

```

- begin
- using Unitful ✓
- using CoolProp ✓
- end

```

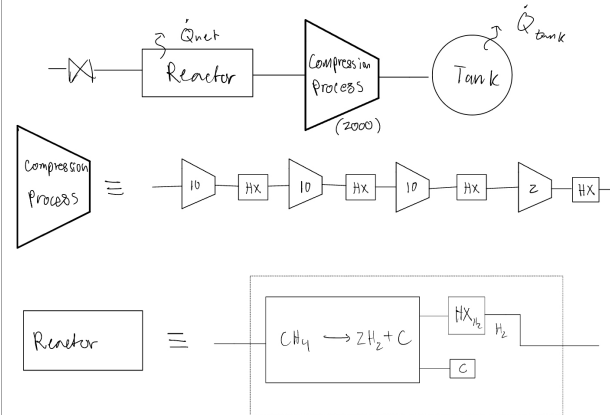
Group Members

Gianna Braga, Brian Burrous, Ky Heon

Project setup

We're using a series of compressors with heat exchangers to cool the gas back to room temperature after each compression. The heat exchanger process is assumed to be isobaric.

Diagram 1

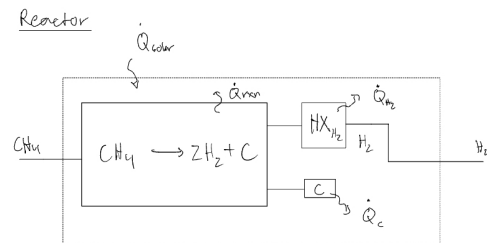


Assumptions

H_2 is a Gas

Solid Carbon in Reactor undergoes ambient cooling

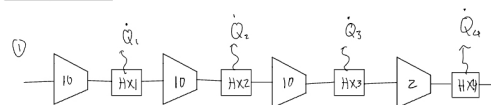
Diagram 2



Exergy Destroyed

$$E_{d_{H_2N}} + E_{d_C} + E_{d_{H_2}}$$

Compressor



\forall pumps, $T_{in} = T_p = 300K$ $P_i = P_{reactor} = 0.1 \text{ bar}$
(Operating Temperature of Pump)

Exergy Destroyed

Sum of E_d \forall Heat Exchangers + Sum of E_d \forall Compressors

```

- # Adiabatic H2 Compressor
- struct Pump
-     W::Any
-     ratio::AbstractFloat
-     P::Any
-     T::Any
-     name::AbstractString
-     η::Number
-
- end

```

```

- # Isenthalpic CH4 Valve
- struct Valve
-     Tin::Any
-     Pin::Any
-     Pex::Any
-     name::AbstractString
- end

```

```

- # ideal Heat Exchanger, approximatly isobaric cooling
- struct Cooler
-     Tin::Any
-     Tex::Any
-     P::Any
-     Tb::Any
-     name::AbstractString
- end

```

```

- # CH4 decomposition reactor
- # Reactor does no work
- struct Reactor
-     Tin::Any
-     Tex::Any
-     P::Any
-     Tb::Any
- end

```

0.01377946 mol s⁻¹

```

- # Assumptions
- begin
-
-     # Reactions is complete: CH4(g) --> 2H2(g) + C(s)
-     # Isenthalpic throttling valve
-
-     # Given Constants
-     P_in = 1u"atm"
-     T_in = 298u"K"
-     P_react = 10u"kPa"
-     T_tank = 300u"K"
-     P_tank_min = 200u"bar"
-     P_tank_max = 220u"bar"
-     V_tank = 1u"m^3"
-     T_pyro = 1600u"K"
-
-     Q_solar = 15u"kW"
-     H_rxn = 74.6u"kJ/mol"
-     Hf_meth = -74850u"kJ/kmol"
-     M_h2 = 2u"mol/g/mol"
-     M_meth = 16.04u"g/mol"
-     M_carbon = 12u"g/mol"
-     C_carbon = 0.71u"J/g/K"
-     R = 8.3145u"J/mol/K"
-
-     MolarMass = Dict{"C"=>12.01u"g/mol", "H2"=>2.02u"g/mol", "CH4"=>16.04u"g/mol"}
-     MODEL2 = Dict{"C"=>410.260u"kJ/kmol", "H2"=>236.100u"kJ/kmol",
-                   "CH4"=>831.650u"kJ/kmol"}
-
-     ## Initial Calcuations
-     n_dot_meth = uconvert(u"kmol/s", 0.1 * Q_solar / H_rxn)
-     n_dot_meth |> println
-     n_dot_h2 = 2 * n_dot_meth
-     n_dot_c = n_dot_meth
-     n_dot_meth = 0.00688973u"mol/s"
-     n_dot_h2 = 2 * n_dot_meth
-
- end

```

2.0107238605898127e-5 kmol s⁻¹

0.006938662225922842 mol s⁻¹

```

- begin
-     massH2 = 1u"kg"
-     massC = 3u"kg"
-
-     day = 10u"hr"
-     molH2 = massH2/MolarMass["H2"]
-     molC = massC/MolarMass["C"]
-     molCH4 = molC
-
-     MolarFlow = Dict{"C"=>molC/day, "H2"=>molH2/day, "CH4"=>molC/day}
-     MolarFlow["C"] = uconvert(u"mol/s", MolarFlow["C"])
-     MolarFlow["H2"] = uconvert(u"mol/s", MolarFlow["H2"])
-     MolarFlow["CH4"] = uconvert(u"mol/s", MolarFlow["CH4"])
-
- end

```

1. Conduct a search of available hydrogen compressors. Does a single compressor exist that serves the required function (gas flow, pressure ratio)? If not, what multiple compressor configuration would satisfy the specifications? Explain and include links where appropriate.

```

- md"""
- 1) Conduct a search of available hydrogen compressors. Does a single compressor exist
- that serves the required function (gas flow, pressure ratio)? If not, what multiple
- compressor configuration would satisfy the specifications? Explain and include links
- where appropriate.
- """

```

We will use a series of 4 compressors, assuming compressor ratios of 10, 10, 10, and 2, to get to the desired tank pressure of 200 bar. The first three stages can be accomplished using the following compressor

<https://www.directindustry.com/prod/fornovo-gas-spa/product-223666-2423388.html>

The final compressor stage exceeds the maximum pressure of this compressor, so we will also be using this compressor for the final compression stage.

<https://www.directindustry.com/prod/jp-sauer-sohn-maschinenbau-gmbh/product-5707-1982415.html>

• Enter cell code...

2. What size of methane mass flow controller (in sccm) is required at nominal efficiency? Find a suitable product.

```
ans2 = 9302.376198653577 cm³ minute⁻¹
• ans2 = let
•   p = PropsSI("D", "T", 273u"K", "P", 1u"atm", "CH4")
•   scfm = MolarFlow["CH4"]*MolarMass["CH4"] / p
•   uconvert(u"cm³/minute", scfm)
• end
```

3. For your compressor configuration in part A, estimate the overall isentropic efficiency of the compression process.

We couldn't find any good data for our specific hydrogen pump, but various papers suggest an isentropic efficiency of 65-85%.

```
• # ans3 = let
• #   pump_size = -1u"kW"
• #   pump = Pump(pump_size/MolarFlow["H2"], 10, P_react, 35u"C", "H2", 0.8)
• #   @show temperature(pump)
• # end
```

4. Calculate the final pressure of the tube cylinder at the end of one day.

```
ans4 = 212.37350437526044 bar
• ans4 = let
•   molH2 = 1u"kg"/M_h2
•   P_H2 = molH2 * R * T_tank / V_tank
•   P_final = uconvert(u"bar", P_tank_min + P_H2)
• end
```

5. Calculate the rate of exergy destruction at the mass flow controller at nominal efficiency

```
ans5 = 0.039785264651772234 kW
• ans5 = let
•   T_o = 298u"K"
•   P_o = 1u"atm"
•   valve = Valve(T_in, P_in, P_react, "CH4")
•   ED = exergyDestroyed(valve, T_o, P_o)*MolarFlow["CH4"]
•   uconvert(u"kW", ED)
• end
```

6. Calculate the rate of exergy destruction in the reactor at nominal efficiency

```
ED_reactor = 2.092470654255285 kW
• ED_reactor = let
•   T_o = 298u"K"
•   P_o = 1u"atm"
•   T_react = 298u"K"
•   T_pump = 300u"K"
•   T_b = 300u"K"
•   #T_b = T_pyro
•   rxn = Reactor(T_react, T_pyro, P_react, T_b)
•   ED_rxn = abs(exergyDestroyed(rxn, T_o, P_o))
•
•   #Hydrogen Cooling
•   hx = Cooler(T_pyro, T_pump, P_react, T_b, "H2")
•   ED_H2 = exergyDestroyed(hx, T_o, P_o)*MolarFlow["H2"]
•
•   #Carbon Cooling
•   Q = massC*C_carbon*(T_pyro - T_o)/day
•   ED_C = Q*(1-T_o/T_b)
•
•   ED_reactor = ED_rxn + ED_H2 + ED_C
•   uconvert(u"kW", ED_reactor)
• end
```

7. What fraction of this reactor exergy destruction is consumed by cooling the graphite from 1600 K to room temperature?

```
ED_C = 0.06268723124999999 kW
• ED_C = let
•   T_o = 298u"K"
•   P_o = 1u"atm"
•   T_b = T_pyro
•   massCarbon = 3u"kg"
•   ΔT = (T_pyro - T_o)
•   Q = massCarbon*C_carbon*ΔT/10u"hr"
•   uconvert(u"kW", (1-T_o/T_b)*Q)
•
• end
```

```
2.9958475700731158
- # Final ratio (percentage)
- (ED_C/ED_reactor)*100
```

Answer:

3% of exergy destruction consumed by cooling graphite from 1600K to room temperature.

8. What fraction of this reactor exergy destruction is consumed by cooling the product hydrogen from 1600 K to room temperature?

```
ED_H2 = 0.7106138732715033 kW
- ED_H2 = let
-   To = 298u"K"
-   Po = 1u"atm"
-   Tpump = 300u"K"
-   Tb = 300u"K"
-   #Tb = T_pyro
-   #Hydrogen Cooling
-   hx = Cooler(T_pyro, Tpump, P_react, Tb, "H2")
-   Ed_H2 = exergyDestroyed(hx, To, Po)*MolarFlow["H2"]
-
-   uconvert(u"kW", Ed_H2)
- end
```

```
ans8 = 33.9605180042256
- ans8 = let
-   uconvert(u"K/K", ED_H2/ED_reactor)*100
- end
```

Answer

34% of the exergy destruction of the reactor is destroyed cooling H₂.

9. Calculate the rate of exergy destruction in the compression process.

```
ans9 = 0.5262926583442024 kW
- ans9 = let
-   To = 298u"K"
-   Po = 1u"atm"
-   Tb = 300u"K"
-   Tp = 300u"K"
-   P = P_react
-   T = Tp
-   power = -5u"kW"
-   pumps = []
-   hxs = []
-   P = P_react
-   T = Tp
-   for i = 1:3
-       pump = Pump(power/MolarFlow["H2"], 10, P, Tp, "H2", 0.65)
-       push!(pumps, pump)
-       P = pump.P * pump.ratio
-       T = temperature(pump)
-       push!(hxs, Cooler(T, Tp, P, Tb, "H2"))
-   end
-   finalPump = Pump(power/MolarFlow["H2"], 2, P, Tp, "H2", 0.65)
-   push!(pumps, finalPump)
-   T = temperature(finalPump)
-   push!(hxs, Cooler(T, Tp, finalPump.ratio*P, Tb, "H2"))
-
-   Ed_pumps = sum([exergyDestroyed(pump, To, Po) for pump in pumps])
-   Ed_hxs = sum([exergyDestroyed(hx, To, Po) for hx in hxs])
-   Ed_compression = MolarFlow["H2"] * (Ed_pumps + Ed_hxs)
-   uconvert(u"kW", Ed_compression)
- end
```

10. Calculate the total exergy destroyed as the pressurized hydrogen loses heat from the tank to the surroundings

Our design uses heat exchangers before and after every compressor stage. This means that the gas enters the tank at ambient temperature and tank pressure. Therefore there is not exergy change/no exergy destruction at this point.

Answer: 0

11:

If the heat lost by the hydrogen stream between the reaction zone and the compressor inlet could be sent completely back into the reaction zone, then by what percentage could the methane mass flow rate increase? What would be the exergy destruction? Would it increase or decrease? By how much?

```
10.474841264052992
- let
-   h1 = PropsSI("Hmolar", "T", T_pyro, "P", P_react, "H2")
-   h2 = PropsSI("Hmolar", "T", 298u"K", "P", 200u"bar", "H2")
-
-   Q_cooling = (h1-h2)*n_dot_h2
-
-   Q_initial = uconvert(u"kW", MolarFlow["CH4"]*H_rxn/0.1)
-   Q_final = uconvert(u"kW", Q_initial + Q_cooling)
-
-   n_final_new = uconvert(u"mol/s", Q_final*0.1/H_rxn)
-   uconvert(u"K/K", (n_final_new-MolarFlow["CH4"])/MolarFlow["CH4"])*100
- end
```

Answer: The molar (and mass) flow rate of methane would increase by 10.5%.

12.

What are the technical and/or societal benefits and drawbacks of using solar heating in this design, as compared to burning methane or hydrogen for pyrolysis?

```
- md"""
- ### 12.
- What are the technical and/or societal benefits and drawbacks of using solar heating
- in this design, as compared to burning methane or hydrogen for pyrolysis?
- """
```

It is assumed that a solar concentrator is being used for this system. A solar concentrator works by having a curved surface or a series of flat surfaces all angled toward one focus, so that the sunlight bounces off the surfaces and reflects all to the same point. At that point a receiver is placed to collect the energy from the sun. This set up is fairly cheap to manufacture and set up. However, there is no way to store the energy so the solar concentrator can only be used when the sun is out and shining. It would be ideal to position this somewhere that the efficiency of this process is not decreased significantly.

If solar panels were being used, a battery can be attached to store the energy that isn't being used during the day, allowing the process to continue, even when the sun is not present. While having a battery solves the issue of the sun's limited availability as an energy source, a new issue is created, cost. The website for the Office of Energy Efficiency and Renewable Energy states that solar batteries can range from \$12,000 to 22,000. In general, there is a high upfront cost with solar panels due to the price of purchasing the panels and their installation if that is required. However, this cost could be made up through the money saved when not paying for other energy sources. The US Government is also starting to offer incentives for using solar panels so those may aid in the initial cost of the solar energy set up.

If the hydrogen and graphite being produced for the assumed 10 hours a day is sufficient, and an irregular production rate due to the sun exposure fluctuation is no issue, then a solar concentrator is a great option. The most significant benefit of solar power over other energy sources, such as burning methane, is that the sun is a renewable energy source. It will never run out of heat to provide, at least not for roughly 5 billion more years. It is also a green energy source. The use of solar energy decreases greenhouse gas production which is vital to slowing the effects of climate change.

Sources:

<https://lightningsolar.com.au/comparative-guide-advantages-disadvantages-of-solar-panels/>

<https://powersolarphoenix.com/commercial-solar-panels-cost/>

<https://www.energy.gov/eere/solar/articles/should-i-get-battery-storage-my-solar-energy-system>

13.

More broadly, what are the technical and societal benefits and drawbacks of using methane (from natural gas) as a source for graphite and hydrogen?

There is no shortage of methane production in our society. The farming and agriculture industries are huge contributors to the methane content in the atmosphere. When manure is produced by livestock, such as pigs or cattle, methane is released. When the manure is spread onto crops for fertilization, methane is released. A fight has begun to reduce meat and dairy consumption in the US has begun. Alternative milks and vegetarian/vegan options are becoming more widespread than ever before. It is apparent however that much more time and effort is needed to change the general population's eating habits so methane production continues.

Another significant source of methane in our society is landfills. As organic materials decompose under piles of waste, there are not significant sources of oxygen to facilitate aerobic decomposition. Bacteria that perform anaerobic decomposition come into play. These bacteria are huge sources of methane through their decomposition processes. Composting can help decrease these methane emissions. By collecting organic materials and allowing them to decompose in environments that provide aeration, organisms that do not produce methane can process the materials. Composting is not a widespread habit. Many communities do not have access to composting programs and especially programs that accept food waste, so much of the organic waste still ends up in landfills, producing methane.

Methane is a significant cause for the trapping of heat within Earth's atmosphere that is leading to climate change. According to UNECE, methane has a warming potential roughly 28-34% higher than that of CO₂. Methane capture is a solution being presented to the high emissions of methane from the above sources. In that set up, perforated tubes are arranged through the methane producing areas to collect the methane and transport it to facilities that will burn it. This will prevent much of the methane being produced in industrial settings from reaching the atmosphere.

A downside of burning methane is that CO₂ is produced by the process. CO₂ in the atmosphere is another cause to the greenhouse effect. However, if the methane being burned is harvested from the atmosphere then the benefits of destroying methane outweighs the drawbacks of CO₂ production. The burning of this collected methane is also beneficial because it eliminates reliance on other energy sources that also produce greenhouse gases. As outlined above, due to the processes used for food production and waste management that this society relies upon, there is an abundance of methane to be utilized for burning and heating. If it is not utilized, it is only making the climate change issue worse.

Sources:

<https://www.epa.gov/lmop/basic-information-about-landfill-gas>

<https://unece.org/challenge>

temperature (generic function with 2 methods)

```
- begin
-   function temperature(pump::Pump)
-       k = 1.4
-       polytropicExp = (k-1)/k
-       Ts = uconvert("K", pump.T)*(pump.ratio)^polytropicExp
-       Hs = PropsSI("Hmolar", "T", Ts, "P", pump.P*pump.ratio, pump.name)
-       H = PropsSI("Hmolar", "T", pump.T, "P", pump.P, pump.name)
-       Hr = H + (Hs-H)/pump.η
-       P2 = pump.P*pump.ratio
-       T = PropsSI("T", "P", P2, "Hmolar", Hr, pump.name)
-       return uconvert("K", T)
-   end
-
-   function temperature(valve::Valve)
-       Hin = PropsSI("H", "T", valve.Tin, "P", valve.Pin, valve.name)
-       return uconvert("K", PropsSI("T", "H", Hin, "P", valve.Pex, valve.name))
-   end
- end
```

pressure (generic function with 1 method)

```
- begin
-   function pressure(hx::Cooler)
-       k = 1.4
-       polytropicExp = k/(k-1)
-       P = hx.P*(hx.Tex/hx.Tin)^polytropicExp
-       return uconvert("bar", P)
-   end
- end
```

exergyDestroyed (generic function with 4 methods)

```
- begin
-   function exergyDestroyed(pump::Pump, To, Po)
-       T = temperature(pump)
-       P = pump.ratio*pump.P
-       e_in = get_flow_exergy(pump.T, pump.P, To, Po, pump.name)
-       e_ex = get_flow_exergy(T, P, To, Po, pump.name)
-
-       Hex = PropsSI("Hmolar", "T", T, "P", P, pump.name)
-       Hin = PropsSI("Hmolar", "T", pump.T, "P", pump.P, pump.name)
-       return uconvert("kJ/mol", Hex-Hin + (e_in - e_ex))
-   end
-
-   function exergyDestroyed(valve::Valve, To, Po)
-       Tex = temperature(valve)
-       e_in = get_flow_exergy(valve.Tin, valve.Pin, To, Po, valve.name)
-       e_ex = get_flow_exergy(Tex, valve.Pex, To, Po, valve.name)
-       return uconvert("kJ/mol", (e_in - e_ex))
-   end
-
-   function exergyDestroyed(react::Reactor, To, Po)
-       Tb = (react.Tex + react.Tin)/2
-       e_in = get_flow_exergy(react.Tin, react.P, To, Po, "CH4")
-       e_ex = get_flow_exergy(react.Tex, react.P, To, Po, "H2")
-       chem_Ex = MODEL2["CH4"] - 2*MODEL2["H2"] - MODEL2["C"]
-       Q = -heat(react)
-       Ed = (1-To/Tb)*Q + MolarFlow["CH4"]*e_in-MolarFlow["H2"]*e_ex +
-           MolarFlow["CH4"]*chem_Ex
-       return uconvert("kW", Ed)
-   end
-
-   function exergyDestroyed(hx::Cooler, To, Po)
-       e_in = get_flow_exergy(hx.Tin, hx.P, To, Po, hx.name)
-       e_ex = get_flow_exergy(hx.Tex, hx.P, To, Po, hx.name)
-       Tb = (hx.Tin + hx.Tex)/2
-       Q = -heat(hx)
-       Ex = (1-To/Tb)*Q + e_in - e_ex
-       return uconvert("kJ/mol", Ex)
-   end
- end
```

heat (generic function with 2 methods)

```
- begin
-   function heat(react::Reactor)
-       Hin = molar_enthalpy(react.Tin, react.P, "CH4", Hf_meth)
-       Hex = molar_enthalpy(react.Tex, react.P, "H2")
-       Q = n_dot_h2*Hex-MolarFlow["CH4"]*Hin
-       return uconvert("kW", Q)
-   end
-
-   function heat(hx::Cooler)
-       Hin = PropsSI("Hmolar", "T", hx.Tin, "P", hx.P, hx.name)
-       Hex = PropsSI("Hmolar", "T", hx.Tex, "P", hx.P, hx.name)
-       return uconvert("kJ/mol", (Hex-Hin))
-   end
- end
```

```
- let
-   #To = 298u"K"
-   #hx = Cooler(T_pyro, To, P_react, T_pyro, "H2")
-   #uconvert("bar/bar", P_react/pressure(hx))
- end
```

molar_enthalpy (generic function with 2 methods)

```
- function molar_enthalpy(T, P, name::String, Hf=0u"kJ/mol")
-   Href = PropsSI("Hmolar", "T", 298.15u"K", "P", 1u"atm", name)
-   H = PropsSI("Hmolar", "T", T, "P", P, name)
-   return uconvert("kJ/mol", Hf + H - Href)
- end
```

get_flow_rate (generic function with 3 methods)

```
- function get_flow_rate(m_dot, T=273.15u"K", P=1u"atm")
-   ρ = PropsSI("D", "T", T, "P", P, "CH4")
-   return uconvert("ft^3/minute", m_dot/ρ)
- end
```

get_flow_exergy (generic function with 1 method)

```
- function get_flow_exergy(T, P, To, Po, name::String)
-   Ho = PropsSI("Hmolar", "T", To, "P", Po, name)
-   So = PropsSI("Smolar", "T", To, "P", Po, name)
-   H = PropsSI("Hmolar", "T", T, "P", P, name)
-   S = PropsSI("Smolar", "T", T, "P", P, name)
-   flow = H - Ho - To*(S - So)
-   return uconvert("kJ/mol", +flow)
- end
```

```

info (generic function with 1 method)
+ function info(n)
+   T_o = 298u"K"
+   P_o = 1u"atm"
+
+   power = -5u"kW"
+   pumps = []
+   P = P_react
+   for i = 1:3
+     pump = Pump(power/n_dot_h2, 10, P, 35u"C", "H2", n)
+     push!(pumps, pump)
+     P = pump.P * pump.ratio
+   end
+   push!(pumps, Pump(power/n_dot_h2, 2, P, 35u"C", "H2", n))
+
+   for pump in pumps
+     pump |> println
+     @show temperature(pump)
+     @show exergyDestroyed(pump, T_o, P_o)
+     "\n" |> print
+   end
+ end

```

Resources: [here]

<https://www.hydrogen.energy.gov/pdfs/9013energyrequirementsforhydrogencompression.pdf>

```

+ md"""
+
+ Resources: [here]
+ https://www.hydrogen.energy.gov/pdfs/9013\_energy\_requirements\_for\_hydrogen\_gas\_compression.pdf
+
+ """

```