

Title:
**Clarifying Process parameters for the
REHOS Cycle Concept.**

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Introduction:

Various forms of the REHOS cycle have been described to make the principles clear. In this regard we refer to [7] that demonstrated the REHOS cycle as baseload power generator making use of waste heat for energy input. Papers [8] and [9] spell out where the REHOS cycle would be derived from and fit into the global renewables energy map, while [10] spell out practical costing of simplifications of the most basic power generation cycles to be used for electricity generation as well as electrical propulsion for marine transport. All process variables provided in the sketches were calculated by simultaneous solutions of the formula's as listed below. Obviously a new set of formulas are compiled for every new process layout, to properly reflect the correct mass-, species- and heat balance for every component, as well as the complete process.

Apart from a detailed concept description of a simple variant of the REHOS Cycle, this paper also spell out the formulas solved together for mass balance, species balance and heat balance of all the named process points on the process layout of the REHOS Heat Balance Model sketched in Figure 1 and 2. Formulas for the calculation of all process parameters like temperature, pressure, enthalpy as well as NH₃ concentration are provided. All these formulas were solved in an Excel Spreadsheet, linked to two files of lookup tables for Saturated Steam, Saturated and Superheated (at 10 Bar Absolute) Ammonia, as well as lookup table process data for saturated NH₃ in Aqua with several different concentrations of ammonia. Over years the lookup table data, referenced in [1] to [5], crosschecked and double checked with numerous other sources have been compiled. The excel files with these "Steam Tables", as I call them, have become quite large over the years, also carrying information on various other substances, but I had to extract only the bare minimum of what is required in order to keep the files small enough for sending by e-mail.

The REHOS Cycle:

The REHOS cycle is made possible by a few physical phenomena found in working with a vertical column of a binary solution of NH₃ dissolved in water. It is well known that any saturated vapor would condense in saturated liquid only if the liquid is sub cooled with respect to the incoming vapor to condense. **Saturated liquid is said to be sub cooled, with respect to the incoming vapor to condense, when the liquid vapor pressure is lower than the vapor pressure of the incoming vapor to condense.** This means that sub cooling is actually defined by the difference in vapor pressures, and not the temperatures of the vapor and liquid.

The consequence of the sub cooling definition above is that saturated water vapor at 30°C (vapor press 4.25 kPa Abs) would condense in sub cooled water at a temperature lower than 30°C, eg. water at 27°C (vapor press 3.57 kPa Abs). The water is said to be sub cooled by 3°C. The same holds true for ammonia (NH₃) saturated vapor at 30°C (vapor press 11.8 Bar Abs) that would condense into saturated liquid NH₃ at 27°C (vapor press 10.8 Bar Abs) as it is sub cooled by 3°C.

Sub cooling, as per above definition, have an interesting consequence when dealing with binary solutions: Should a pure saturated NH₃ vapor at -19°C (vapor pressure 2 Bar Abs) come into contact with a saturated solution of 80% NH₃ in aqua, (water) at a temperature of -15°C (vapor pressure 1.85 Bar Abs), the vapor will condense, or be absorbed, as the saturation pressure of this binary solution would be 2 Bar Abs at a temperature of -13°C, which means the solution at -15°C is actually sub cooled by 2°C, although it is 4°C warmer than the condensing vapor! Should the liquid solution concentration of NH₃ be 50% NH₃ in aqua, instead of the 80% mentioned above, the liquid saturation temperature (where the vapor pressure is 2 Bar Abs) would be 13°C, which have the result that the incoming cold, (-19°C) vapor would condense in the liquid as long as the liquid temperature stay below 13°C. Similarly, the saturation pressure of a 5% NH₃ in aqua solution is 2 Bar Abs at a temperature of 103°C, having the effect of absorbing the cold (-19°C) vapor even at 100°C (which is then sub cooled by 3°C). This concept of increase in temperature by the absorption of cold vapor into a sub cooled binary solution has been used extensively in absorption refrigeration and absorption heat transformers (AHT) for years already, as also described in my paper ref [10] written in August 2017.

From a publication made for the Kalina cycle, by L. Kielasa et al [11] made in 1996 already, ammonia-water mixtures have four primary differences from the pure NH₃ and H₂O state. The third primary difference mentioned in this paper, spell out that **"A binary mixture has thermo-physical properties that causes mixed fluid temperatures to increase or decrease without a change in heat content. The temperature of pure substances like NH₃ or H₂O cannot change without a change in energy."** This create a further interesting phenomena with binary solutions in the density relation with NH₃ concentration and solution temperature. Saturated solution of 80% NH₃ in Aqua at -13°C have a density of 711 kg/m³ and an enthalpy of $H_{top} = -1.932e^5 J / kg$, in stark contrast to the much higher density of 916 kg/m³ of a 5% NH₃ in aqua solution at 103°C and an enthalpy of $H_{bottom} = 3.97e^5 J / kg$, while the saturation vapor pressure is 2 Bar Abs for both example solutions. This result in a binary column where the hot (high enthalpy) solution migrate to the bottom of the column and is trapped there, while the cooler, higher concentration NH₃ solution with lower density (and low enthalpy) would rise to the top of the column. This saturated binary column, cold at the top (-13°C) and hot (103°C) at the bottom, while any external heat added anywhere along the length of the saturated column would boil off (desorb) some NH₃ vapor, which would rise as bubbles to the colder, higher concentration solution higher up in the column to be absorbed again to replenish any heat lost in the column, maintaining the temperature and concentration gradients. Once the concentration- and temperature gradients have been established, only conduction heat flowing from the hot bottom to the cold top (as well as through the reactor walls) would have to be replenished with external heat to maintain the gradients. The actual mechanism of this principle can be visualized as follows:

Should heat be added anywhere along the length of the saturated reactor with established temperature and concentration gradients,

- an amount of NH₃ vapor would be boiled of (desorbed) from the binary solution at the point of external heat entry;

- the vapor bubble would immediately start rising due to density difference with the liquid;
- additional vapor (as bubble) generated locally in the reactor would increase the pressure in the reactor;
- the increased pressure implies an increase in saturation temperature, implying an immediate sub cooling close to the point of external heat input;
- the generated vapor bubble would be re-absorbed in the sub cooled region directly above where the bubble was formed;
- re-absorption of the vapor increase the NH₃ concentration directly above the original heat entry point, as well as decrease the local pressure again to close to where it was.
- the higher concentration NH₃ solution so formed, have a lower enthalpy at the same original pressure, decreasing the solution temperature to match this enthalpy;
- at the same time, the original solution releasing NH₃ vapor, now have a lower concentration NH₃, with a corresponding higher density;
- this higher density solution would migrate downwards, displacing higher concentration solution below it;
- the lower concentration NH₃ have a higher enthalpy at the same pressure, by the same amount as the enthalpy drop of the upwards migrating higher concentration solution, increasing the solution temperature to match this enthalpy;
- the rising higher concentration solution enthalpy decrease amount, stays balanced with the downwards flowing lower concentration solution enthalpy gained, so that the complete reactor stay in energy balance, even though any heat entering the reactor, end up as establishing a higher bottom temperature (with higher enthalpy) and lower top temperature (with lower enthalpy), as well as a higher NH₃ concentration at the top than the bottom of the reactor.

The amount of heat required to establish the temperature and concentration gradients for the -13°C to 103°C example reactor, amounts to:

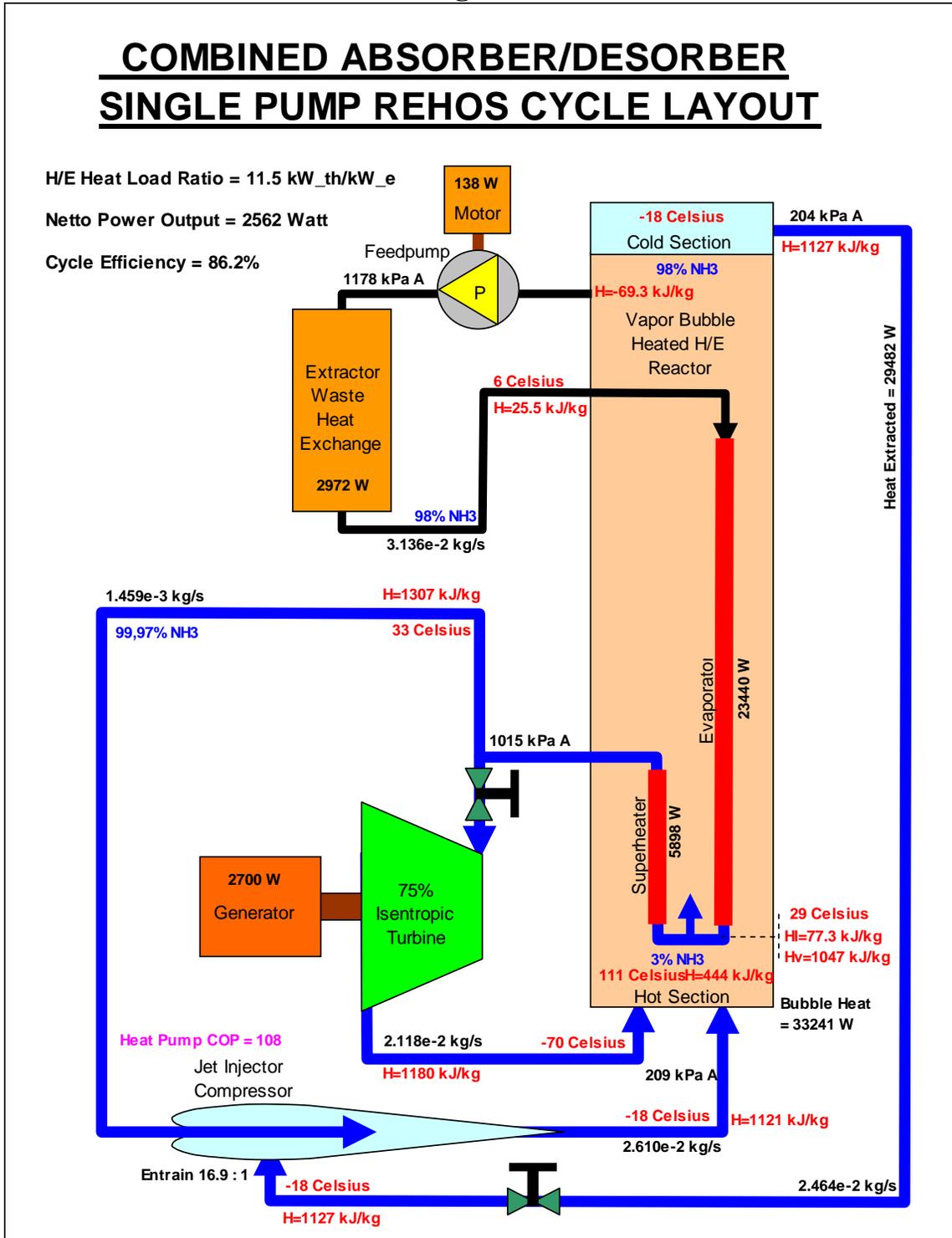
$$\text{Gradient Establishing Heat} = (H_{\text{bottom}} - H_{\text{top}}) = [(3.97e^5) - (-1.932e^5)] = 516.32e^3 \text{ J / kg}$$

This high amount of heat is only required to establish the temperature and concentration gradient, and maintaining the gradients take a lot less energy, as only the heat extracted from the reactor, as well as the minimal radiant and conduction heat loss need to be replenished. The average pressure in the saturated reactor would increase slowly with an unbalanced addition of heat, as would the temperature differential, but the rise in bottom to top differential temperature would lead to higher heat losses, countering the imbalance again. Without any external heat input, the top and bottom temperatures would slowly come closer together with a corresponding decrease in average pressure in the reactor, until the temperature and concentration gradients inside the reactor cease altogether.

To put the stepwise explanation above in different words, should heat be extracted (by heat exchange coils) from the hot bottom of the reactor, the area would become sub cooled, and NH₃ vapor entering from the bottom as bubbles would be absorbed in the hot

sub cooled solution to re-heat it again to the saturated condition. This added high concentration ammonia being absorbed (dissolved) at the bottom of the reactor, still have a very high enthalpy, and would migrate upwards due to solution density reasons as stepwise described above. As it migrates upwards, it is also cooled by the direct contact

Figure 1



high rates of heat transfer, to allow high efficiency heat exchange, as it is critical to the efficient operation of the REHOS cycle.

Adding a heat pump compressor to extract NH₃ vapor (flashing liquid into vapor and cooling the top area of the column) and pumping compressed vapor (at a pressure high enough to overcome the column hydraulic height) into the bottom area of the column, create this bubble reactor, where the heat pump continuously extract heat from the top and add it to the bottom by vapor bubbles being absorbed in sub cooled regions along the complete length of the column. The low pressure ratio required for the compressor ensure a very high COP heat pump, most practically manufactured as a vapor injector type (see reference [6]) compressor. The energy used by this heat pump compressor is very low, and is designed to only supplement heat used from the reactor and radiant heat lost to the environment, both of which would sub cool certain area's of the reactor. Note that the vapor bubbles rising vertically in the reactor would only be absorbed (and generate heat in the process) in area's of the column which is sub cooled. Heat generated by the condensing vapor bubbles is the sum of the latent heat of condensation, as well as the heat of solution (HOS) of the NH₃ dissolving into the solution.

The heart of the REHOS cycle is this absorption powered reactor as described above, with vapor injector type compressor with a low compression ratio. The high COP heat pump formed by the vapor injector type compressor, establish and maintain a temperature and concentration gradient in the reactor, extracting heat from the top of the reactor as liquid ammonia flash into vapor, and pumping heat into the reactor bottom by direct contact vapor bubble absorption into the sub cooled binary solution. The pressure the reactor operate on is a function of the NH₃ concentration as well as the average temperature, but would in general be chosen fairly low, as eg. about 2 Bar absolute.

The low reactor top temperature facilitate waste heat absorption from the environment below ambient temperatures, allowing the environmental heat exchanger near the cold top of the reactor to extract waste heat from external sources, adding this heat to the cycle. The low top temperature also ensure during operation that the liquid present there, has a very high concentration NH₃, used direct by the pressure pump to feed the evaporator/superheater heat exchanger coils in the reactor bottom to form the high pressure vapor used both for powering the power turbine and a small percentage for driving the injector compressor.

High reactor bottom temperature facilitate the evaporation and superheating of the high pressure pumped turbine drive vapor (NH₃) in the heat exchanger coils integrated into the hot reactor bottom. The heat absorbed for evaporation and superheating the pumped high pressure NH₃, is extracted from the hot bottom of the reactor by the heat exchanger coils, sub cooling the reactor bottom area, allowing vapor bubbles from the heat pump injector compressor (as well as turbine exhaust) to be absorbed in that area, transferring large amounts of absorption heat from the low pressure vapor bubbles to the hot bottom of the reactor. As mentioned before, the slow upwards migration of the absorbed NH₃ is cooled by the slow downwards migration of the higher density lower concentration

solution, balancing the reactor internally as far as mass, species as well as heat is concerned.

The low pressure, but high temperature bottom of the reactor also facilitate the main thermodynamic cycle efficiency gain, by absorbing all the low pressure expanded turbine exhaust vapor direct into the reactor bottom, regeneratively recovering all the latent heat in the exhaust vapor that would have been rejected to a cooling tower if this was a conventional organic rankine cycle. This create the extremely high cycle efficiency of the REHOS cycle in excess of 85%, only reduced by the energy used for pumping as well as the energy in the small percentage high pressure vapor used for driving the injector compressor. This regeneration is also the reason why the thermodynamic cycle efficiency is nearly independent of the turbine isentropic efficiency, shown in the paper titled "The Simplified REHOS Cycle" ref [10], written August 2017. The graphical representation of the Simplified REHOS Cycle is represented in Figure 1, above.

The high pressure, superheated NH₃ vapor is expanded in a standard isentropic turbine coupled to an electrical generator for delivering electrical power output. See more detailed descriptions in the referenced documents [9] and [10], summarized graphically by the sketch in Figure 1 above. Process variables shown in the line diagram of Figure 1 above, have all been calculated by simultaneously solving all the formulas shown below for complete mass-, species- and heat balance of each process component individually as well as the combination of the complete thermodynamic cycle. This was done using the Excel spreadsheet (macro program for Optimization included), named "REHOS Experiments_Export_Version", and should be read with this document, although the values generated in the excel spreadsheet have been included in this revision of this document.

In the schematic of Figure 2 above, all process lines have been labeled alphabetically, making it easier to relate process variables to the label. Note that liquid flows are sketched as black lines, while vapor flow is sketched as blue lines. Heat exchange tubing have been sketched as thick red lines, and the NH₃ in aqua solution both in the bubble reactor as the vapor/liquid float splitter are drawn as dark blue. In the reactor some vapor bubbles rising in the liquid are also drawn as light-blue small circles.

The Jet Injector type compressor was designed on the mentioned excel spreadsheet by using most of the formulas presented in the paper of Chen et al [6], but not all calculations are listed here as formulas, as this is not part of new technology. It has been used for decades already.

Nomenclature:

A_{jet} = Supersonic injector inflow nozzle flow area in m^2 .

M_A = Mass flow in kg/s at position A. (Subscript reflect position, A, B, C etc.)

P_A = Pressure in Pa Abs at position A.

T_A = Temperature in °Celsius at position A.

R_A = Gas constant in N.m/kg.K at position A.

k_A = Specific heat ratio C_p / C_v at position A.

C_{pM} = Specific heat at constant pressure in j/kg.K at position M.

η_{pn} = Isentropic efficiency coefficient for the injector nozzle.

$\eta_{turbine}$ = Turbine isentropic efficiency.

η_{pump} = Hydraulic pressure pump isentropic efficiency.

ρ_A = Media density in kg / m^3 at position A.

H_A = Enthalpy in J/kg at position A. (Enthalpy of all lookup tables (H_2O and NH_3) have been adjusted for liquid at 0°C to have an enthalpy of zero J/kg.)

H_{vE} = Vapor enthalpy of the solution at position E.

H_{lE} = Liquid enthalpy of the solution at position E.

$\%NH3_A$ = Concentration ammonia in media at position A.

(Turbine_Power) = Isentropic turbine expansion power in Watt.

(Evap_Heat) = Heat Energy for the heating and evaporation of liquid, in Watt.

All the equations for mass balance, species balance and heat balance are listed below in equation section (1), (2) and (3) respectively. These should all be solved together for proper balancing of the REHOS cycle.

The equations in section (4) are just a convenient listing of the temperatures at each process position in alphabetical order, A to N, while section (5) does the same for the enthalpy at all process positions in alphabetical order, A to N. Similarly, equation section (6) list all the concentration values (%NH3 in aqua) of all the process positions alphabetically A to N.

Mass Balance Formula's: **Equations section (1)**

Mass flow of vapor into the supersonic injector nozzle as drive medium calculated as per formula (2) of the design paper by Chen et al [6]:

$$M_A = \left(\frac{A_{jet} \cdot P_A}{\sqrt{(T_A + 273)}} \right) \cdot \sqrt{\left(\frac{k_m}{R_m} \right) \cdot \left(\frac{2}{(k_M + 1)} \right)^{\frac{(k_M + 1)}{(k_M - 1)}}} \cdot \sqrt{\eta_{pn}} \quad (1.1)$$

$$M_A = \left[\frac{(7.854e^{-7}) \cdot (1.015e^6)}{\sqrt{(33 + 273)}} \right] \cdot \sqrt{\left(\frac{(1.44)}{(444)} \right) \cdot \left(\frac{2}{(1.44 + 1)} \right)^{\frac{(1.44 + 1)}{(1.44 - 1)}}} \cdot \sqrt{(95\%)} = 1.459e^{-3}$$

The injector jet nozzle flow area A_{jet} is calculated after the jet nozzle opening was chosen as 1mm diameter and η_{pn} is chosen as 95%, even more conservative than the 98% recommended by Chen et al [6].

$$M_B = M_G + M_C - M_F \quad (1.2)$$

$$M_B = (3.162e^{-2}) + (2.469e^{-2}) - (8.935e^{-3}) = 4.737e^{-2}$$

$$M_C = M_A \cdot (\text{Injector_Entrainment_Ratio}) \quad (1.3)$$

$$M_C = (1.459e^{-3}) \cdot (16.926) = 2.469e^{-2}$$

The mass flow at position C is adjusted by the optimization macro by throttling the compressor inlet pressure, so that the amount of heat extracted from the top of the reactor nearly correspond to the heat of evaporation and the superheat extracted from the hot lower area of the reactor. This is done to guarantee enough heat of absorption in the lower area of the reactor for delivering the evaporation and superheat energy at the higher temperature is available.

$$M_D = M_E + (\text{Small_Decimal_Error_of_} - 2.38e^{-4}) \quad (1.4)$$

$$M_D = (3.162e^{-2}) + (-2.38e^{-4}) = 3.138e^{-2}$$

$$M_E = M_F + M_L = (8.935e^{-3}) + (2.269e^{-2}) = 3.162e^{-2} \quad (1.5)$$

$$M_B = M_N + M_H = (2.123e^{-2}) + (2.615e^{-2}) = 4.737e^{-2} \quad (1.6)$$

$$M_G = M_D - (\text{Small_Decimal_Error_of_} - 2.38e^{-4}) \quad (1.7)$$

$$M_G = (3.138e^{-2}) - (-2.38e^{-4}) = 3.162e^{-2}$$

The lookup tables are indexed to 1°C intervals, making exact balancing of all the different variables difficult. The optimization macro manipulate several temperature values up and down by 1°C intervals to find the best balance, but when all balancing are completed, a small error existed with overall energy balance. The total calculated absorbed heat does not add up to the injector compressor energy used and the turbine bruto power developed. An error of a few watt (some ~30W) could be zeroed by adjusting these small errors to the mass flows reflected in formula (1.4) and (1.7) as a last step in the optimization macro instruction list.

$$M_H = M_A + M_C = (1.459e^{-3}) + (2.469e^{-2}) = 2.615e^{-2} \quad (1.8)$$

$$M_I = (\text{Chosen_Mass_for_} 2700\text{Watt_Bruto_Power}) \quad (1.9)$$

$$M_L = M_I = 2.269e^{-2} \quad (1.10)$$

$$M_M = M_I - M_A = (2.269e^{-2}) - (1.459e^{-3}) = 2.123e^{-2} \quad (1.11)$$

$$M_N = M_M = 2.123e^{-2} \quad (1.12)$$

Species Balance Formula's. The actual calculated values for all variables are listed lower in formula section 6. Equations section (2)

$$M_B \cdot \%NH3_B + M_F \cdot \%NH3_F = M_G \cdot \%NH3_G + M_C \cdot \%NH3_C \quad (2.1)$$

$$M_A \cdot \%NH3_A + M_M \cdot \%NH3_M = M_I \cdot \%NH3_I \quad (2.2)$$

$$M_F \cdot \%NH3_F + M_L \cdot \%NH3_L = M_E \cdot \%NH3_E \quad (2.3)$$

$$M_A \cdot \%NH3_A + M_C \cdot \%NH3_C = M_H \cdot \%NH3_H \quad (2.4)$$

$$M_B \cdot \%NH3_B = M_N \cdot \%NH3_N + M_H \cdot \%NH3_H \quad (2.5)$$

Heat Balance Formula's. Some values as calculated by the spreadsheet is shown in red, but all Mass and Enthalpy values are listed in formula section 1 and 5 respectively. Equations section (3)

$$M_H \cdot H_H + M_N \cdot H_N = M_B \cdot H_B \quad (3.1)$$

$$M_A \cdot H_A + M_M \cdot H_M = M_I \cdot H_I \quad (3.2)$$

$$M_A \cdot H_A + M_C \cdot H_C - (Compress_Power) = M_H \cdot H_H \quad (3.3)$$

The heat balance formula used for the reactor, equation (3.4) below, only calculate external heat added to the reactor by lines B and F, balancing against heat extracted from the reactor by lines G and C, as well as heat absorbed out of the reactor, namely (*SHT*) and (*Evap_Heat*). Reactor internal heat exchange between the upwards migrating high concentration absorbed NH3 decreasing enthalpy with decreasing temperature, stays in balance with the downwards migrating lower concentration (but higher density) solution increasing enthalpy with increasing temperature, maintaining the temperature and concentration gradients with direct contact heat exchange in the body of the reactor, while slowly circulating the vertical up-and-down countercurrent mass flows. The direct contact liquid-liquid heat exchange to maintain the gradients under operational conditions require the internal volume (and mass) of the reactor vertical column to be large enough for high heat exchange efficiency and to have very small temperature differences driving the heat exchange. Total reactor mass balance is given by formula (1.2), while the species (amount of NH3) balance is calculated by equation (2.1) above.

$$M_G.H_G + M_C.H_C + (SHT) + (Evap_Heat) = M_B.H_B + M_F.H_F \quad (3.4)$$

$$M_F.H_F + M_L.H_L = M_E.H_E \quad (3.5)$$

$$(Evap_Heat) = M_D.(H_E - H_D) = 23454 \quad (3.6)$$

$$(SHT) = M_L.(H_I - H_L) = 5910 \quad (3.7)$$

$$(Turbine_Power) = M_M.(H_M - H_N) = 2700 \quad (3.8)$$

$$(Compress_Power) = M_A.(H_A - H_H) = 274 \quad (3.9)$$

$$(Heat_Extract_from_Reactor_Top) = (Heat_Top) = M_C.(H_C - H_K) \quad (3.10)$$

$$(Heat_Top) = 29542$$

$$(Heat_Delivered_to_Reactor_Bottom) = (Heat_Bottom) = M_B.(H_B - H_J) \quad (3.11)$$

$$(Heat_Bottom) = 33275$$

$$Heat_Pump_COP = \frac{(Heat_Top)}{(Compress_Power)} = \frac{(29542)}{(274)} = 108 \quad (3.12)$$

$$(Pump_Power) = [(P_D - P_G).M_G / \rho_G] / \eta_{pump} \quad (3.13)$$

$$(Pump_Power) = \left[\frac{(1.110e^6 - 2.04e^5).(3.162e^{-2})}{(676)} \right] / (30.7\%) = 138$$

$$(Input_Heat) = M_D.(H_D - H_G) = (3.138e^{-2}).[(2.548e^4) - (-6.929e^4)] \quad (3.14)$$

$$\text{Externally Absorbed Heat} = (Input_Heat) = 2974$$

$$(REHOS_Cycle_Efficiency) = \eta_{REHOS} = \frac{[(Turbine_Power) - (Pump_Power)]}{(Input_Heat)} \quad (3.15)$$

$$\eta_{REHOS} = \frac{[(2700) - (138)]}{(2974)} = 86.1\%$$

Temperature Formula's with values in red as calculated by the spreadsheet. Equations section (4)

$$\text{Heat_Exch_Drop_J} \rightarrow \text{A/I/M} = (\delta T_{\text{Sht_Exch}}) = 78^\circ\text{C} \quad (4.1)$$

$$\text{Heat_Exch_Drop_J} \rightarrow \text{E} = (\delta T_{\text{Evap_Exch}}) = 82^\circ\text{C} \quad (4.2)$$

$$T_A = T_J - (\delta T_{\text{Sht_Exch}}) = 111^\circ\text{C} - 78^\circ\text{C} = 33^\circ\text{C} \quad (4.3)$$

$$T_B = \text{Average}(T_H, T_N) = \text{Average}(-18^\circ\text{C}, -69.6^\circ\text{C}) = -43.8^\circ\text{C} \quad (4.4)$$

$$T_C = T_K = -18^\circ\text{C} \quad (4.5)$$

$$T_D = (\text{chosen_by_optimization_makro}) = 6^\circ\text{C} \quad (4.6)$$

$$T_E = T_J - (\delta T_{\text{Evap_Exch}}) = 111^\circ\text{C} - 82^\circ\text{C} = 29^\circ\text{C} \quad (4.7)$$

$$T_F = T_E = 29^\circ\text{C} \quad (4.8)$$

$$T_G = T_K = -18^\circ\text{C} \quad (4.9)$$

$$T_H = (\text{chosen_by_optimization_makro}) = -18^\circ\text{C} \quad (4.10)$$

$$T_I = T_J - (\delta T_{\text{Sht_Exch}}) = 111^\circ\text{C} - 78^\circ\text{C} = 33^\circ\text{C} \quad (4.11)$$

$$T_J = (\text{chosen_by_optimization_makro}) = 111^\circ\text{C} \quad (4.12)$$

$$T_L = T_F = 29^\circ\text{C} \quad (4.13)$$

$$T_M = T_I = 33^\circ\text{C} \quad (4.14)$$

$$T_N = \frac{(T_M + 273)}{\left[\left(\frac{P_M}{P_N} \right)^{\frac{(k_M - 1)}{k_M}} \right]} - 273 + \left[\frac{(\text{Turbine_Power})}{M_N} / \eta_{\text{turbine}} \right] \cdot \frac{(1 - \eta_{\text{turbine}})}{C_{pM}} \quad (4.15)$$

$$T_N = \frac{(33 + 273)}{\left[\left(\frac{(1.015e^6)}{(2.104e^5)} \right)^{\frac{(1.44 - 1)}{1.44}} \right]} - (273) + \left[\frac{(2700)}{(2.1228e^{-2})} / (75\%) \right] \cdot \frac{(1 - 75\%)}{(2969)} = -69.6^\circ\text{C}$$

Although the temperature calculated in formula (4.15) may be very low, the minimum temperature available on the lookup tables are -39°C , and therefore at the lookup table reference this temperature is limited to a minimum of -39°C , even though the calculation (4.15) give a lower value. It is not so important, as this temperature is not used by further calculations, and is therefore deemed acceptable.

**Enthalpy Formula's with values in red as calculated by the spreadsheet.
Equations section (5)**

$$H_A = (\text{Lookup_Table}) = (\text{NH3_10Bar_SHT @ 33}^\circ\text{C}) = 1.307e^6 \quad (5.1)$$

$$H_B = (M_G.H_G + M_C.H_C + (\text{SHT}) + (\text{Evap_Heat}) - M_F.H_F) / M_B \quad (5.2)$$

$$H_B = \frac{[(3.162e^{-2}).(-6.929e^4) + (2.469e^{-2}).(1.127e^6) + (5910) + (23454) - (8.935e^{-3}).(7.730e^4)]}{(4.737e^{-2})}$$

$$H_B = 1.146e^6$$

$$H_C = (\text{Lookup_Table}) = (\text{NH3_98\% @ -18}^\circ\text{C}) = 1.127e^6 \quad (5.3)$$

$$H_D = (\text{Lookup_Table}) = (\text{NH3_98\% @ 6}^\circ\text{C}) = 2.548e^4 \quad (5.4)$$

$$H_E = x.H_{vE} + (1-x).H_{lE} = (71.07\%).(1.037e^6) + (1-71.07\%).(1.238e^5) = 7.728e^5 \quad (5.5)$$

with x chosen by the optimization macro, while H_{vE} and H_{lE} are looked up in the lookup tables.

$$H_F = (\text{Lookup_Table}) = (\text{NH3_93\% @ 29}^\circ\text{C}) = 7.730e^4 \quad (5.6)$$

$$H_G = (\text{Lookup_Table}) = (\text{NH3_98\% @ -18}^\circ\text{C}) = -6.929e^4 \quad (5.7)$$

$$H_H = (M_B.H_B - M_N.H_N) / M_H \quad (5.8)$$

$$H_H = \frac{[(4.737e^{-2}).(1.146e^6) - (2.123e^{-2}).(1.180e^6)]}{(2.615e^{-2})} = 1.119e^6$$

$$H_I = (\text{Lookup_Table}) = (\text{NH3_10Bar_SHT @ 33}^\circ\text{C}) = 1.307e^6 \quad (5.9)$$

$$H_J = (\text{Lookup_Table}) = (\text{NH3_3\% @ 111}^\circ\text{C}) = 4.441e^5 \quad (5.10)$$

$$H_K = (\text{Lookup_Table}) = (\text{NH3_98\% @ -18}^\circ\text{C}) = -6.929e^4 \quad (5.11)$$

$$H_L = (\text{Lookup_Table}) = (\text{NH3_93\% @ 29}^\circ\text{C}) = 1.047e^6 \quad (5.12)$$

$$H_M = (\text{Lookup_Table}) = (\text{NH3_10Bar SHT @ 33}^\circ\text{C}) = 1.307e^6 \quad (5.13)$$

$$H_N = H_M - [R_M \cdot (T_M + 273) \cdot k_M / (k_M - 1)] \cdot [1 - (\frac{P_N}{P_M})^{\frac{(k_M - 1)}{k_M}}] \cdot \eta_{turbine} \quad (5.14)$$

$$H_N = (1.307e^6) - [\frac{(444) \cdot (33 + 273) \cdot (1.44)}{(1.44 - 1)}] \cdot [1 - (\frac{(2.104e^5)}{(1.015e^6)})^{\frac{(1.44 - 1)}{1.44}}] \cdot (75\%)$$

$$H_N = 1.180e^6$$

Ammonia Concentration Formula's with values in red as calculated by the spreadsheet. Equations section (6)

$$\%NH3_A = (Lookup_Table) = (NH3_93\% @ 29^\circ C) = 99.97\% \quad (6.1)$$

$$\%NH3_B = (M_G \cdot \%NH3_G + M_C \cdot \%NH3_C - M_F \cdot \%NH3_F) / M_B \quad (6.2)$$

$$\%NH3_B = \frac{[(3.162e^{-2}) \cdot (98\%) + (2.469e^{-2}) \cdot (100\%) - (8.935e^{-3}) \cdot (93\%)]}{(4.737e^{-2})}$$

$$\%NH3_B = 99.99\%$$

$$\%NH3_C = (Lookup_Tables) = (NH3_98\% @ -18^\circ C) = 100\% \quad (6.3)$$

$$\%NH3_D = (Lookup_Table) = (NH3_98\% @ -18^\circ C) = 98\% \quad (6.4)$$

$$\%NH3_E = \%NH3_D = 98\% \quad (6.5)$$

$$\%NH3_F = (M_E \cdot \%NH3_E - M_L \cdot \%NH3_L) / M_F \quad (6.6)$$

$$\%NH3_F = \frac{[(3.162e^{-2}) \cdot (98\%) - (2.269e^{-2}) \cdot (99.97\%)]}{(8.935e^{-3})} = 93\%$$

$$\%NH3_G = (Lookup_Table) = (NH3_98\% @ -18^\circ C) = 98\% \quad (6.7)$$

$$\%NH3_H = (M_A \cdot \%NH3_A + M_C \cdot \%NH3_C) / M_H \quad (6.8)$$

$$\%NH3_H = \frac{[(1.459e^{-3}) \cdot (99.97\%) + (2.469e^{-2}) \cdot (100\%)]}{(2.615e^{-2})} = 100\%$$

$$\%NH3_I = (Lookup_Table) = (NH3_93\% @ 29^\circ C) = 99.97\% \quad (6.9)$$

$$\%NH3_J = (Lookup_Table) = (NH3_3\% @ 111^\circ C) = 3\% \quad (6.10)$$

$$\%NH3_K = (Lookup_Table) = (NH3_98\% @ -18^\circ C) = 98\% \quad (6.11)$$

$$\%NH3_L = (Lookup_Table) = (NH3_93\% @ 29^\circ C) = 99.97\% \quad (6.12)$$

$$\%NH3_M = (Lookup_Table) = (NH3_93\% @ 29^\circ C) = 99.97\% \quad (6.13)$$

$$\%NH3_N = (Lookup_Table) = (NH3_93\% @ 29^\circ C) = 99.97\% \quad (6.14)$$

Assumptions and starting points:

In the excel spreadsheets, a general color coding was used. Normally a yellow block contain a formula, while a neon-green block contain a fixed value, either put in as a starting point, or adjusted by the optimization macro. The dark green and lighter green is used to indicate the value comes from a lookup table.

As a starting point, the injector jet nozzle opening diameter was chosen as 1mm, while the nozzle outflow isentropic efficiency was chosen as 95%. The turbine isentropic efficiency was chosen as 75%, while the pressure pump use a 30.7% efficiency, which come from the actual efficiency of a certain gear pump I bought.

The values of heat exchanger temperature delta's was chosen as $(\delta T_{Evap_Exch}) = 82^\circ C$, while the superheater exchanger, $(\delta T_{Sht_Exch}) = 78^\circ C$. These values are specifically chosen to be fairly high, to make it easier for the heat exchanger tubing inside the reactor design. The reactor top temperature was chosen as $-18^\circ C$, as this was regarded as a realistic assumption, with the reactor top solution concentration assumed to be 98% NH_3 in aqua, and the reactor hot bottom solution concentration assumed to be 3% NH_3 in aqua for this example calculation. The reactor height was assumed to be 0.8m. Various other concentration values may be chosen, but for each specific case, a different set of process variables will have to be calculated.

During optimization the macro also adjust the throttling of the vapor pressure at position (C) to fit the mass flow requirements of the injector compressor by manipulating the compressor inlet pressure.

From the mass-, species- and heat balance of the complete REHOS cycle, it becomes clear that no heat is rejected out of the cycle, yet it balance perfectly!

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