MATERIAL AND ENERGY BALANCE

We produce acetaldehyde by dehydrogenation of ethanol. Flow chart is as shown in the figure.

Reaction:

$$C_2H_5OH \rightarrow CH_3CHO + H_2$$

Catalyst: Cu -Co-Cr_2o_3

Temperature: 280 – 350^0 C.

Process description: The raw material i.e., ethanol is vaporized and the vapors, so generated, are heated in a heat exchanger to the reaction temperature by hot product stream. The product stream is cooled to -10^0 C and in doing it, all unreacted ethanol and acetaldehyde are condensed. The out going gaseous stream, containing hydrogen mainly, is scrubbed with dilute alcohol (alcohol + water) to remove uncondensed products and the undissolved gas. The remaining pure hydrogen (98%) is burnt in stack.

The material and energy balance in a plant design is necessary because this fixes the relative flow rates of different flow streams and temperatures in the flow sheet.

Notations used:

M_{steam} = Mass flow rate of steam.

▲H_{steam} = enthalpy of steam.

E = Mass flow rate of ethanol.

A = Mass flow rate of acetaldehyde.

H = Mass flow rate of hydrogen.

C_p = specific heat capacity.

λ = Latent heat of vaporization.

Basis: One hour of operation.

Amount of acetaldehyde to be produced = 150 TPD = 6250kg/hr.

Molecular weight of ethanol = 46 kg/kmol.

Molecular weight of acetaldehyde = 44 kg/kmol.

Molecular weight of hydrogen = 2 kg/kmol.

Therefore, amount of acetaldehyde to be produced = 142.04 kmol/hr.

Let conversion be 94%.

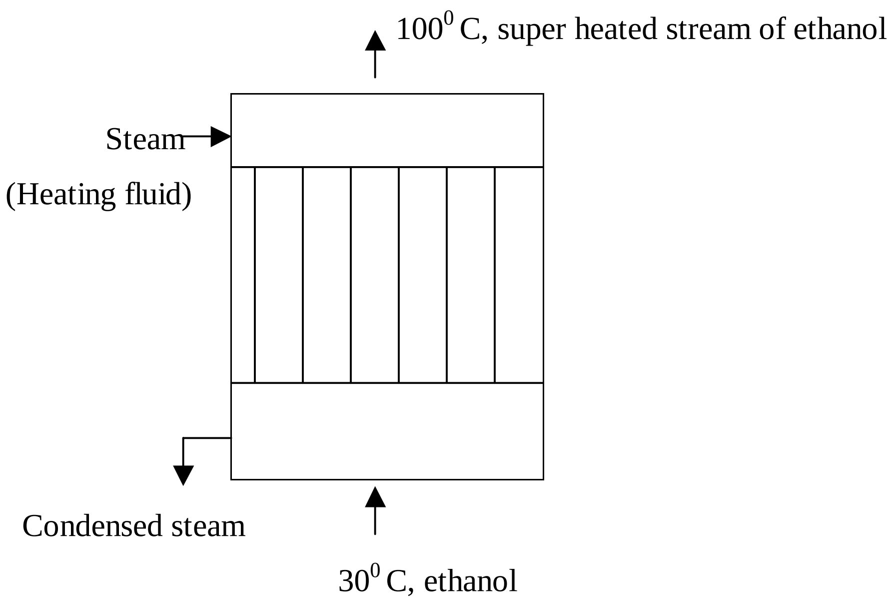
Taking into account the losses let, the acetaldehyde produced to be some extra.

Let acetaldehyde to be produced = 6500 kg/hr.

Amount of ethanol required for 100% conversion = 6795.45 kg/hr.

Therefore, ethanol required for 94% conversion = 7229.2 kg/hr.

Vaporizer:



As shown in the figure,

Ethanol liquid inlet temperature = T_i=30^0 C.

Ethanol leaves as superheated steam at 100^0 C = T_o

Heating fluid is assumed to be saturated steam here and to provide sufficient temperature gradient; it is taken to be about 3 atmospheric pressure. At this pressure it condenses at 133.89^0 C and because process streams are normally available at this pressure.

Condensing temperature of ethanol = 133.89^0 C.

From steam table enthalpy of steam at this temperature = ΔH_{steam} = 514.9 kcal/kg.

Boiling point of ethanol = T_b = 78.4^0 C.

Specific heat of ethanol, at 30^0 C = Cpi = 0.5976 kcal/kg ^{0}C.

at 100^0 C = C_{po} = 0.4382 kcal/kg ^{0}C.

Latent heat of vaporization of ethanol = $\lambda_{ethanol}$ = 200.6 kcal/kg.

From heat balance we have,

$M_{steam} * \Delta H_{steam} + E * C_{pi} * (T_i - T_b) = E * \lambda_{ethanol} + E * C_{po} * (T_o - T_b)$

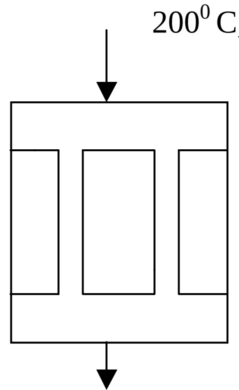
Therefore, $M_{steam} = E * [\ C_{pi} * (T_b - T_i) + \lambda_{ethanol} +\ C_{po} * (T_o - T_b)] / \Delta H_{steam.}$

$M_{steam} = 7229.2 * [0.5976 * (78.4 - 30) + 200.6 + 0.4382 * (100 - 78.4)] / 514.9$

$= 3355.40$ kg.

Reactor:

200^0 C, ethanol



310^0 C, A = 6500 kg.

E = 295.45 kg.

The reaction in the reactor:

$$C_2H_5OH \rightarrow CH_3CHO + H_2$$

Optimum reaction temperature = 310^0 C.

Conversion = 94%.

From material balance we have,

Amount of acetaldehyde produced = .94 * 44* 7229.2 / 46 = 6500 kg.

Amount of hydrogen produced = .94 * 2* 7229.2 / 46 = 295.45 kg.

Amount of ethanol unreacted = 7229.2 – (6500 + 295.45) = 433.74 kg.

If it is decided to use saturated steam at 133 atm. (steam at this pressure condenses at 335.5^0 C), it means that the reactor should be a pressure vessel. This proposition is rejected because of high costs and it is decided to use saturated vapors of dowtherm, condensing at 350^0 C, for heating purposes.

$\lambda_{dowtherm} = 56.5$ kcal / kg.

Heat of reaction = $\Delta H_r = 332.64$ kcal / kg.

Assuming ethanol vapors enter the reactor at 200^0 C.

From heat balance we can found amount of dowtherm required = M_d.

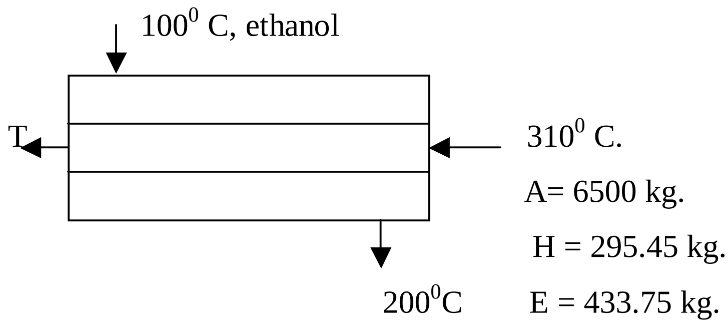
Specific heat capacity of ethanol = 0.539 kcal / kg ^{0}C.

$M_d * \lambda_{dowtherm} = E * C_p * (310 – 200) + E * \blacktriangle H_r * 0.94$

Therefore, $M_d = 7229.2 * [0.539 * (310 – 200) + 332.64 * 0.94] / 56.5$

$= 47.594 * 10^3$ kg.

Heat exchanger:



This is used only for heat recovery. Since it is assumed vapor is heated up to 200^0 C by the product stream of the reactor at 300^0 C.

Let outlet temperature = T^0 C.

C_p of ethanol at 310^0 C = 0.549 kcal / kg ^{0}C.

C_p of acetaldehyde at 310^0 C = 0.528 kcal / kg ^{0}C.

C_p of hydrogen at 310^0 C = 2.485 kcal / kg ^{0}C.

From heat balance we can find the outlet temperature.

$E*C_{p, ethanol}*(200 – 100) = E*C_{p,ethanol}*(310 – T) + H*C_{p,hydrogen}*(310 –T) + A*C_{p,acet}$

7229.2*0.471*(200-100) = 433.75*0.549*(310-T) + 295.45*2.485*(310-T)+6500*0.528

Therefore, T = 232.69^0 C.

Condenser C_1:

In condenser 1 it is decided to use cooling water at 300^0 C. the outlet temperature of cooling water is not allowed to go above 50^0C, because above this temperature, there is a problem of vaporization. Normally the approach temp difference is about 10^0C. Since the product can at best be cooled to 40^0C, at this temperature the product stream would be a two-phase mixture and the mixture composition can be found out from VLE data.

We make an approximate that; the information given at 699 mmHg is taken.

At 400^0C, ethanol in vapor phase = 4.1 mol%.

Ethanol in liquid phase = 55 mol%.

Let, m_l = moles of liquid consisting of ethanol and acetaldehyde.

m_v = moles of vapor consisting of ethanol and acetaldehyde.

Therefore from mole balance we have,

$0.55 * m_l + 0.041 * m_v = 9.43$

$0.45 * m_l + 0.959 * m_v = 147.42$

On solving above two equations we get, m_l = 5.868 kmol.

m_v = 151.283 kmol.

Vapor phase composition,

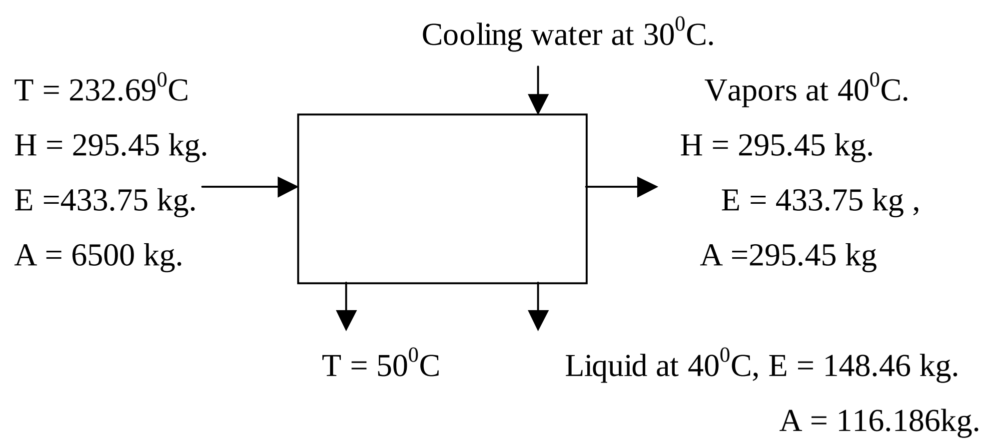
Acetaldehyde = 145.08 kmol = 6383.52 kg.

Ethanol = 6.2026 kmol = 285.32 kg.

Liquid phase composition,

Acetaldehyde = 2.6406 kmol = 116.186 kg.

Ethanol = 3.2274 kmol = 148.460 kg



Heat balance,

At 232.69^0C,

$C_{p,\ hydrogen}$ = 2.485 kcal / kg ^0C.

$C_{p,\ acetaldehyde}$ = 0.417 kcal / kg ^0C.

$C_{p,\ ethanol}$ = 0.5415 kcal / kg ^0C.

$\lambda_{acetaldehyde}$ = 139.5 kcal / kg.

$\lambda_{ethanol}$ = 200.6 kcal / kg.

Heat given out by hydrogen = 295.45 * 2.485 * (232.69 – 40) = 141.47 * 10^3 kcal.

Heat given out by acetaldehyde = 6500* 0.417 * (232.69 – 40) + 116.186 * 139.5

= 538.5 * 10^3 kcal.

Heat given out by ethanol = 433.75* 0.5415 * (232.69 – 40) + 148.46 * 200.6

= 75.04 * 10^3 kcal.

Total heat given out = 755.01 * 10^3 kcal.

Let, M_w = mass flow rate of cooling water.

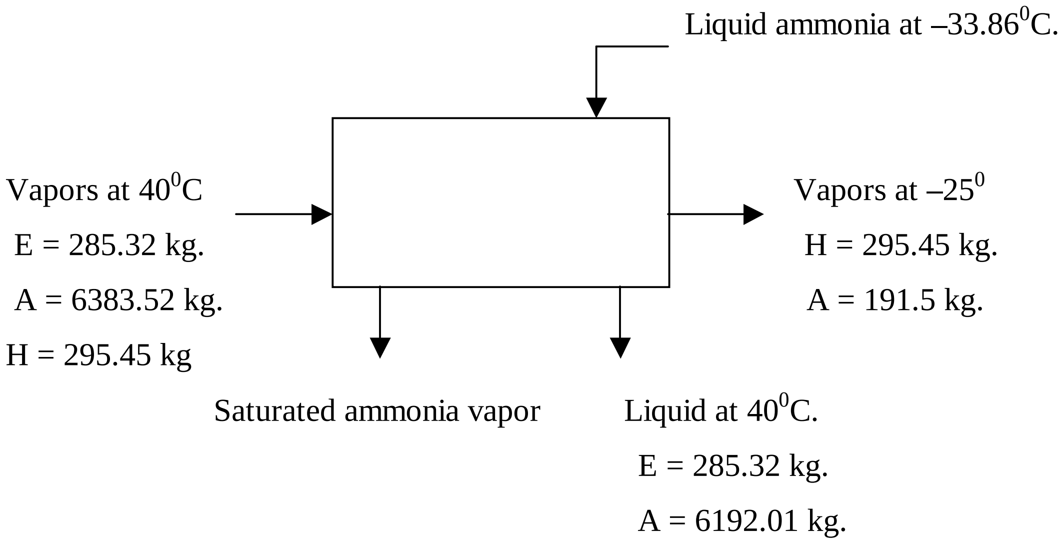
C_p of water = 1 kcal / kg ^0C.

Therefore, Mw = 755.01 * 10^3 / (1 * (50-30)).

= 37.75 * 10^3 kg.

Condenser 2:

In condenser c_2, it is desired to condense all ethanol and acetaldehyde. If the working pressure is 1 atm. From the equilibrium data it is seen that for temperatures below 30^0C, there is going to be no ethanol in vapor phase and acetaldehyde would exert its vapor pressure at that temperature. If it is desired to achieve about 97% recovery of acetaldehyde, the outlet temperature of the product stream should be about $–25^0C$.This is because at $–22.6^0C$, its vapor pressure is 100 mmHg and the vapor phase will consists of 13.15 mol%. In view of this, the cooling fluid chosen is saturated NH_3 at 1 atm. At which it boils at $–33.6^0C$.



Heat balance,

At 40^0C,

$C_{p,\ hydrogen}$ = 3.399 kcal / kg ^{0}C.

$C_{p,\ acetaldehyde}$ = 0.347 kcal / kg ^{0}C.

$C_{p,\ ethanol}$ = 0.616 kcal / kg ^{0}C.

$\lambda_{acetaldehyde}$ = 139.5 kcal / kg.

$\lambda_{ethanol}$ = 200.6 kcal / kg.

$\lambda_{ammonia}$ = 590 kcal / kg.

Heat given out by hydrogen = 295.45 * 3.399 * (40 + 25) = 65.275 * 10^3 kcal.

Heat given out by acetaldehyde = 6383.52* 0.347 * (40+ 25) + 6192.01 * 139.5

= 1007.765 * 10^3 kcal.

Heat given out by ethanol = 285.32* 0.616 * (40+25) + 285.32 * 200.6

= 68.659 * 10^3 kcal.

Total heat given out = 1141.699 * 10^3 kcal.

Let $M_{ammonia}$ = mass flow rate of ammonia.

Therefore, $M_{ammonia}$ = 1141.699 * 10^3 / 590.

= 1935.083 kg.

Preheater:

The preheater to the distillation column is necessary because the feed plate will be completely chilled if the feed is not heated. The water stream from condenser c_1 is available at 50^0C and is used in the preheater. If the maximum approach temperature difference is 10^0C, the product stream can at best be heated to 40^0C. the distillation column pressure is chosen to be 1158 mmHg so that pure acetaldehyde is obtained as liquid product at 40^0C. In view of this, the stream coming out of the preheater is liquid.

Heat balance,

At 40^0C,

$C_{p,\ acetaldehyde}$ = 0.347 kcal / kg ^{0}C.

$C_{p,\ ethanol}$ = 0.616 kcal / kg ^{0}C.

Let, M_w = mass flow rate of cooling water.

M_w * (50-30) = 433.78 * (40 + 25)* 0.616 + 6308.196*(40+25)*0.347

Therefore, M_w = 7982.49 kg.

Distillation column:

In distillation column acetaldehyde condenses at 40^0C. since vapor pressure data's of pure gas is not available, it is estimated using Antoine's equation.

ln P = A + B/T

Where, A and B are constants, they can be determined from boiling point data at,

Pressures 760 mmHg and 400 mmHg.

At 760 mmHg T = 20.2^0C= 293.2^0K.

400 mmHg T = 4.9^0C = 277.9^0K.

Therefore, ln 760 = A + B/293.2

ln 760 = A + B/277.9

On solving above two equations we get,

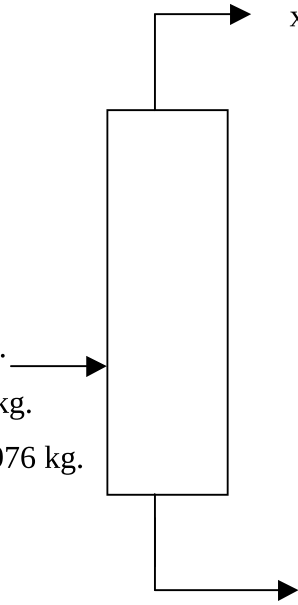
A = 18.29 and B = -3418.2

Therefore, ln P = 18.29 – 3418.2/T

Therefore at 40^0C, P = 1586.41 mmHg.

D = 6372.56 kg.

$x_d = 0.99$



E = 433.78 kg.

A = 6308.196 kg.

Total feed = F = 6741.976 kg.

$x_f = 0.93$

W = 369.416 kg.

$x_w = 0.06$

Assume 99% acetaldehyde recovery in overhead product.

Assume $x_d = 0.99$

In overhead:

Acetaldehyde = 6245.11 kg.

Ethanol = 127.45 kg.

Total D = 6372.56 kg.

In bottom:

Acetaldehyde = 63.082 kg.

Ethanol = 306.334 kg.

Total W = 369.416 kg.

F = D + W

$F * x_f = D * x_d + W * x_w$

Therefore, $x_w = \frac{F * x_f - D * x_d}{W * x_w}$

$$x_w = \frac{6741.976 * 0.93 - 6372.56 * 0.99}{369.416} = 0.06$$

Assume reflux ratio = 0.3

Therefore L / D = 0.3

L = 0.3 * 6372.56 = 1911.768 kg.

Vapor going to the condenser = L + D = 1911.768 + 6372.56

= 8284.328 kg.

Of this 99% is acetaldehyde.

Therefore, vapor composition going to the condenser:

Acetaldehyde = 8118.64 kg.

Ethanol = 165.68 kg.

Heat load to the condenser = $M_{ethanol} * \lambda_{ethanol} + M_{acetaldehyde} * \lambda_{acetaldehyde}$

= 165.68 * 200.6 + 8118.64 * 139.5

= $1165.7856 * 10^3$ kcal.

Reboiler load:

Let "m" be the amount of liquid vaporized.

Let "$\bar{L}$" be liquid going into the reboiler.

Let $\bar{L}$ / W = 10

Therefore, $\bar{L}$ = 369.416 * 10 = 3694.16 kg.

Therefore, m = $\bar{L}$ – W

= 3694.16 – 369.416 = 3324.744 kg.

Of which about 10% is acetaldehyde.

Therefore, Acetaldehyde = 332.47 kg.

Ethanol = 2992. 27 kg.

Therefore, heat load in the reboiler = Methanol $* \lambda_{ethanol} + M_{acetaldehyde} * \lambda_{acetaldehyde}$

= 2992.27 * 200.6 + 332.47 * 139.5

= $646.629 * 10^3$ kcal.