kyle A, et al., Cost and performance of PC and IGCC plants for a range of carbon dioxide capture, DOE, 2013

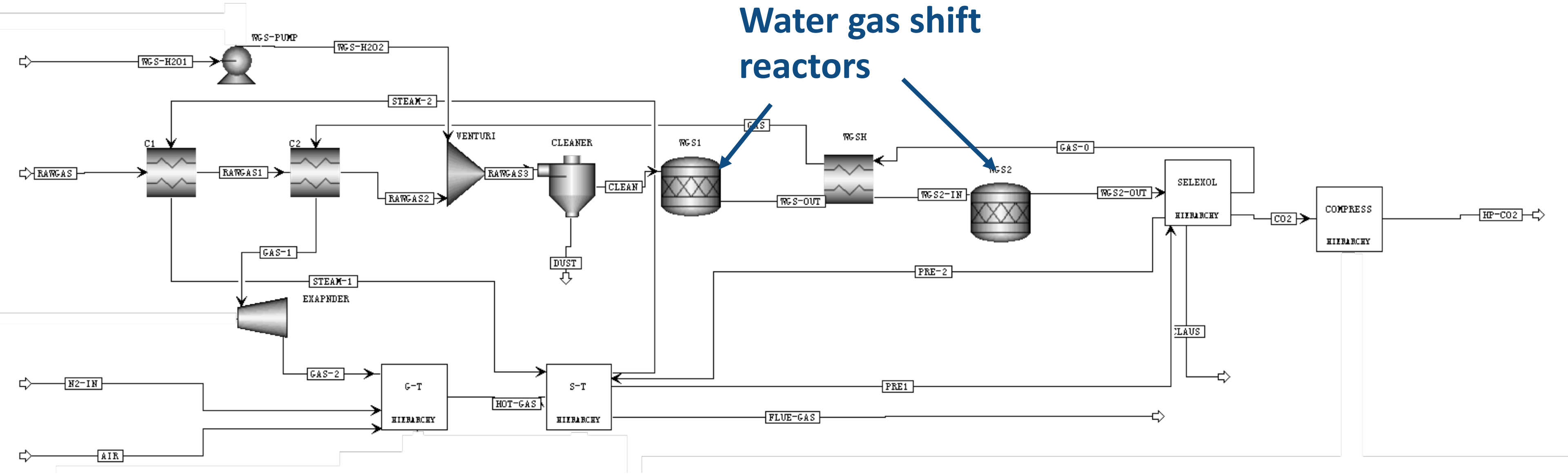
To capture CO_2, water gas shift reactors and acid gas removal systems are installed

- Water gas shift reactor converts CO into CO_2: $CO + H_2O \rightarrow CO_2 + H_2$
- Selexol processes separate CO_2 and H_2S

Gasification products



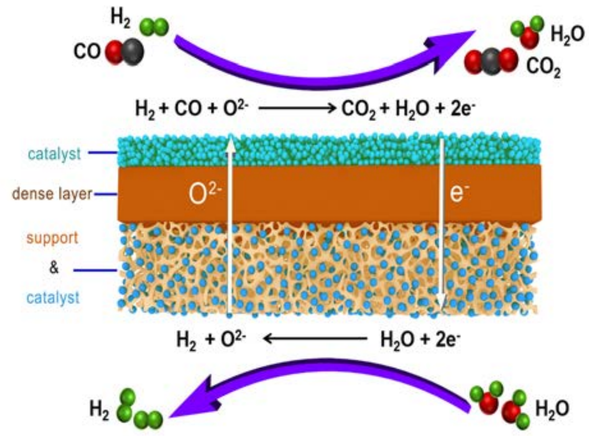
IGCC-WGS

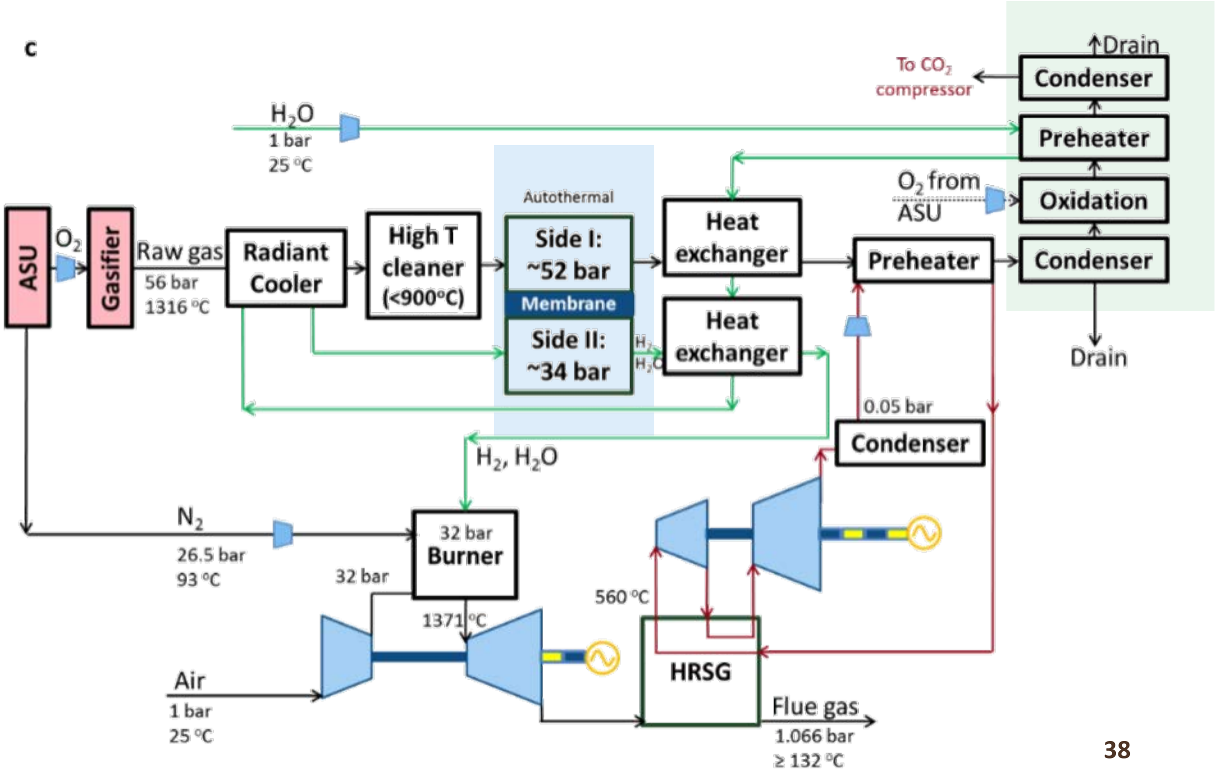


Water gas shift reactors

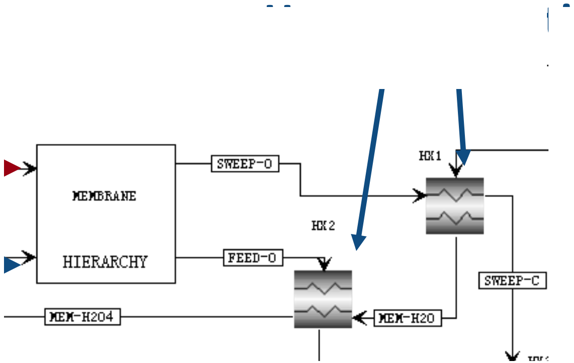
Instead, IGCC-OTM system uses a membrane to produce high purity H_2 with CC

- An oxygen permeable membrane can produce H_2 from water splitting and oxidize the fuel in one unit



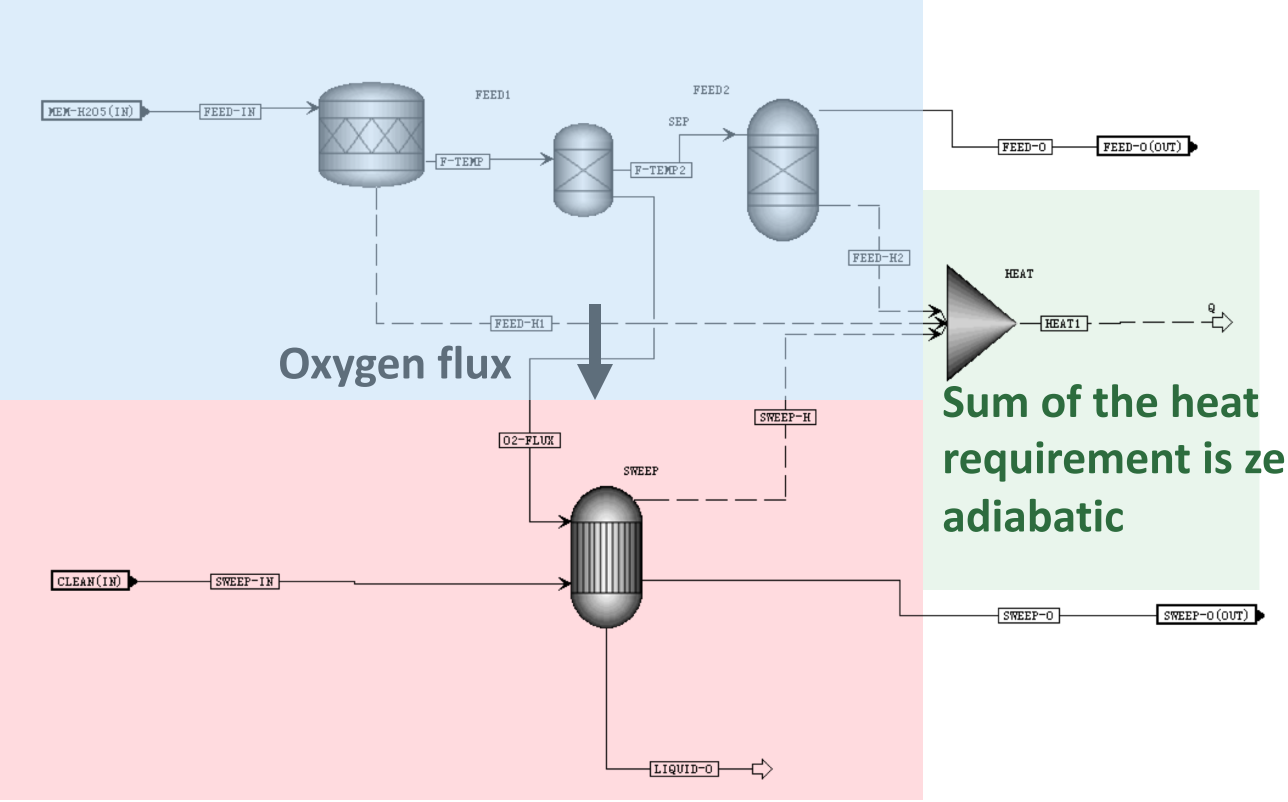


IGCC-OTM


MEMBRANE
HIERARCHY
SWEEP-O
FEED-O
HX1
HX2
SWEEP-C
MEM-H204
MEM-H20

Membrane reactor

Water splitting side



Oxygen flux

Sum of the heat requirement is zero: adiabatic

Syngas oxidation side

Operating conditions

- After connecting all the components in Aspen Plus, the operating conditions and parameters have to be entered

Fuel	
Coal rank	High-volatile A bituminous (Illinois No. 6) HHV (as-received) = 27.135 MJ kg^{-1}
Raw gas composition	Shown in Table 1
Gasifier	
Technology	GEE gasification technology
T **(^{o}C)**	1316
P **(MPa)**	5.6
Gas Turbine	
TIT* (^{o}C)	1371
Combustor pressure (MPa)	3.2
Isentropic efficiency (%)	85

Compressor (air or N_2)	
Isentropic efficiency (%)	84
Heat exchangers	
Minimum internal temperature approach (MITA) (^{o}C)	20 Heat recovery steam generators (HRSG): 10 ^{o}C
Pressure drop (%)	5
Steam cycle	
TIT (^{o}C)	560
HP turbine inlet pressure (MPa)	12.5
HP turbine outlet pressure (MPa)	0.568
Turbine efficiencies (%)	90
Pump efficiency (%)	75
Flue gas outlet temperature (^{o}C)	132 (or higher due to constraint of MITA in HRSG)

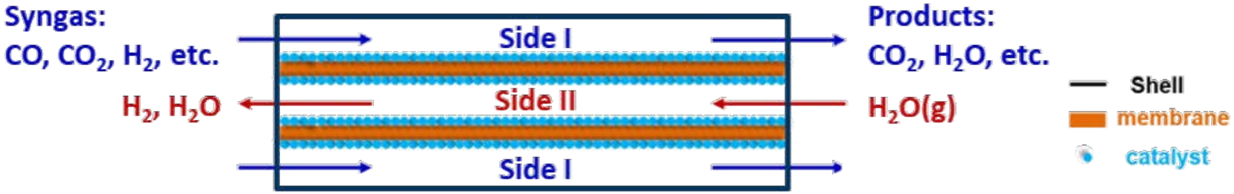
Operating conditions (cont.)

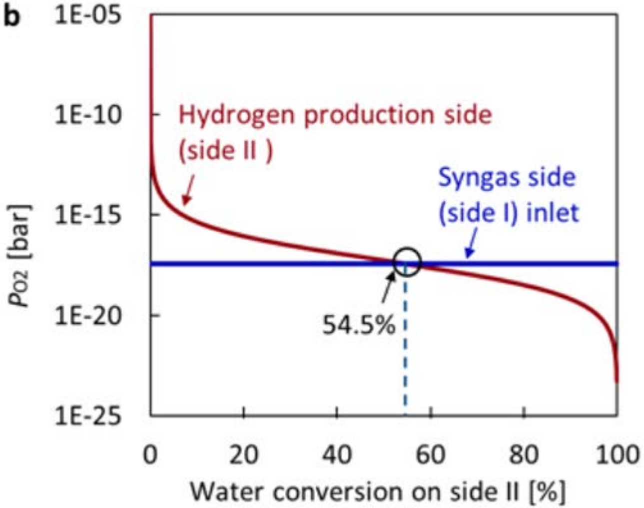
Selexol process	
Work consumption	Calculated from literature
CO_2 removal efficiency (%)	90
H_2S removal efficiency (%)	99.6
H_2 recovery efficiency (%)	99.4
High temperature gas cleaning	
Operating temperature (^oC)	~900 ^oC

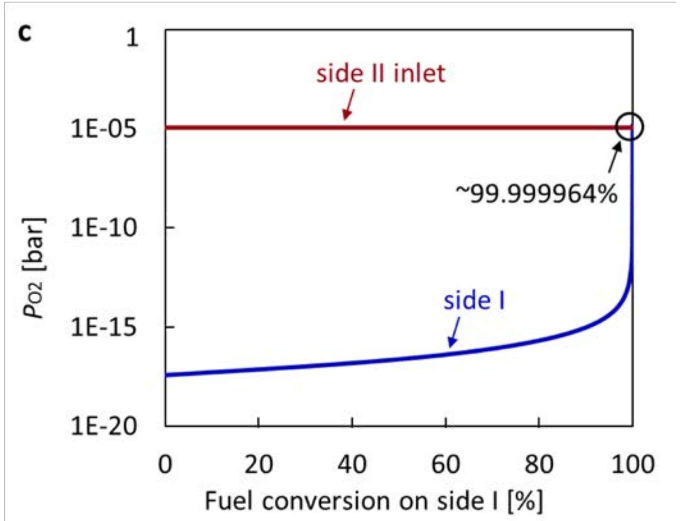
Membrane reactor	
Operating temperature (^oC)	850 ^oC
Raw gas conversion on side I (%)	99**
Water conversion on side II (%)	54**
Reactor design	See Figure 2 (a)
CO_2 compressor	
CO_2 delivery pressure (MPa)	12
Exit CO_2 stream composition (mol%)	>99% CO_2 (EOR ready)
Isentropic efficiency (%)	84

Membrane is a user-defined component and its performance has to be determined

- For a counter-flow configuration, the maximum conversion ratios on side I and II are determined





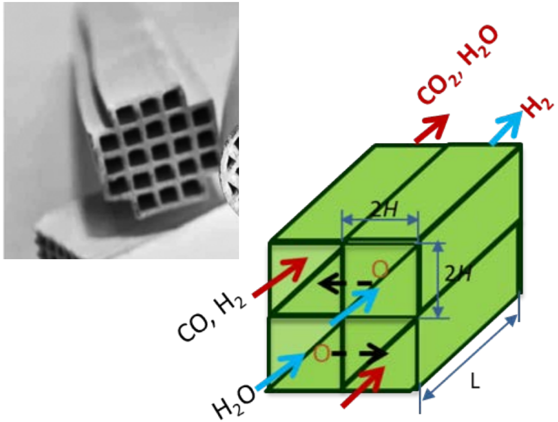


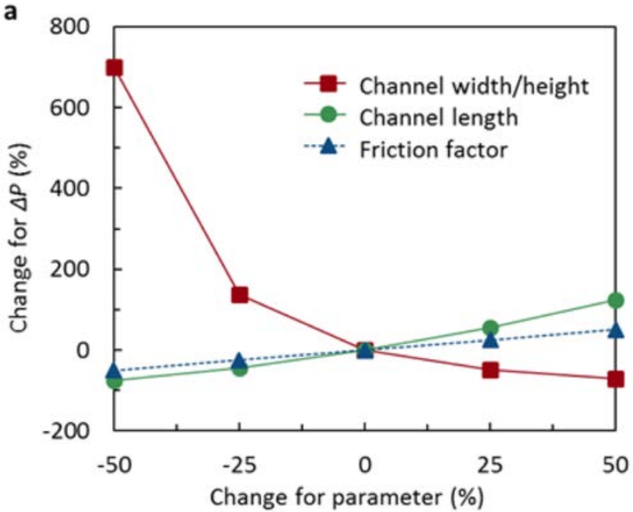
Pressure drop inside the membrane reactor

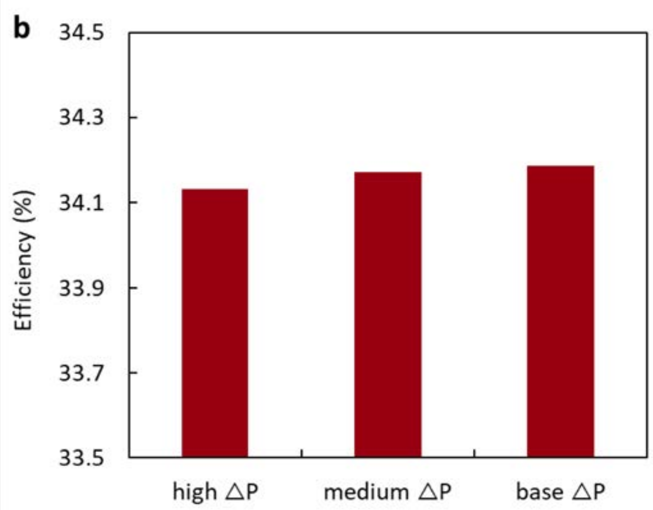
- A monolith membrane reactor configuration is used to estimate the pressure drop

$$\Delta P_{tot} = \left(\frac{1}{2} \frac{\rho V^2}{D_h} \right) \cdot f \cdot L$$

- Sensitivity analysis is carried out to identify the most sensitive membrane parameter and its impacts on the overall efficiency



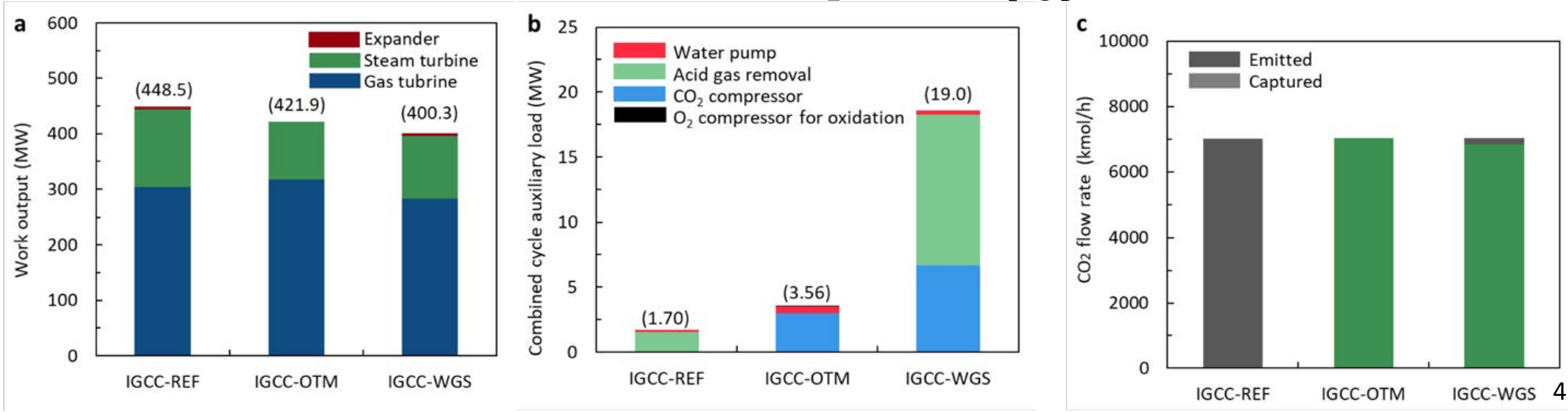




Performance comparison among the systems

- We can see that the IGCC-OTM can capture more CO_2, while require less auxiliary load than IGCC-WGS
- This leads to higher efficiency of IGCC-OTM than IGCC-WGS (34.2% v.s. 30.6%)
- The specific primary energy consumption for CO_2 avoided (SPECCA) of this novel technology is 1.08 MJ $kgCO_2^{-1}$, which is 59% lower than that of the IGCC-WGS

$$SPECCA = \frac{Energy\ consumption\ due\ to\ CC\ [MJ]}{reduction\ in\ CO_2\ emission\ [kg]}$$



Some examples

- 1. Thermodynamic efficiency of a novel IGCC-CC power plant integrated with an oxygen permeable membrane for hydrogen production and carbon capture (CC)

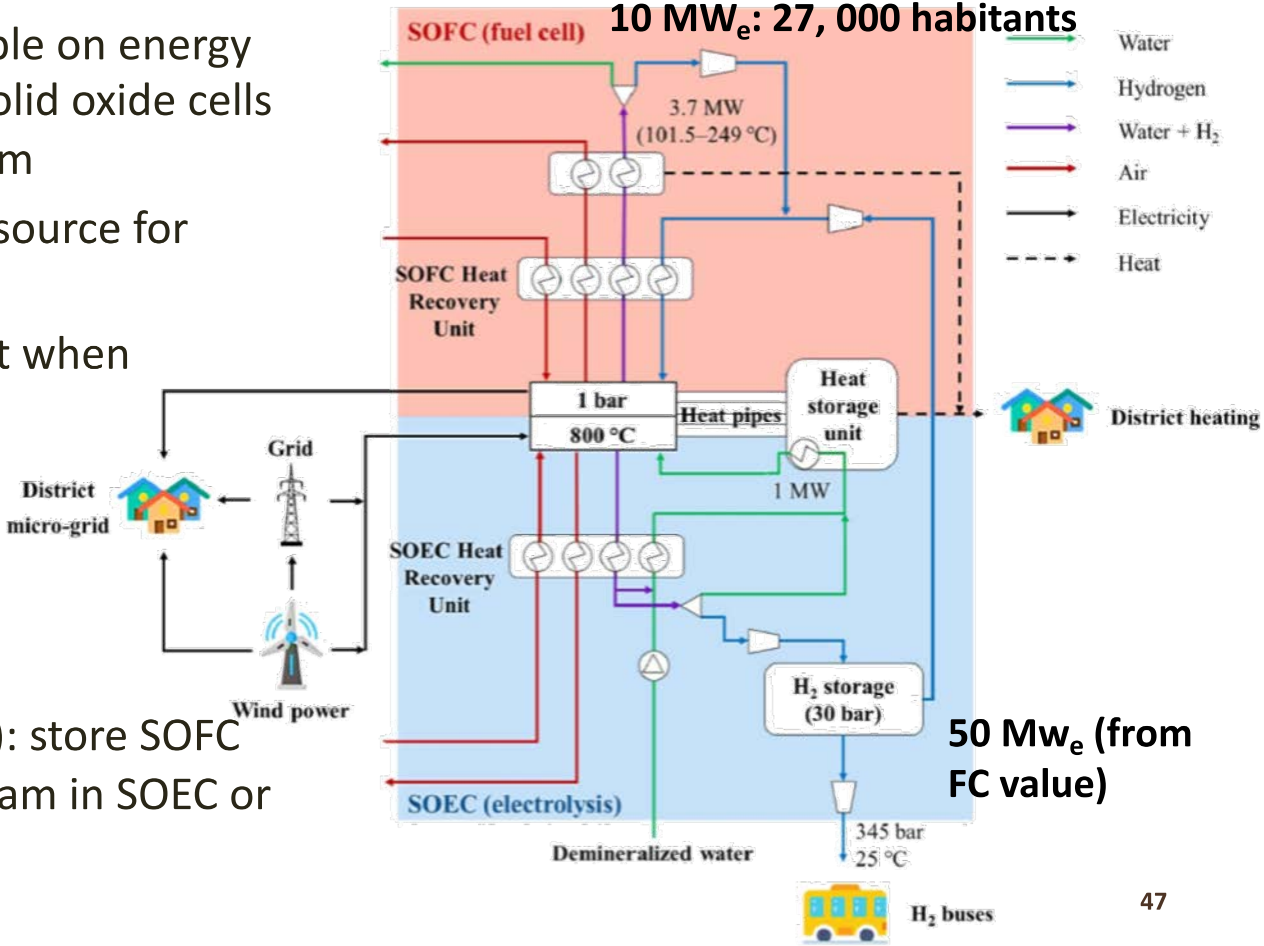
(XY Wu, et al., Journal of Advanced Manufacturing and Processing, 2020, under review)

- 2. Dynamic modeling of a flexible Power-to-X plant

(G Buffo, et al., Journal of Energy Storage, 2020, 29, 101314)

Example 2: Dynamic simulation

- Here we discuss an example on energy storage using reversible solid oxide cells in a poly-generation system
- Wind power is the major source for energy
- Grid energy is supplement when needed
- Energy consumption:
    - H_2 buses fleet
    - District micro-grid
    - District heating
- Heat storage (molten salt): store SOFC waste heat to preheat steam in SOEC or for district heating



10 MW_e: 27, 000 habitants

50 Mw_e (from FC value)

Energy generation

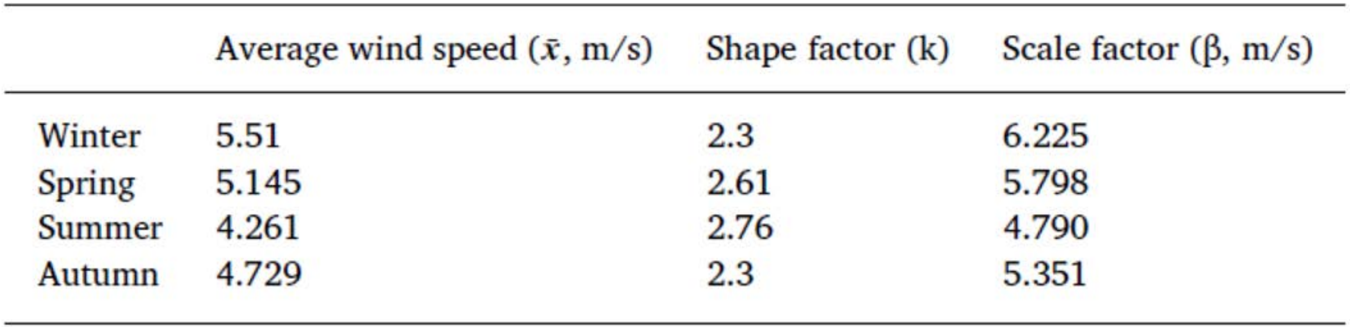
- The wind turbine generation is the kinetic energy of the wind, whose speed distribution follows Weibull distribution:

Shape factor **Wind speed**

$$f(x) = \frac{k}{\beta}\left(\frac{x}{\beta}\right)^{k-1} exp\left[-\left(\frac{x}{\beta}\right)^{k}\right]$$

Probability **Scale factor**

Data for an observational site in Nottingham, UK[1]



	Average wind speed ($\bar{x}$, m/s)	Shape factor (k)	Scale factor (β, m/s)
Winter	5.51	2.3	6.225
Spring	5.145	2.61	5.798
Summer	4.261	2.76	4.790
Autumn	4.729	2.3	5.351

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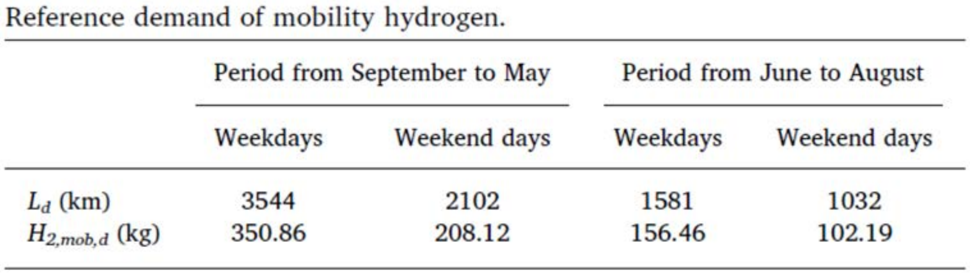
[1] S.E. George, United Kingdom Windspeed - Measurement, Climatology, Predictability and Link to Tropical Atlantic Variability

Demand modeling

- Electricity demand
  - Monte Carlo bottom-up stochastic model

- H_2 bus fleet demand (high priority)
  - 9 kg-H_2/100 km with 10% excess H_2 in the tank for emergency
  - Base case: 1 million km/year (~ Bus 1 mileage)



Reference demand of mobility hydrogen.

	Period from September to May		Period from June to August	
	Weekdays	Weekend days	Weekdays	Weekend days
L_d (km)	3544	2102	1581	1032
$H_{2,mob,d}$ (kg)	350.86	208.12	156.46	102.19

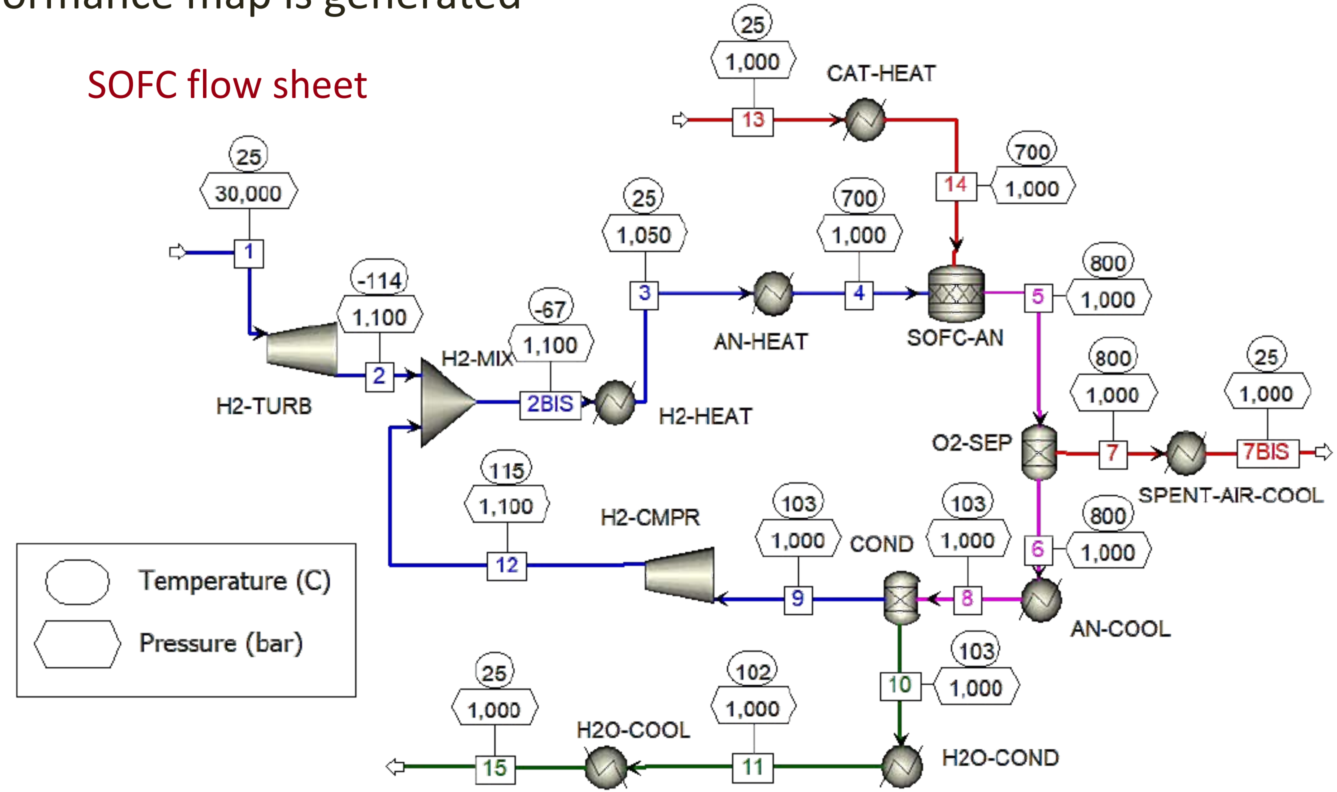
- H_2 storage for SOFC (medium)

- District heating demand (low)
  - Stochastic model

Plant simulation - Steady

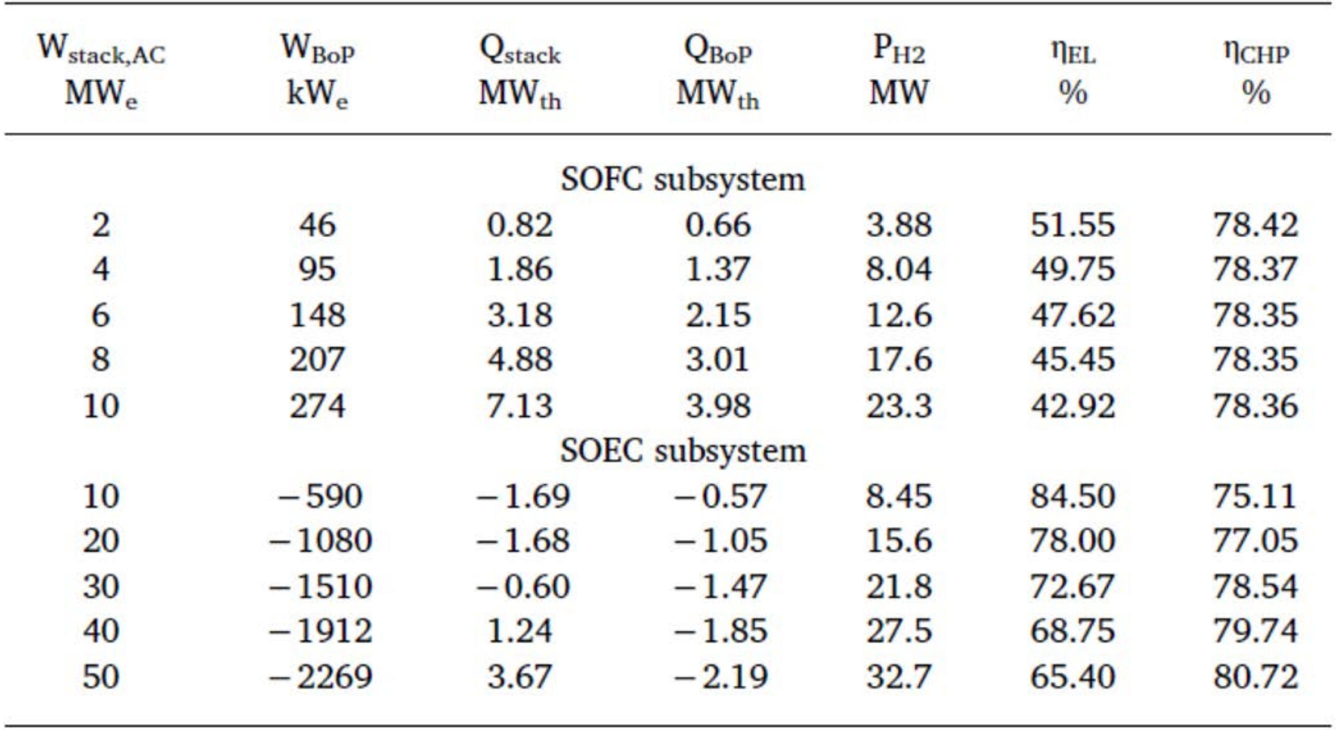
- The steady operation of the rSOC plant is modeled using Aspen Plus^{TM}
- A performance map is generated

SOFC flow sheet



Performance map of the rSOC system

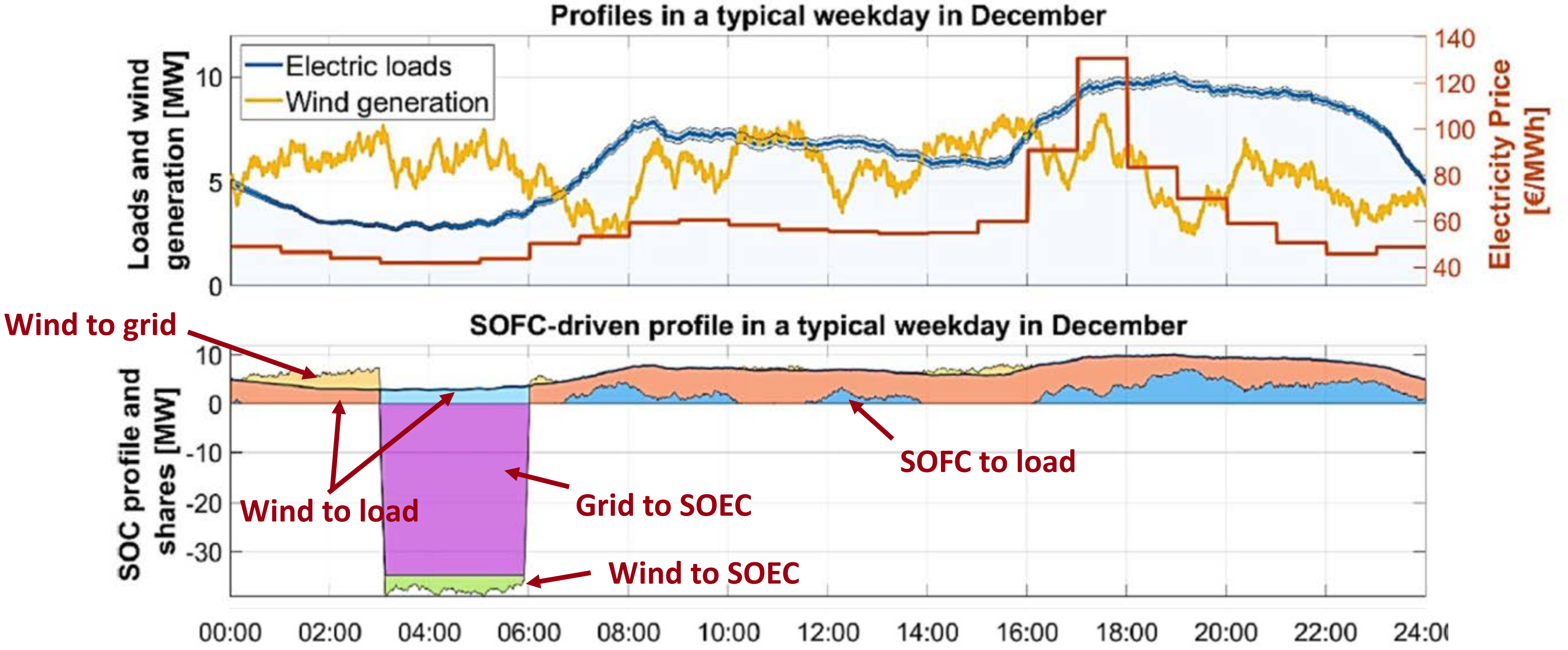
- A time-resolved model can interact with the steady state performance map with the temporal profiles of energy demand of the residential district and wind power generation



$W_{stack,AC}$ MW_e	W_{BoP} kW_e	Q_{stack} MW_{th}	Q_{BoP} MW_{th}	P_{H2} MW	η_{EL} %	η_{CHP} %
			SOFC subsystem			
2	46	0.82	0.66	3.88	51.55	78.42
4	95	1.86	1.37	8.04	49.75	78.37
6	148	3.18	2.15	12.6	47.62	78.35
8	207	4.88	3.01	17.6	45.45	78.35
10	274	7.13	3.98	23.3	42.92	78.36
			SOEC subsystem			
10	−590	−1.69	−0.57	8.45	84.50	75.11
20	−1080	−1.68	−1.05	15.6	78.00	77.05
30	−1510	−0.60	−1.47	21.8	72.67	78.54
40	−1912	1.24	−1.85	27.5	68.75	79.74
50	−2269	3.67	−2.19	32.7	65.40	80.72

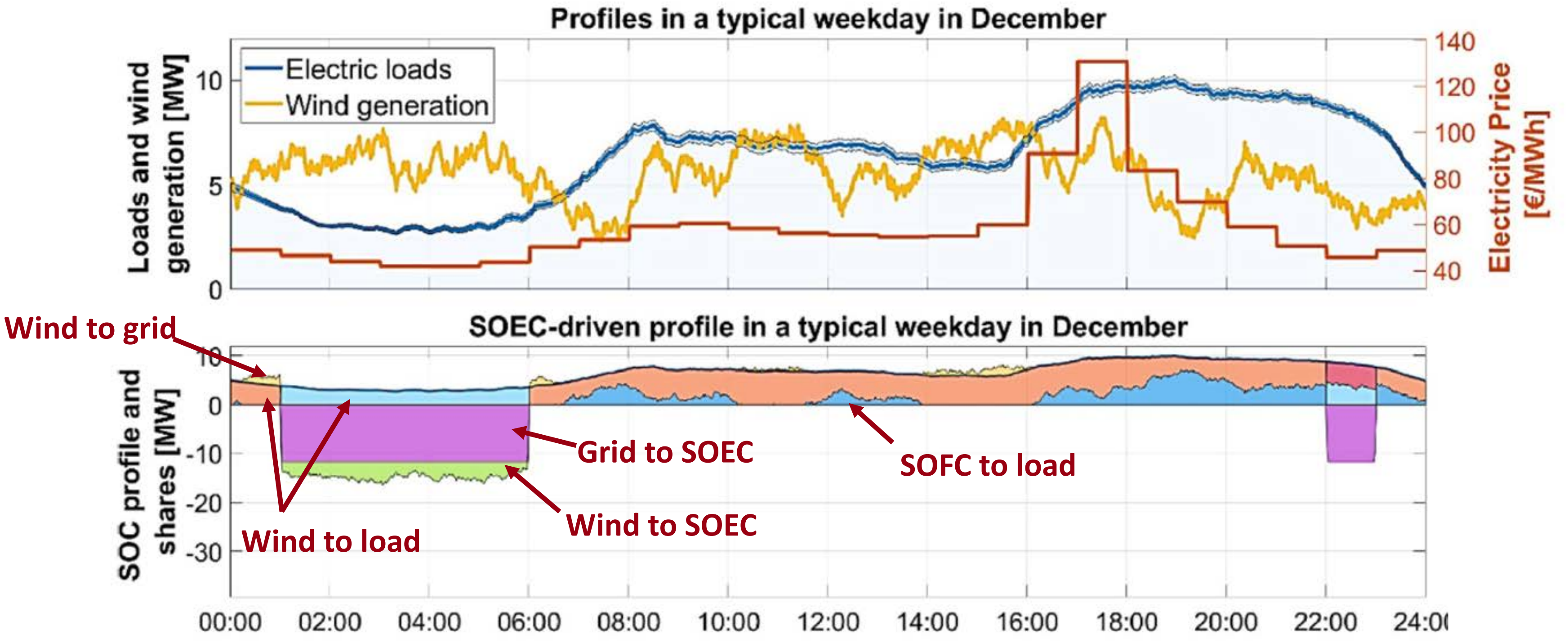
System dispatch profile

- SOFC-driven: Maximum SOFC operating hours



System dispatch profile

- SOEC-driven: Maximum SOEC operating hours



Wind to grid

Grid to SOEC

SOFC to load

Wind to SOEC

Wind to load

Based on the operating dispatch profile, some performance criteria can be evaluated

- Capacity factor

$$CF = \frac{Yearly\ energy\ produced\ (consumed)}{nominal\ size \times operating\ hours}$$

- Efficiency
  - Daily efficiency

$$\eta_{d,p} = \frac{E_{SOFC,d,p} + E_{BOP,\ SOFC,d,p}}{|E_{SOEC,d,p} + E_{BOP,SOEC,d,p}|}$$

(Energy production is positive)

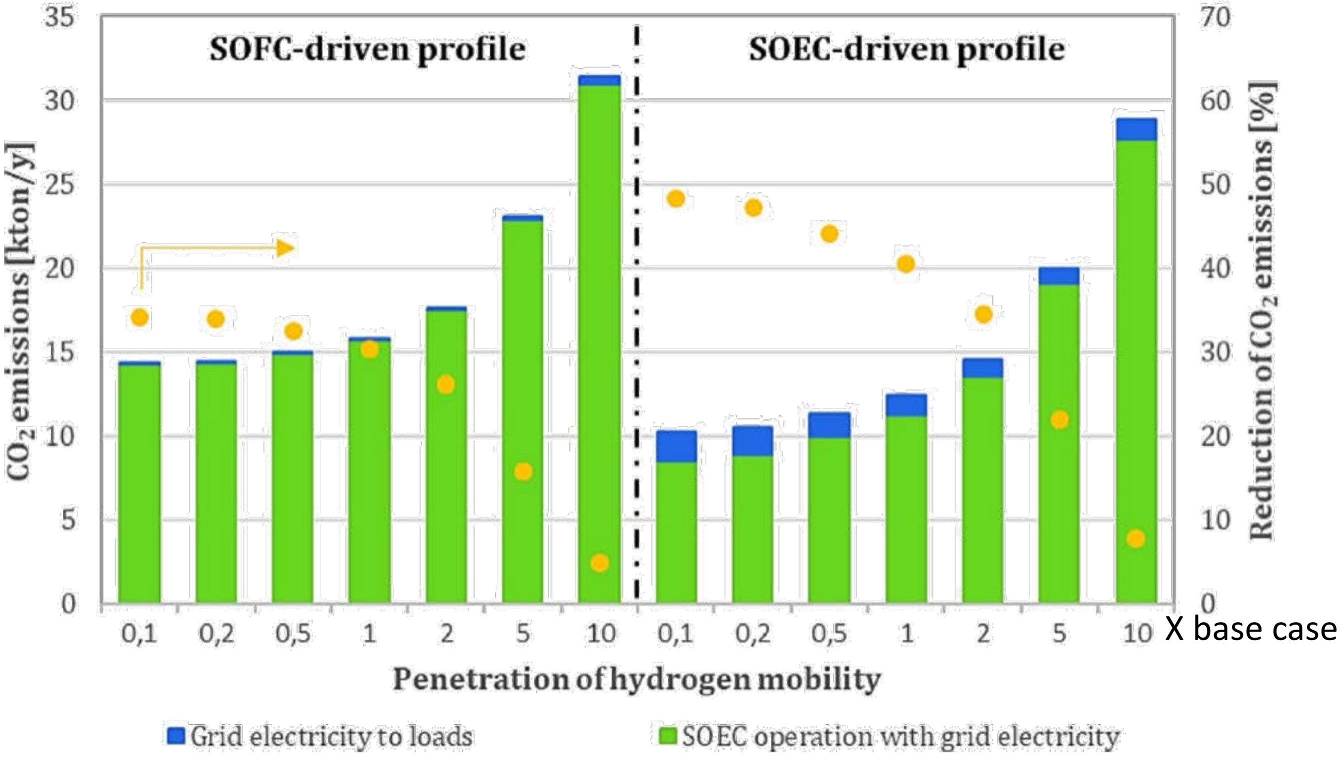
  - Annual efficiency

$$\eta_y^* = \frac{(E_{SOFC,load,y} + E_{BOP,\ SOFC,y}) + H_{2,mob,y} \cdot LHV_{H_2} + E_{DH,y}}{|E_{SOEC,y} + E_{BOP,SOEC,y}|}$$

- Total CO_2 emission
  - Emission due to the use of grid electricity
  - Emission reduction due to elimination of gas boilers for heating and diesel buses

The potential of CO_2 reduction depends on the hydrogen required for buses

- The system has 30-50% CO_2 reduction potential
- The potential drops when more hydrogen is required for the bus fleet



Base case:
1 million km/year
(~ bus 1 mileage)

Recap

- Energy systems: production, conversion, delivery, and use of energy
- System analysis: efficiency, emissions, economics, societal impacts
- Aspen Plus^{TM}: interface and components
- Examples to do thermodynamic analysis and dynamic simulations

Thanks!

2.60/2.62 lecture

Energy system modeling and examples

Xiao-Yu Wu

2.60J Fundamentals of Advanced Energy Conversion
Spring 2020