Calculations for Calcium Carbide / Acetylene Reactor Block Diagram (Class Example)

November 1, 2011

1 Introduction

You have inherited the world's largest storehouse of calcium carbide (CaC_2) from your grandfather, who made a fortune starting precious metal mining companies. You wish to use this free (?) source of energy to provide process heat to a liquid sodium refinery down the street, as there aren't any more mining companies that use CaC_2 for lanterns, and what used to be vehicle carbide lamps are now filament or LED lights. The sodium refiners will pay you handsomely for your services and process heat, as long as you can provide what they need.

2 Problem Statement

The sodium refiners require you to provide a steady stream of process heat to their system in order to heat up liquid sodium metal. They require you to heat $10 \frac{\text{kg}}{\text{sec}}$ of sodium from 100C to 500C. They are asking you to provide the heat exchanger to perform this operation.

Design, characterize, and optimize a system to provide this process heat in the most efficient manner. Start by defining a system, make educated guesses for key missing parameters, and iterate along your design to reduce cost, material strain, resource consumption, and anything else that could reduce your profit margins or safety margins.

3 Starting the Solution

Start by constructing a block diagram. An example of one that (at first) solves the problem is shown in Figure 1.

3.1 CaC_2 Reactor

Think about what components you need in order to get energy from calcium carbide into the liquid sodium. Since you have an inexhaustible supply of CaC_2, let's start with that. Looking up typical reactions for calcium carbide, we can find one that is used in carbide lamps (and many other CaC_2 devices). It involves a reaction with water to produce acetylene (C_2H_2), which is very energy dense & unstable, and lime slurry:

$$CaC_2(s) + 2H_2O(l,g) \rightarrow C_2H_2(g) + Ca\left(OH\right)_2(s) \qquad \Delta H_{RXN} = ??? \tag{1}$$

Let's start by drawing a block for the CaC_2 reactor as shown on the upper left of Figure 1, where it will react with water to produce acetylene. Write the reaction in Equation 1 inside the block so the readers know what's happening inside. You can also draw an input line for CaC_2 and an output line for $Ca\left(OH\right)_2$ at this point, as you know they will have to be inputs and outputs, respectively.

Let's also assume that we want gaseous water entering the CaC_2 reactor, which will help increase the reactivity of this system. Draw a line representing steam entering the CaC_2 reactor. We will finish connecting this line later, in Section 3.6.

Block Diagram for Calcium Carbide / Acetylene Heating System
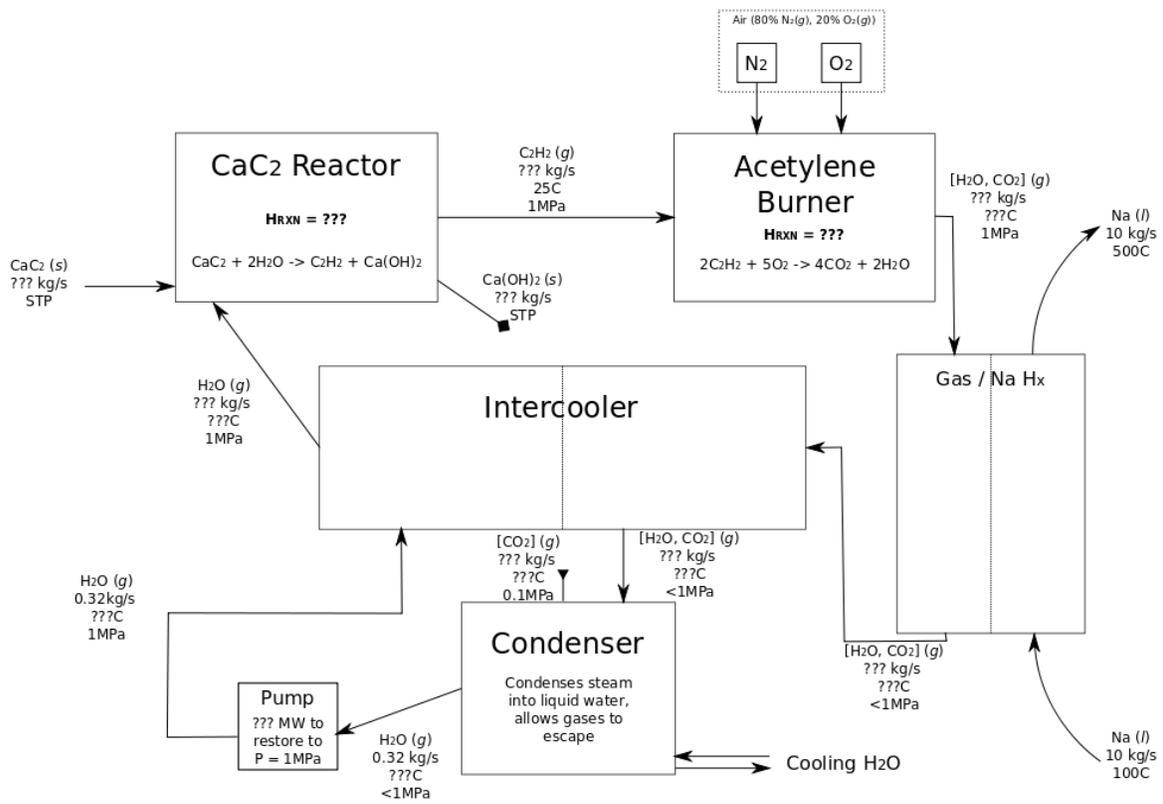
Figure 1: Block diagram for initial setup of this system. Note that a number of parameters are missing, and it seems that there are many more variables than equations to solve.

3.2 Acetylene Burner

Next, we want to extract as much energy as possible from the acetylene gas. Acetylene is commonly used in high temperature welding torches as oxy-acetylene, where flame temperatures can exceed 3,000C. Acetylene burns (combusts) with oxygen to produce water vapor and carbon dioxide:

$$2C_2H_2(g) + 5O_2(g) \rightarrow 4CO_2(g) + 2H_2O(g) \qquad \Delta H_{RXN} = ??? \tag{2}$$
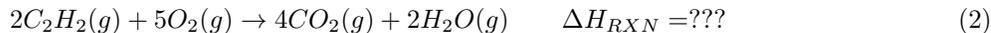
We expect that this reaction will have a very large, negative enthalpy of reaction, as we know it is very exothermic. We'll worry about finding out how exothermic it is later. Draw a block for the acetylene burner, as shown in the upper right of Figure 1. Write the reaction in Equation 2 inside the block so the readers know what's happening in the burner.

You can now draw a line showing acetylene flowing out of the CaC_2 reactor and into the acetylene burner. We will want the acetylene gas to be at room temperature (25C), since it is technically thermodynamically unstable (positive enthalpy of formation).

You may have noticed that the oxygen in Equation 2 has to come from somewhere. Rather than supply the burner with pure oxygen, which would be expensive, you can just add air. Draw a block for an input of air into the acetylene burner. For simplicity's sake, let's model the air as 80% nitrogen (N_2) and 20% oxygen (O_2). Draw two sub-boxes to indicate each of these gases, so that the reader knows how you are modeling this mixture of gases better known as air.

Now draw a line leaving the acetylene reactor, that will contain the heated gaseous products (carbon dioxide and water vapor) with it. This will be what actually transfers heat into the sodium via a heat exchanger.

3.3 Heat Exchanger with Sodium

Now that we have a very hot stream of gases, let's use it to transfer heat into the molten sodium (Na). Draw a box for the gas/Na heat exchanger, with a dotted line down the middle to represent the physical separation between the fluid streams, as seen on the right of Figure 1. You can now draw arrows to represent the flow of Na, leading in and out of the heat exchanger. Write down the key parameters of the Na given to you by your partner in industry. Let's use a counterflow heat exchanger, as those tend to be more compact than comparable parallel flow heat exchangers. We will make educated guesses as to the temperatures of the gases entering and exiting the heat exchanger soon.

3.4 Steam Recovery and Gas Separation

It is also desired to keep the steam inside the cycle, as higher purity steam will result in less corrosion in the system, and require fewer inputs as a whole. A condenser will work well to separate the condensable gases (water vapor) from the non-condensable gases (carbon dioxide).

Draw a box to represent the condenser, as shown at the bottom of Figure 1. You can now draw a line that represents the carbon dioxide leaving the condenser, and showing liquid water (which has been *condensed*) leaving the condenser.

3.5 The Pump

In order to keep the system flowing and pressurized, we need to add a pump. Now is a good time to set an initial system pressure. Let's assume the system is at or near 1 MPa (10 bar), a modest pressure for these systems. Draw a box to represent the pump, as shown in the lower left of Figure 1. Connect the liquid water leaving the condenser to one side of the pump, and draw liquid water leaving the pump from the other side.

Now is a good time to fill in pressures for each node. The liquid water leaving the pump will be at 1 MPa, while the gas stream leaving the heat exchanger will certainly undergo some pressure losses. Represent these by penciling in a gas pressure of "<1 MPa." We'll calculate this actual number later, but we'll assume that it is close to 1 MPa for enthalpy calculations.

3.6 Add an Intercooler

Remember the water vapor entering the CaC_2 reactor in Section 3.1? Notice that we have liquid water leaving the pump and gaseous water entering the CaC_2 reactor. Also notice that the gas stream that would have entered the condenser is probably coming in at a very high temperature, which will be well over 100C. This is a good place to add an *intercooler*, which removes heat from one fluid stream and transfers it to another. An intercooler is essentially a heat exchanger between two parts of the same loop.

Draw a box with a dotted line in the middle to represent the intercooler, as shown in the center of Figure 1. Connect the output of the gas/Na heat exchanger and the input of the condenser to one side of the intercooler. Now connect the output of the pump and the steam input to the CaC_2 reactor to the other side. Notice that the water enters as a liquid and leaves as a solid. The heat from the intercooler will be boiling this water. Keep this in mind when we guess the temperatures entering and leaving the intercooler, which we will do soon.

3.7 Accumulate Useful Parameters

Now is the best time to use lookup tables and correlations to get whatever thermodynamic and physical properties you think you will need. For this example, this would include the following:

- Saturation temperature for $1\,\mathrm{MPa}$ steam (180C)

- Molar masses $\left(\frac{\mathrm{kg}}{\mathrm{mol}}\right)$ for all chemical compounds in the system

- Enthalpies of formation $\left(\frac{\mathrm{kJ}}{\mathrm{mol}}\right)$ for all chemical compounds in the system

- Specific heat constants *at constant pressure* $\left(c_{p_l}, c_{p_g} \; \left[\frac{\mathrm{kJ}}{\mathrm{kg \cdot K}}\right] \& \left[\frac{\mathrm{kJ}}{\mathrm{mol \cdot K}}\right]\right)$ for all chemical compounds in the system

- Enthalpy of vaporization $\left(h_{fg} \; \left[\frac{\mathrm{kJ}}{\mathrm{kg}}\right]\right)$ for any compounds that may undergo a phase change in the system

- Key enthalpies of compounds that will be tracked as they flow through the system

  - Here, "enthalpy" is a relative term. It refers to the enthalpy *above* the enthalpy of formation at 25C $\left(\Delta_0 H^f\right)$ for the compound. This includes the terms for heating. Remember that $\Delta_0 H^f$ is the enthalpy released upon creating that compound from its constituent elemental species, and that it is *different* for liquid and gaseous phases. That also means that $\Delta_0 H^f$ is *zero* for elements.

Tables of useful numbers for this problem have been compiled in Table 1.

3.8 Summary

You should now have a block diagram very similar to that in Figure 1. It seems that we have a complete loop, with everything accounted for. We'll see how true this is in the next section.

Before proceeding, fill in any parameters that you know from the start without performing any detailed calculations. These would include approximate system pressures ($1\,\mathrm{MPa}$ in the loop, $0.1\,\mathrm{MPa}$ for gases leaving the condenser and entering the atmosphere), all parameters for sodium, and any temperatures that you want to specify (25C acetylene, for example).

Keep EVERYTHING in the same unit system, preferably SI.

4 Iteration #1

We will now begin filling in the missing parameters for the system, by computing what we can from properties both guessed and given. Educated guesses based on the physics of each sub-system will be used to fill in missing parameters to proceed.

The methodology will involve performing the easiest calculation that we can do, and working either one step forward or backward in our thermodynamic loop to get more of the parameters we are looking for. Changes made to the block diagram from Figure 1 in this iteration will be marked in **blue**.

Useful thermodynamic and chemical properties				
Compound	$c_p \;\; \frac{kJ}{kg \cdot K}$	$c_p \;\; \frac{kJ}{mol \cdot K}$	M.M. $\;\; \frac{kg}{mol}$	$\Delta_0 H^f \;\; \frac{kJ}{mol}$
H_2O (g)	2.44	0.044	0.018	-241.8
CO_2 (g)	0.843	0.037	0.044	-393.5
N_2 (g)	1.039	0.029	0.028	
O_2 (g)			0.032	0
CaC_2 (s)			0.064	-59.8
C_2H_2 (g)		0.0875	0.026	+227.4
$Ca(OH)_2$ (s)		0.044	0.074	-985.2

Enthalpies from fluid tables at 1 MPa		
Compound	$H \;\; \frac{kJ}{kg}$ at 300 C	$H \;\; \frac{kJ}{kg}$ at 900 C
H_2O (g)	3055.4	4340
CO_2 (g)	771.6	1485
N_2 (g)	600.3	1287

Sat. H_2O at 1 MPa ($T_{sat} = 180$ C)	
Property	Value
$c_{pl} \;\; \frac{kJ}{kg \cdot K}$	4.405
$c_{pg} \;\; \frac{kJ}{kg \cdot K}$	2.713
$h_{fg} \;\; \frac{kJ}{kg}$	2014.5

Table 1: Useful tables of properties from lookup tables for the CaC_2/acetylene reactor example

4.1 Heat Transfer Across the Gas/Na Heat Exchanger

We know the temperature change and mass flow rate across the sodium side of this heat exchanger, so we can calculate its heat transfer with the following formula:

$$\dot{Q} = \dot{m} c_p \left(T_{out} - T_{in} \right) \tag{3}$$

where $\dot{Q}$ is the heat transfer rate in megawatts (MW), $\dot{m}$ is the mass flow rate in $\frac{kg}{sec}$, c_p is the heat capacity in $\frac{kJ}{kg \cdot K}$, and T_{out} & T_{in} are the outlet and inlet temperatures, respectively. We know $\dot{m}$, T_{out} & T_{in}. We can look up that $c_{p_{Na}} = 1.228 \frac{kJ}{kg \cdot K}$. Plugging in all these values gives us $\dot{Q} = 4.912 \, MW$. Write this number inside the gas/Na heat exchanger.

4.2 Molar Gas Fractions

We can now find the molar gas fractions of the gas streams entering the gas/Na heat exchanger. From Equation 2, we know that there are two moles of CO_2 created for each mole of H_2O created. We also know that there are five moles of O_2 consumed for every four moles of CO_2 created. Finally, we are modeling air as an 80-20 mix of $N_2 - O_2$, so we know that there are four moles of N_2 consumed for every mole of O_2 consumed. That means that if five moles of O_2 must enter the reaction, then twenty moles of N_2 get taken along for the ride.

We can use this information to modify Equation 2 to get the new total equation:

$$2C_2H_2(g) + 5O_2(g) + 20N_2(g) \rightarrow 4CO_2(g) + 2H_2O(g) + 20N_2(g) \qquad \Delta H_{RXN} = ??? \tag{4}$$
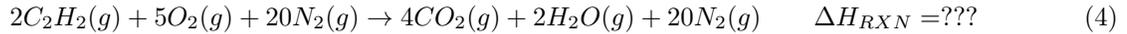
It is important to note that nitrogen is present in this reactor, even though it is not reacting. We will see why very soon. Add the twenty moles of nitrogen to each side of the equation in the acetylene burner on the block diagram, and add $N_2(g)$ to each gas stream from the acetylene reactor to the condenser, where the nitrogen will escape into the atmosphere.

Now is a good time to get the mass fractions of the gases in this stream from their molar ratios and their molar masses. We just found their molar ratios, and the molar masses were compiled in Table 1. Using that information, we get the following information:

$$(4 \, mol \, CO_2) \cdot \left(0.044 \frac{kg}{mol} \right) = 0.176 \, kg \, CO_2 \; for \; every$$

$$(2 \, mol \, H_2O) \cdot \left(0.018 \frac{kg}{mol} \right) = 0.036 \, kg \, H_2O \; for \; every \tag{5}$$
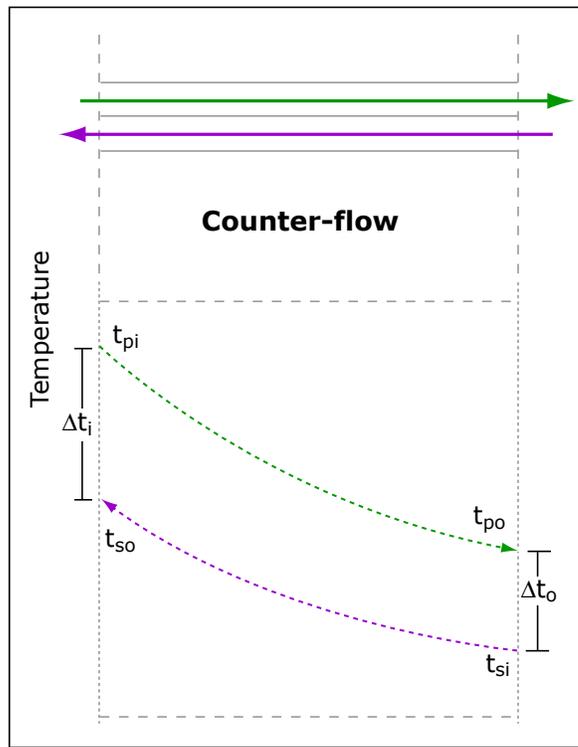
Image by MIT OpenCourseWare.

Figure 2: Typical temperature distribution in a counterflow heat exchanger

$$(20 \, mol \, N_2) \cdot \quad 0.028 \frac{kg}{mol} \quad = 0.560 \, kg \, H_2O$$

If we find the relative mass percentages from the numbers in Equation 5, we get a mix of 22.8% CO_2, 4.7% H_2O, and 72.5% N_2. As a sanity check, make sure these fractions add up to 100%. These mass fractions will be useful when calculating the mass flow rate of the gas stream in Section 4.4 below, especially since the enthalpies in Table 1 are given in $\frac{kJ}{kg}$.

4.3   Gas/Na Heat Exchanger Temperatures

We don't yet know the temperatures of the gases entering and leaving the gas/Na heat exchanger. Now is the time to make an educated guess. Recall that for a counterflow heat exchanger, the graph of the temperatures looks like that in Figure 2. The gas stream's outlet temperature $T_{out_{gas}}$ cannot lie below the inlet temperature of the sodium ($T_{in_{Na}}$), and the gas stream's inlet temperature $T_{in_{gas}}$ must lie above the sodium's outlet temperature ($T_{out_{Na}}$). Since the sodium enters at 100C and leaves at 500C, and $T_{out_{gas}}$ will probably be between them, let's choose the midpoint of 300C for $T_{out_{gas}}$ for now. Also, since $T_{in_{gas}}$ must exceed $T_{out_{Na}}$, and the gases will be coming from a hot acetylene flame, let's just assume that $T_{in_{gas}} = 900C$. Note that the actual guess for these parameters are not important now, as they will be iterated upon and refined later.

4.4   Mass Flow Rate Leaving the Acetylene Burner

Now we have enough information to find the mass flow rate of the three-gas mixture leaving the acetylene burner, and consequently the mass flow rate of each of the three consituent gases. We can modify Equation 3 to use specific enthalpies as follows:

$$\dot{Q} = \dot{m} \left(h_{out} - h_{in} \right) \tag{6}$$

where h_{out} and h_{in} are the average specific enthalpies of the gas mixture outlet and inlet, respectively. Since we have three gases, their mass fractions and the enthalpies at the outlet & inlet temperatures, we can modify

Equation 6 to account for these three gases:

$$\dot{Q} = \dot{m}_{total} \sum_{n=1}^{3} \left[x_n \left(h_{o_n} - h_{i_n} \right) \right] \tag{7}$$

where $\dot{m_{total}}$ is the total mass flow rate of the gas stream in $\frac{kg}{sec}$, x_n is the mass fraction of one gas, and h_{o_n} & h_{i_n} are the outlet and inlet enthalpies, respectively, of that gas. Substituting in the gas mass fractions and enthalpies, along with the heat exchanger's heat transfer rate from Section 4.1, we get:

$$4,912\,kW = \dot{m}_{total} \cdot \left[(0.228)\,(1485 - 771.6) + (0.047)\,(4340 - 3055.4) + (0.725)\,(1287 - 600.3) \right] \tag{8}$$

$$\Downarrow$$

$$4912\,kW = \dot{m}_{total} \cdot \left[162.66 + 60.38 + 497.86 \right]$$

$$\Downarrow$$

$$\dot{m}_{total} = \frac{4912\,kW}{720.92\frac{kJ}{kg}} = 6.814\,\frac{kg}{sec}$$

Write this mass flow rate as that leaving the acetylene reactor and entering the gas/Na heat exchanger. This is also the mass flow rate entering & leaving the intercooler. Now, since we have the mass fraction of water (4.7%), we know that

$$\dot{m}_{H_2O} = \dot{m}_{total} \times 0.047 = 0.320\,\frac{kg}{sec} \tag{9}$$

Write this as the mass flow rate of water leaving the condenser, entering and leaving the pump, entering and leaving the intercooler, and entering the CaC_2 reactor.

4.5 Mass Flow Rates of Acetylene and Remaining Species

The only major mass flow rate missing inside the loop is that of acetylene gas. To find it, we note that the mass flow rate of water ($0.320\,\frac{kg}{sec}$) corresponds to $17.78\,\frac{mol}{sec}$ (see Table 1 for water's molar mass). We also know that the molar ratios of H_2O and C_2H_2 in the acetylene burner are 1:1, so $17.78\,\frac{mol}{sec}$ of C_2H_2 flow through the loop. Using the molar mass of C_2H_2 from Table 1, we find a mass flow rate of $0.462\,\frac{kg}{sec}$ for C_2H_2. Write this as the mass flow rate of C_2H_2 on the block diagram.

We can easily find the mass flow rates of CaC_2 in and $Ca\,(OH)_2$ out of the CaC_2 reactor, since they are all in a 1:1:1 molar ratio with C_2H_2. Using the molar masses in Table 1, we find mass flow rates of $1.138\,\frac{kg}{sec}$ for CaC_2 and $1.316\,\frac{kg}{sec}$ for $Ca\,(OH)_2$. Write these down on the block diagram, as they are key inputs and outputs for the system.

We can also use these molar ratios to find the mass flow rate of air required by the acetylene burner, and therefore the individual mass flow rates of nitrogen and oxygen into the acetylene burner. Note that acetylene has a 2:5 molar ratio with oxygen, so there are $\frac{5}{2}\cdot 17.78 = 44.45\,\frac{mol}{sec}$ of oxygen entering, or $1.42\,\frac{kg}{sec}$. Nitrogen has a 4:1 molar ratio with oxygen, so it requires $(4)\cdot 44.45 = 177.8\,\frac{mol}{sec}$ of flow, which corresponds to $4.98\,\frac{kg}{sec}$ of nitrogen. Write these down on the block diagram, as they will determine the size and power of the air intake unit to be specified.

4.6 Water/Steam Temperatures Entering & Leaving the Intercooler

We haven't yet specified the temperatures of the water entering and the steam leaving the intercooler. We know from Section 3.5 that the water entering the intercooler is a liquid, and we have assumed in Section 3.1 that the water leaving the intercooler must be a gas. The saturation temperature of water at $1\,MPa$ was found to be 180C. Let us assume that the liquid water is cooled as little as possible with some small margin, say to 170C. Let us also assume that the intercooler will provide just enough heat to vaporize this water, plus ten degrees of sensible heat. This gives an exit temperature of 190C. Write these two temperatures down on the block diagram.

4.7 Intercooler Power

We now have enough information to find the power transferred in the intercooler. We know that enough heat has to be transferred to transform 170C liquid water to 190C water vapor at 1 MPa. The equation for heat transfer across the intercooler is as follows:

$$\dot{Q}_{Intercooler} = m_{H_2O} \cdot c_{p_l}(180C - 170C) + \dot{h}_{fg} + c_{p_g}(190C - 180C) \tag{10}$$

We know every term on the right side of Equation 10, from a combination of values from Section 4.4 and Table 1. Plugging these values in, we arrive at $\dot{Q}_{Intercooler} = 667.4$ kW. Write this number inside the intercooler on the block diagram. You can now use this value to determine the temperature of the gas stream leaving the hot side of the intercooler, as well as the temperature of the exhaust gases leaving the condenser.

4.8 Something Is Missing!

Look carefully at the inputs and outputs for the CaC_2 reactor. Does conservation of mass apply? The answer is NO! Note that we only have half the required water entering the CaC_2 reactor! Check the number of moles of acetylene leaving the CaC_2 reactor, compared with the number of moles of water entering it. This water must come from somewhere.

Add an extra $0.320 \frac{kg}{sec}$ of water entering the CaC_2 reactor. Let's assume that we've heated it to 190C, and pressurized it to 1 MPa for simplicity's sake. Draw this as a new input on your block diagram.

4.9 Summary of Iteration #1

Now your block diagram should resemble that in Figure 3. At this point, we have balanced the loop from a thermofluid point of view. However, note that there are still a few key missing features to the diagram. The enthalpies of reaction have not been filled in, so we don't know the outlet temperatures from either the CaC_2 reactor *or* the acetylene burner. We will have to find these missing numbers, figure out how hot the outlet gas streams are, and check our assumptions accordingly.

5 Iteration #2

As we mentioned in Section 4.9, we will be advancing our diagram from a purely thermofluid analysis to a combined thermofluid and *thermochemical* balance. This will involve finding the enthalpies of reaction for each major chemical reaction occurring, and propagating the consequences along our loop. Changes made to the block diagram from Figure 3 in this iteration will be marked in **red**.

5.1 Enthalpy of Reaction for Acetylene Combustion

Using the enthalpies of formation from Table 1, we can determine the enthalpy of reaction per mole of acetylene. This enthalpy is the energy available for heating the products (*both* chemical products and those "coming along for the ride") leaving the acetylene burner. Recall Equation 2, and substitute the enthalpies of formation for each chemical species, leaving the stoichiometric constants in place. To save a step, we will divide each stoichiometric constant by two, since two moles of acetylene are consumed, and this equation gives the enthalpy *per mole* of acetylene:

$$\Delta H_{RXN} = \sum H_{Prodcuts} - \sum H_{Reactants} \tag{11}$$

$$\Delta H_{RXN} = \underbrace{2(-393.5)}_{2CO_2} + \underbrace{1(-241.8)}_{H_2O} - \underbrace{1(227.4)}_{C_2H_2} - \underbrace{2.5(0)}_{2.5O_2} = -1256.4 \frac{kJ}{mol\,C_2H_2}$$

We can ignore nitrogen for now, since in either case it would cancel out. Write this enthalpy of reaction on the block diagram. This enthalpy is now available to heat up the CO_2, H_2O, and N_2 leaving the acetylene
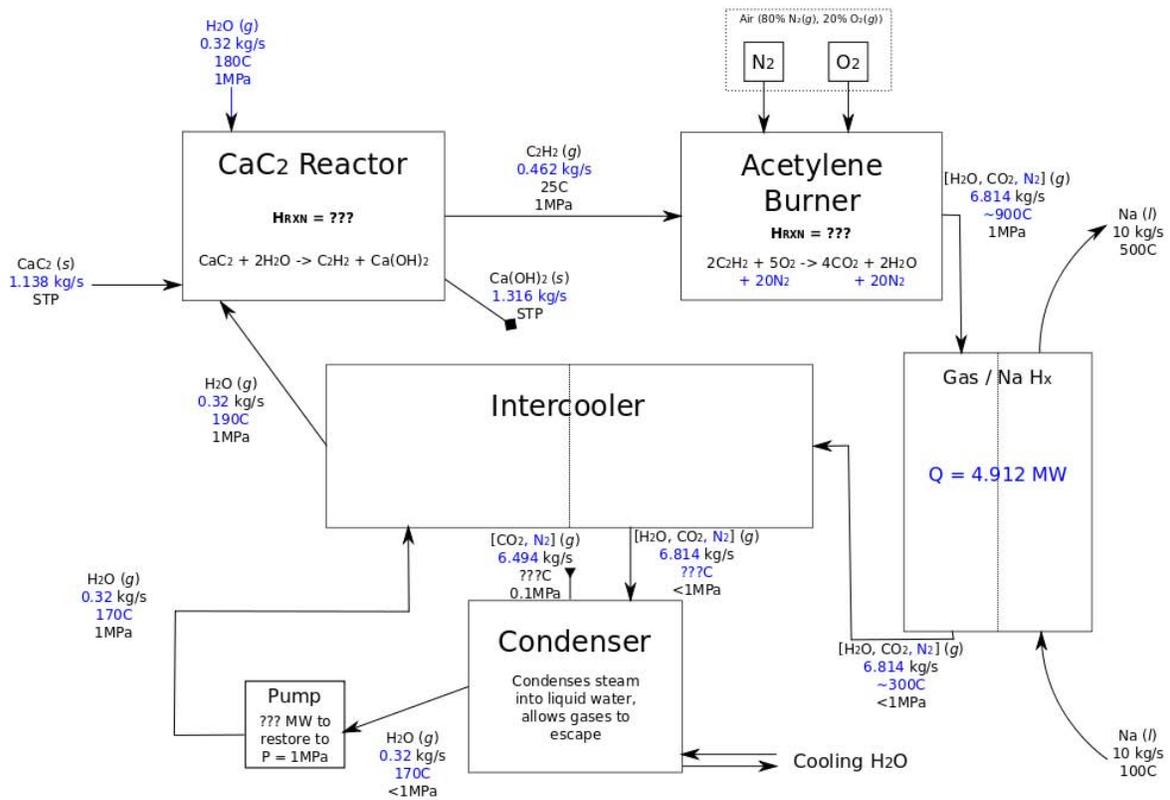
Figure 3: Block diagram for iteration #1 of this system. Changes since initial setup have been marked in **blue**.

burner. Using a variant of Equation 7, but using *mole fractions* instead of mass fractions (because our values for c_p in Table 1 are given in $\frac{kJ}{mol \cdot K}$), we arrive at the following equation:

$$\dot{Q} = \Delta T \cdot \left[\sum_{n=1}^{3} \left[\frac{\# \, moles_n}{\# \, moles_{C_2 H_2}} \cdot c_{p_n} \right] \right] \tag{12}$$

$$1256.4 \, kJ = (T_{out} - 25C) \cdot \left[\underbrace{\frac{(2) \, (0.037)}{2CO_2}}_{} + \underbrace{\frac{(1) \, (0.044)}{H_2 O}}_{} + \underbrace{\frac{(10) \, (0.029)}{10 N_2}}_{} \right]$$

$$T_{out} = 3054C$$

That's quite hot, FAAAAR hotter than our assumed outlet temperature of 900C! As a sanity check, we can look up that the flame temperature of an air-acetylene mixture is indeed in the range of 2400C, since there are some losses (radiative and other) in the real world.

5.2   What Do We Do Now?

Either way, we will have to change *something* to avoid gases entering our heat exchanger at 3054C, which would surely melt it. There are a number of possibilities, some more elegant that others. A few include:

- Changing fuel sources
- Dumping the excess heat
- Limiting the combustion efficiency (incomplete reaction)
- Storing excess heat
- Adding thermal mass to absorb energy

The first option is not an option, since the free calcium carbide is the reason we're here in the first place! Dumping the excess heat through a heat sink is possible, though we would be wasting a large amount of our power. Limiting the combustion efficiency doesn't dump any heat, but it DOES pump explosive acetylene through our system, which we must avoid. Storing excess heat only works as long as there is storage capacity available. The only option that seems elegant enough is to add extra thermal mass to absorb energy, keeping all of our energy at a lower temperature.

5.3   Adding Thermal Mass to the Acetylene Burner

Take a close look at the reaction in Equation 4. As we mentioned in Section 5.1, nitrogen is "going along for the ride" in this system. It doesn't react, but it DOES absorb heat and lower the overall temperature of the products, as the *same enthalpy* is available to heat *more products*. This explains the difference in flame temperatures between air-acetylene (~2400C) and oxy-acetylene (~3050C).

If we want to keep our flame outlet temperature at 900C, where we would like it to be, we need to figure out how much extra thermal mass to add to lower the temperature. Let's assume that we have more water (we must be near a lake or a river!), entering as 25C cooling water. This would require a complex burner/boiler design, but we'll ignore the specifics for now.

We can modify Equation 12 to include this new amount of water ($x \, more \, moles$), by fixing the outlet temperature of the acetylene burner at 900C:

$$1256.4 \, kJ = (900C - 25C) \cdot \left[\underbrace{\frac{(2) \, (0.037)}{2CO_2}}_{} + \underbrace{\frac{(1 + x) \, (0.044)}{H_2 O}}_{} + \underbrace{\frac{(10) \, (0.029)}{10 N_2}}_{} \right] \tag{13}$$

We find that x must equal 24.88 mol of excess water *per mole of acetylene*. Remember that Equation 13 is normalized to one mole of acetylene. If we multiply this number by the actual moles of acetylene flowing through the system (17.88 mol), we arrive at a required 442.37 $\frac{mol}{sec}$, or 7.97 $\frac{kg}{sec}$, of water entering the acetylene burner. Write this as a new input to the acetylene burner on the block diagram.

10
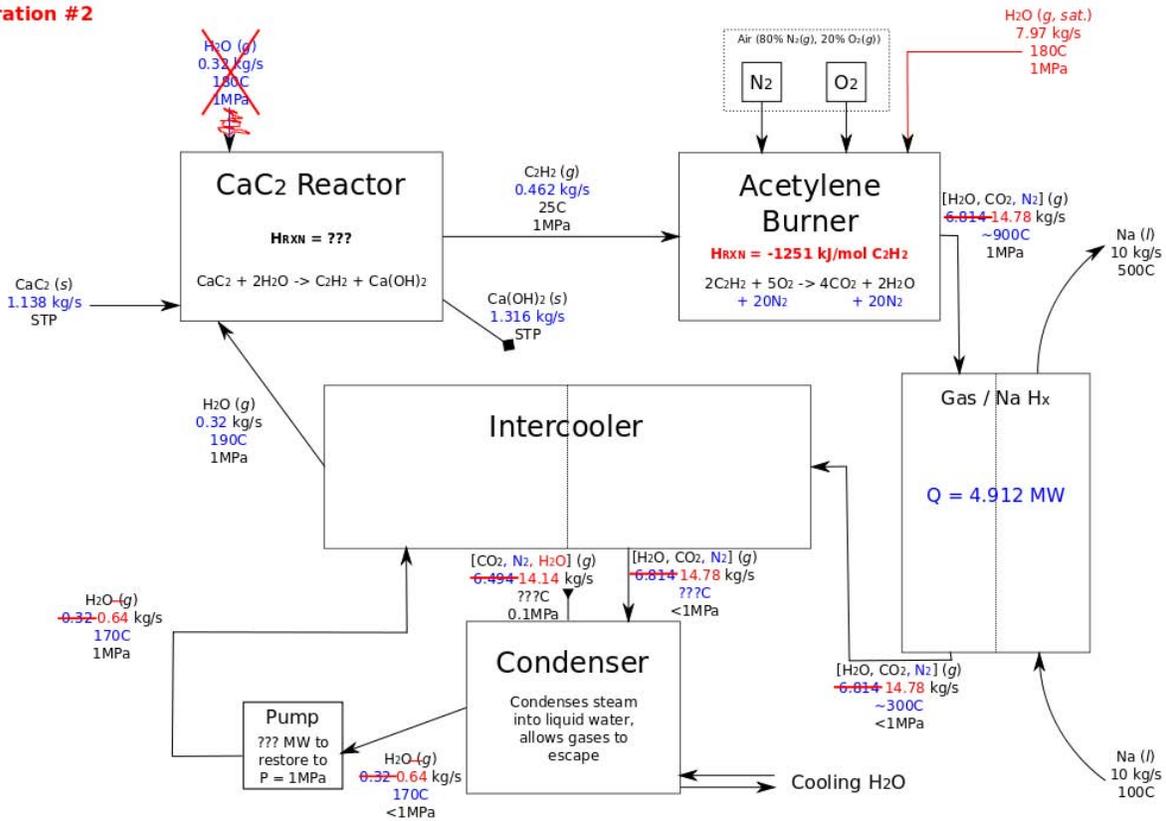
Figure 4: Block diagram for iteration #2 of this system. Changes since Iteration #1 have been marked in **red**.

5.4 Propagating the Change Along the Loop

The added steam from Section 5.3 changes the mass flow characteristics of the rest of the loop. We must now add this extra $7.97 \frac{\text{kg}}{\text{sec}}$ to the original gas mixture flow rate of $6.814 \frac{\text{kg}}{\text{sec}}$ for a total of $14.78 \frac{\text{kg}}{\text{sec}}$. Change the appropriate mass flow rates on your diagram to reflect this change.

5.4.1 Simplifying the System

Now notice that we've got tons of extra steam flowing through the system! That means we no longer need the $0.320 \frac{\text{kg}}{\text{sec}}$ of steam entering the CaC_2 reactor. Cross out that input from Iteration #1, as it's no longer necessary. Instead, you can fix the mass flow rate of steam out of the condenser at the required $0.64 \frac{\text{kg}}{\text{sec}}$, and dump the excess steam as evaporation out of the condenser.

5.5 Summary of Iteration #2

Now your block diagram should resemble that in Figure 4. At this point, we have balanced the loop from a thermofluid point of view, and partially from a thermochemical perspective. The next iteration will focus on finding the last major unknown in the system and propagating its consequences.

6 Iteration #3

Now we will be advancing our diagram to a complete thermofluid and thermochemical balance. This will involve finding the enthalpies of reaction for each remaining major chemical reaction occurring, and propagating the consequences along our loop. Changes made to the block diagram from Figure 4 in this iteration will be marked in green.

6.1 Enthalpy of Reaction for Calcium Carbide Reaction

Using the enthalpies of formation from Table 1, we can determine the enthalpy of reaction per mole of calcium carbide reacted. Using the methodology from Equations 11 and 12, we find that the enthalpy of the reaction in Equation 1 is -315.26 $\frac{kJ}{mol}$. Since some reactants and products remain solid, finding a true outlet temperature isn't easy, but it is clear that it will be high. We want the acetylene to stay *cool*, so we must add cooling water to the CaC_2 reactor. Draw this on the block diagram to explicitly show that this reaction must be cooled.

6.2 Propagating the Change

Now that we know there is *no* reason to heat the water entering the CaC_2 reactor, there's no need for it to be steam. *That means there's no need for an intercooler at all!!!* Cross out the intercooler, and re-route any flow lines to reflect this change. You can also specify that the water leaving the condenser can be quite cool, around 30-40C, since the cooler the inlet water is, the less cooling water will be required. Remember from Section 3.4 that we chose a closed loop for reasons of water purity and corrosion resistance, so we don't want to switch to an open loop now.

Write the enthalpy of reaction from Section 6.1 on the block diagram, and don't forget to change the temperatures & phases of water leaving the condenser.

6.3 Summary of Iteration #3

Now your block diagram should resemble that in Figure 5. At this point, we have balanced the loop from a thermofluid and thermochemical point of view.

7 What's Next?

Further iterations are necessary to optimize and fine-tune this design. Examples of directions in which to proceed include:

- Determine the new gas/Na heat exchanger outlet temperature

- Relax assumptions about ideal reactor mixing

- Relax assumptions about adiabatic components

- Design the heat exchangers

  - Calculate an approximate pressure loss, and see if it changes any state variables down the loop
  - Consider how to address problems of fouling, especially from incomplete combustion of acetylene

- Design the condenser

  - Calculate an approximate pressure loss, and see if it changes any state variables down the loop

- Calculate the pressure loss across the loop, and calculate the required pumping power needed to pump the system

- Explore materials choices and concerns for each component of the system
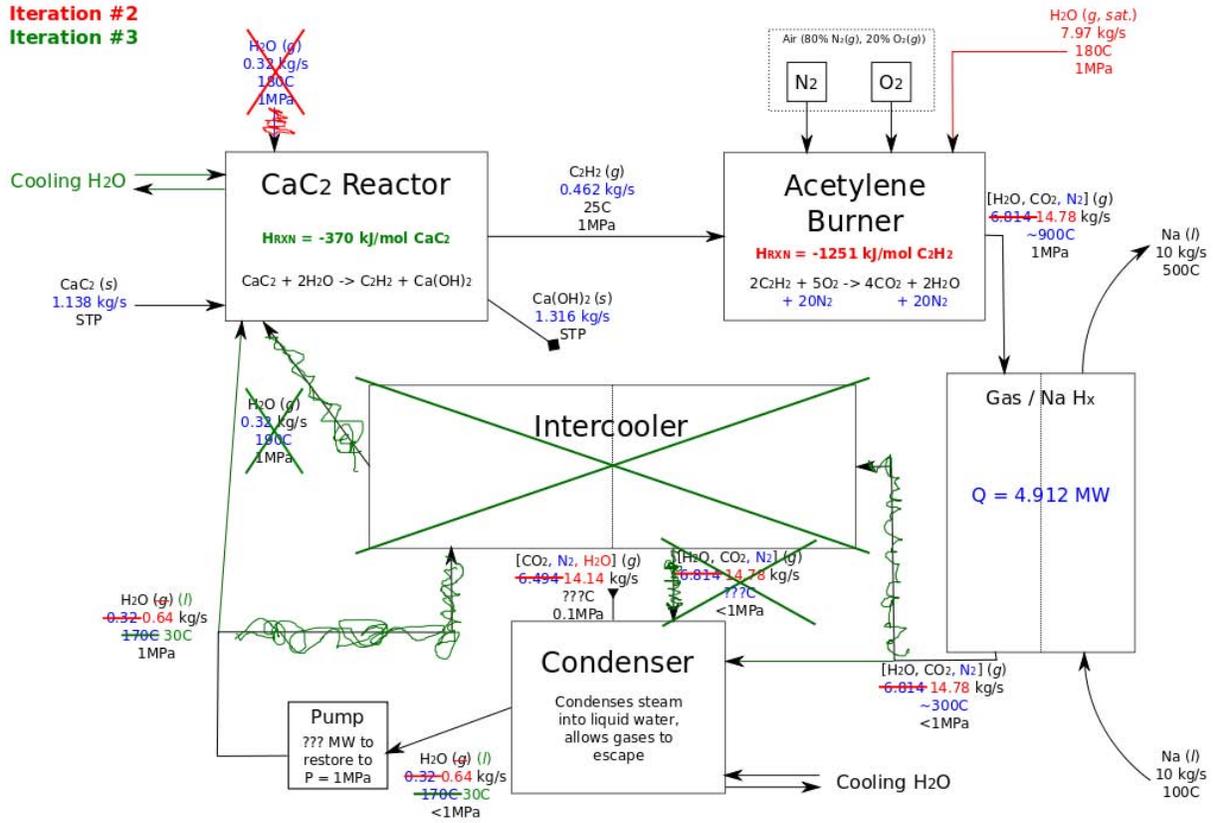
Figure 5: Block diagram for iteration #3 of this system. Changes since Iteration #2 have been marked in **green**.

- – Estimate corrosion losses and mechanisms for each component

- Plan for accidents, such as gas explosions, leaks, primary/secondary heat exchanger leakage, safety valves & systems, startup, shutdown, and combustion transients

- Explore how to clean and maintain the two reactors, the heat exchanger, and the condenser

- Design the calcium carbide input system - i.e. how will you ensure a constant input stream of calcium carbide?

- Relax the assumption of pure calcium carbide, as "technical grade" is only 75-85% pure

  - – Explore what the impurities will do to your reaction

- Calculate pressure losses through piping in the system

- Calculate Reynolds numbers for key components (heat exchanger, condenser) and explore if you are nearing Mach 1, entering turbulent flow, and how that will affect heat transfer

- Calculate the true effectiveness of the heat exchangers

- *Think of more!*

These would all be considered finer details of the design. Even so, they should be addressed in some way, and the relative importances of each should be weighed in when choosing how to address them.

22.033 / 22.33 Nuclear Systems Design Project
Fall 2011