

Chlorine condenser-evaporator simulation

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Abstract. Refrigeration machines are an integral part of chemical engineering. Coldness in mechanical engineering is used to improve the properties of steels, to stabilize the shape and size of steel parts, to restore the dimensions of worn steel hardened parts, to fasten the parts to be machined during cutting and grinding, to ensure fixed planting during assembly, bending pipelines, deep drawing and stamping parts from sheet materials, in the manufacture and processing of rubber parts, with solid anodizing of aluminum alloy parts.

1. Introduction

Refrigeration machines are widely used for liquefying gases, such as liquid oxygen, nitrogen, chlorine and methane. They have long been widely used in chemistry, engineering and metallurgy. Chlorine in both liquid and gaseous states at low and moderate temperatures (up to 100 °C) practically does not interact with metals and alloys widely used in chemical engineering. This property of chlorine ensures the safety of the operation of high-pressure chlorine vessels, chemical equipment and pipelines (in chlorine warehouses) made of carbonaceous and low-alloyed manganese steels. The condenser-evaporator occupies a central place in the chlorine liquefaction system. Let us consider the simulation of this apparatus for further development of its control system.

2. The basis of the mathematical model

Pressure, density, and heat capacity of freon are known to depend on temperature [1]. They are represented by graphic data, which are approximated and represented in the form of analytical expressions. Accordingly, let us add these dependencies to the dynamic model being developed.

The dependence of freon density in kg/m³ on temperature and pressure assumes the following expression:

$$\rho(T, p) = (-0.6259 \cdot T^2 - 25.353 \cdot T \cdot 1572.3) \cdot bf^{\left(\frac{p}{101325} - 1\right)},$$

where T – freon temperature in °C;

bf – the freon compression ratio, $bf = 0.995$;

p – freon pressure in Pa.

The dependence of the freon specific heat on the temperature in J/kg·K assumes the following expression:

$$Cp_{fg}(T) = 0.5583 T^2 + 7.9825 T + 866.61,$$

where T – freon temperature in °C.



The dependence of the freon partial pressure on temperature in Pa assumes the following expression:

$$\text{Pr}f(T) = (7 \cdot 10^{-6} \cdot T^3 + 0.0014 T^2 \cdot 0.1001 T + 3.9588) \cdot 10^5,$$

where T – freon temperature in °C.

Let us now turn to a description of the equations simulating the chlorine behavior in condenser-evaporator. In the reference data, two curves were found from which it is possible to approximate the partial pressure of chlorine depending on the temperature range. Let us set the condition that if the chlorine temperature is less than 239.4 K, then one uses the first equation of the approximated curve; otherwise — the second one.

Then the equation for finding the partial pressure of chlorine in Pa takes the form:

$$\text{Pr}h(T) = \begin{cases} nT = T + 273.15 \\ 10^{\frac{8.0213 - \frac{530.591}{nT - 64.63}}{}} \text{ IF } nT < 239.4, \\ 10^{\frac{9.28814 - \frac{969.992}{nT - 12.791}}{}} \text{ ELSE} \end{cases}$$

where nT – the chlorine temperature in K.

The heat of condensation of chlorine depends only on its temperature, and, therefore, this curve is approximated by the graph presented in the reference data [2] and is represented by an analytical expression.

The heat of condensation of chlorine owing to its temperature is represented in J / kg:

$$C_{\text{cond}h}(T) = -0.0298 T^3 - 1.643 \cdot T^2 - 517.06 \cdot T + 267940,$$

where nT – the chlorine temperature in °C.

The mathematical model must take into account the norms of the procedure for carrying out the process of liquefying chlorine. Therefore, one should not allow the level to tend to exceed the maximum value. In addition, one can not possibly keep freon from being present in the condenser-evaporator. For these purposes, let us write the interlockings of the maximum and minimum freon levels in the apparatus. Interlockings will come in action when the level in the apparatus will reach either a minimum or maximum mark.

The variable p1 stores the level value in the evaporator condenser as a percentage of the volume of the intertubular space. If the volume percentage reaches at a certain instant of time less than 100 percent, then one can continue to fill it, the logical "1" is now in action; otherwise the logical "0" is in action.

The variable p2 stores the current value of the pressure in the apparatus in Pa if it is less than the partial freon pressure at a present temperature, which is accounted for the result of the function of the freon partial pressure of Prf (p3) of the temperature p3, which is the indication of that the freon condenses. Otherwise, it evaporates. The p4 variable stores the values of the chlorine temperature in °C.

Thus, Lf1(p) accounts for interlocking of the freon level in keeping with its supply, whereas Lf2(p) is keeping with freon evaporation and condensation, which will depend on the partial pressure value of and pressure in the apparatus.

The above-stated is the basis for the development of an analytical expression for interlocking maximum and minimum levels in the condenser-evaporator

$$Lf_1(p) = \begin{cases} 1 & \text{IF } p_1 < 100 \\ 0 & \text{ELSE} \end{cases}, \quad Lf_2(p) = \begin{cases} \begin{cases} 1 & \text{IF } (\Pr f(p_3) - p_2) > 0 \\ 0 & \text{ELSE} \end{cases} & \text{IF } p_1 > 0 \\ 0 & \text{ELSE} \end{cases}.$$

Let us define the volumes of evaporated and condensed refrigerant per 1 second of time. These processes will depend on the freon diffusion coefficient k_1 (it stands for its rate evaporation) of the intertubular space Vf . For condensation, an inverse process will occur, so let us indicate a negative expression for the relation.

Let us use the interlocking $Lf_2(p)$ which will stop the condensation or evaporation of freon in the mathematical model, if the level approaches the maximum and minimum values. Coefficient k_1 is govern by the freon physical properties and shows the rapidity of its evaporation (condensation). Taking into account the atmospheric pressure factor, the condition is reduced to the form $\Pr f(p_3) > p_2 + 101325$. Formula $(1 - \frac{p_2 + 101325}{\Pr f(p_3)})$ shows the evaporation intensity. To find the

current values of the volume filled, let us perform $\frac{p_1}{100} \cdot Vf$.

The above-stated is the basis for the development of an analytical expression for the volume of evaporated (condensed) refrigerant in m^3 per 1 second, represented by the formula:

$$Visp(p) = \begin{cases} Lf_2(p) \cdot k_1 \cdot (1 - \frac{p_2 + 101325}{\Pr f(p_3)}) \cdot \frac{p_1}{100} \cdot Vf, & \text{IF } \Pr f(p_3) > p_2 + 101325 \\ -Lf_2(p) \cdot k_1 \cdot (1 - \frac{\Pr f(p_3)}{p_2 + 101325}) \cdot \frac{p_1}{100} \cdot Vf & \text{ELSE} \end{cases},$$

where k_1 – freon diffusion coefficient;

Vf – intertubular space volume of condenser-evaporator, m^3 .

Further calculations will take a value, equal to the product of the heat capacity per mass for both liquid and gaseous freon together, measured in $\frac{J \cdot kg}{K}$:

$$Cpf(p, dm) = Cpf_g(p_3) \cdot \left[Vf \cdot \frac{p_1}{100} \cdot pof(p_3, p_2) + Vf \cdot \frac{100 - p_1}{100} \cdot \frac{(p_2 + 101325) \cdot Mf}{10^5 \cdot R \cdot (273.15 + p_3)} + dm \right],$$

where Mf – freon molar mass of, kg / mol ;

dm – incoming liquid freon mass, kg .

The volumetric chlorine flow rate will depend directly on the chlorine flow rate in the condenser. Multiply the concentration of chlorine in chlorine gas by the chlorine pressure depending on its temperature (on the p_4 variable), because the p_4 variable accounts for storing data on the chlorine temperature in $^{\circ}C$. We get $\frac{Conc}{100} \cdot \Pr h(p_4)$. If this value is less than the chlorine pressure in one

atmosphere system $Ph + 101325$, then chlorine begins to condensate. Let us express this dependence in m^3 per second. It is worth noting that if the above condition is not met, then chlorine condensation will not occur.

Therefore, it is fair to assert that the dependencies will assume the following relations:

$$Gcond(p) = \begin{cases} k_3 \cdot (1 - \frac{\frac{Conc}{100} \cdot \Pr h(p_4)}{Ph + 101325}) \cdot Vh \cdot \frac{Conc}{100}, & \text{IF } \frac{Conc}{100} \cdot \Pr h(p_4) < Ph + 101325, \\ 0 & \text{ELSE} \end{cases}$$

where k_3 - the chlorine diffusion coefficient;

$Conc$ – chlorine concentration in chlorine gas, percent;

Ph – chlorine pressure in chlorine gas, Pa;

Vh – intertubular space volume, m^3 .

The amount of chlorine condensed is expressed in mol /sec:

$$Vhg(p) = \frac{\left(\frac{Gh}{Mh}\right) \cdot R \cdot (p_4 + 273.15)}{(Ph + 1) \cdot 101325},$$

where Gh – the chlorine flow rate, m^3/sec ;

Mh – the chlorine molar mass, kg /mol;

R – the universal gas constant, $R = 8.314 \text{ J/(mol} \cdot \text{K)}$;

Vh – the intertubular space volume, m^3 .

3. Mathematical model of condenser-evaporator

Thus, on the basis of the above mentioned, there is a complete basis of dependencies for the determination of equations describing the processes in the condenser-evaporator. Let us consider each of the equations in more detail. The equation for the level in percent will be determined by the difference between the freon entering the condenser-evaporator and the vapor of its evaporation:

$$dL(p) = Lf_1(p) \cdot \frac{Gf \cdot a1}{Vf} - Visp(p),$$

where Gf – freon flow rate, m^3/s ;

$a1$ – the valve opening gap for the liquid freon supply, percentage.

$$\frac{Gf \cdot a1}{Vf}.$$

The amount of incoming freon will be determined by the fraction

This fraction, where the numerator is the product of the freon flow rate Gf , is the valve opening gap for the fluid freon supply of $a1$, and the denominator Vf is the intertubular space volume. Accordingly, this ratio will enable to find the apparatus extent with freon. Let us multiply this expression by $Lf_1(p)$ – interlocking the freon supply on entering, in order to prevent apparatus overflow.

The subtracted $Visp(p)$ is the amount of evaporated or condensed Freon. Evaporation will proceed at the moment when the freon vapor partial pressure is greater than the saturated vapor pressure at a given temperature, when these pressures are equal to each other, evaporation and condensation processes are in equilibrium. Otherwise, condensation will occur [5].

The equation for determining the freon temperature in $^{\circ}\text{C}$ takes the form:

$$dTf(p) = \frac{-Visp(p) \cdot pof(p_3, p_2) \cdot Cisp + (Tatm - p_3) \cdot Tp + (p_4 - p_3) \cdot alfa \cdot S1}{Cpf(p, 0) + Cp} + \frac{p_3 \cdot Cpf(p, 0) + Tf1 \cdot Cpf_g(Tf1) \cdot Gf \cdot a1 \cdot pof(Tf1, Pf1) + p_3 \cdot Cp}{Cpf(p, Gf \cdot a1 \cdot pof(Tf1, Pf1)) + Cp} - p_3,$$

where $Cisp$ – heat of chlorine condensation of, J/kg;

$Tatm$ – ambient air temperature, $^{\circ}\text{C}$;

Tp – heat loss at a temperature difference of 1°C , J/K;

$S1$ – surface area of heat transfer from freon to chlorine, m^2 ;

$Alfa$ – the thermal conductivity coefficient, $\text{J} / (\text{m}^2 \cdot \text{K})$;

Cp – heat capacity of the apparatus walling, $\text{J} / (\text{kg} \cdot \text{K})$;

$Tf1$ – fluid freon temperature at the condenser-evaporator inlet, $^{\circ}\text{C}$;

$Pf1$ – fluid freon pressure at the condenser-evaporator inlet, Pa.

The first fraction in the equation shows the freon temperature variation without regard for the supply of its new liquid phase.

Let us consider the terms in the numerator:

- $-Visp(p) \cdot pof(p_3, p_2) \cdot Cisp$ – heat consumption during evaporation, J;
- $(T_{atm} - p_3) \cdot Tp$ – loss of heat into the atmosphere, J;
- $(p_4 - p_3) \cdot alfa \cdot S1$ – heat taken from chlorine, J.

The freon temperature in °C is found as the ratio of the total amount of heat to the sum of the specific heat of the current freon and the heat capacity of the condenser-evaporator $\frac{-Visp(p) \cdot pof(p_3, p_2) \cdot Cisp + (T_{atm} - p_3) \cdot Tp + (p_4 - p_3) \cdot alfa \cdot S1}{Cpf(p, 0) + Cp}$. It is to be noted that the heat

capacity of the walls of the apparatus Cp is taken into account. The second fraction in the equation shows the freon temperature variation, taking into account the supply of its new liquid phase.

Let us consider the terms in the numerator:

- $p_3 \cdot Cpf(p, 0)$ – the heat obtained by the freon is already in the apparatus, J;
- $Tf1 \cdot Cpf(Tf1) \cdot Gf \cdot a1 \cdot pof(Tf1, Pf1)$ – heat from incoming freon, J;
- $p_3 \cdot Cp$ – heat, given to the walls of the apparatus, J.

The freon temperature °C is found as the ratio of the total amount of heat to the sum of the heat capacity of the incoming (decreasing) freon and the heat capacity of the walls of the condenser-evaporator is:

$$\frac{p_3 \cdot Cpf(p, 0) + Tf1 \cdot Cpf(Tf1) \cdot Gf \cdot a1 \cdot pof(Tf1, Pf1) + p_3 \cdot Cp}{Cpf(p, Gf \cdot a1 \cdot pof(Tf1, Pf1)) + Cp}$$

It is to be noted that the heat capacity of the walling of the apparatus Cp is taken into account.

So that to find the temperature variation from the sum of fractions (the current temperature value) let us subtract the previous temperature p3 in °C.

To find the pressure, let us consider four terms of the formula:

$$dP(p) = \left[\frac{(p_2 + 101325) \cdot (100 - p_1)}{100 - \left[p_1 + Lf_1(p) \cdot \frac{Gf \cdot a1}{Vf} - Visp(p) \right]} - p_2 - 101325 \right] + \frac{R \cdot (273,15 + p_3) \cdot \frac{Visp(p) \cdot pof(p_3, p_2)}{Mf}}{Vf \cdot 101325} + \frac{(p_2 + 101325) \cdot dTf(p)}{273,15 + p_3} - (p_2 - Pf2) \cdot \frac{a2}{100} \cdot k2,$$

where k2 – the throughput of the freon nozzle from the apparatus;

a2 – valve opening gap of freon vapor outlet, percentage;

Pf2 – freon vapor pressure upstream the compressor, Pa.

The term $\left[\frac{(p_2 + 101325) \cdot (100 - p_1)}{100 - \left[p_1 + Lf_1(p) \cdot \frac{Gf \cdot a1}{Vf} - Visp(p) \right]} - p_2 - 101325 \right]$ shows the dependence of the pressure variation change on the level. The expression $\frac{(p_2 + 101325) \cdot (100 - p_1)}{100 - \left[p_1 + Lf_1(p) \cdot \frac{Gf \cdot a1}{Vf} - Visp(p) \right]}$ is derived from the

Boyle–Mariotte law.

The fraction $\frac{R \cdot (273,15 + p_3) \cdot \frac{Visp(p) \cdot pof(p_3, p_2)}{Mf}}{Vf \cdot 101325}$ shows the pressure variation during evaporation. It is

obtained from the law of Mendeleev–Klaiperon.

The term $\frac{(p_2 + 101325) \cdot dTf(p)}{273,15 + p_3}$ takes into account the pressure variation depending on temperature. It is derived from the law of Charles.

The fraction $(p_2 - Pf2) \cdot \frac{a2}{100}$ shows the pressure variation depending on gaseous freon output. Let us develop an equation for describing the chlorine temperature variation:

$$dTh(p) = \frac{-(p_4 - p_3) \cdot \alpha \cdot S1 + Gcond(p) \cdot Ccondh(p_4)}{Cpgh \cdot \frac{(Ph + 101325) \cdot Vh}{R \cdot (273,15 + p_4)}} - \frac{Vhg(p) \cdot (p_4 - Th1)}{Vh - Vhg(p)},$$

where Cpgh – the heat capacity of liquid chlorine, J / (kg · K);

Th1 – chlorine temperature at the apparatus inlet, percentage;

Pf2 – freon vapor pressure of the compressor upstream, Pa.

Let us consider the first fraction. In the numerator, the term $-(p_4 - p_3) \cdot \alpha \cdot S1$ shows the heat transferred to freon, $Gcond(p) \cdot Ccondh(p_4)$ takes into account the heat of chlorine condensation. The denominator $Cpgh \cdot \frac{(Ph + 101325) \cdot Vh}{R \cdot (273,15 + p_4)}$ is the chlorine heat capacity [4]. The second fraction $\frac{Vhg(p) \cdot (p_4 - Th1)}{Vh - Vhg(p)}$ shows the change in the chlorine temperature due to its entry from the chlorine compressor.

4. Conclusion

A mathematical model of the CO is developed. The model describes the key processes in the apparatus: evaporation of freon, condensation of chlorine, freon level and pressure variation in the apparatus. The model is based on the equations characterizing the above-described processes, which makes it possible to use it for designing and calculating heat transfer apparatus through a wall with phase transitions of coolants of various characteristics.

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