

## MODELING OF PROCESSES OF GAS COOLING BY CONTACT WITH A LIQUID AND UPDATING OF COLUMN APPARATUSES

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The process of gas cooling with a liquid in a countercurrent packed column (scrubber), where the phases are in direct contact, is described. The system of differential equations for heat transfer in gas and liquid phases and moisture mass transfer is given. Equations for determining the fields of gas enthalpy distribution, liquid temperature, moisture content in the gas along the packed bed height are derived through transition to a cellular model. The adequacy of the proposed equations is validated in practice. The packed column is updated, which involved replacement of plates by packings produced by OOO IVTs Inzhekhim (EPC Chemical Engineering LLC), which enhanced the efficiency of pyrogas cooling with water in ethylene production.

**Keywords:** gas cooling, heat and mass transfer, packed columns, packed scrubbers, mathematical modeling, apparatus updating.

In fuel and power engineering undertakings, spraying, vortex, and plate apparatuses as well as Venturi scrubbers and packed scrubbers are used to clean and cool gases. For enhancing efficiency of gas cooling processes, it is essential to improve the methods of calculation of these processes, to develop new designs of apparatuses, and to update the conventional designs [1–3]. Mathematical modeling of processes of wet cooling of flue and technological gases is particularly important.

The process of gas cooling by liquids with direct contact of the phases is characterized by mass and energy transfer through the interface. In this process, the gas stream is a continuous phase that contains a substantial quantity of disperse inclusions, such as droplets, sprays, and films of the liquid. It is impossible to describe heat and mass transfer precisely at the level of individual disperse inclusions because of large number of these inclusions and unknown area of distribution of contact of the phases in space.

For practical calculations, however, only some average values are of interest. For modeling two-phase streams, an approach based on macroscopic balancing and averaging of local single-phase conservation equations and conditions of contact at the phase interface with use of the source terms of interphase transfer is used. Here, source terms are expressed in terms of macroscopic determinate variables [4].

For calculating the fields and efficiency of heat and mass transfer in industrial apparatuses, the most widely used are various models of flow pattern [5, 6]. In such models, average phase velocities are used and nonuniformity of distribution of field variables is taken account of by introducing coefficients of longitudinal (reverse) and transverse mixing. In such a formulation, the salient task of modeling of two-phase flows boils down to experimental determination of mixing factors and parameters of source terms of interphase transfer.

In this study, this approach was used for modeling combined heat and mass transfer during cooling of gases with water in packed scrubbers.

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## Diffusion Model

Let us consider the process of gas cooling with a liquid in a countercurrent packed column (scrubber) in film-flow operation mode.

Let us write the equations of monoparametric diffusion models of heat and mass transfer with interphase sources of heat and mass:

$$\rho_1 c_1 W_1 \frac{dT_1}{dz} = \rho_1 c_1 D_{m.l} \frac{d^2 T_1}{dz^2} - \frac{Q(z)}{V_b(z)}; \quad (1)$$

$$\rho_g W_g \frac{dI_g}{dz} = \rho_g c_g D_{m.g} \frac{d^2 T_g}{dz^2} + \frac{Q(z)}{V_b(z)}; \quad (2)$$

$$W_g \frac{dx}{dz} = D_{m.g} \frac{d^2 x}{dz^2} \pm (\beta_g a_v)(x_{if} - x^*), \quad (3)$$

where (1), (2), and (3) are equations of heat transfer in liquid phase, heat transfer in vapor-gas phase, and moisture mass transfer in gas phase, respectively;  $\rho_1$  and  $\rho_g$  are liquid and gas densities,  $\text{kg/m}^3$ ;  $c_1$  and  $c_g$  are heat capacities of liquid and gas phases,  $\text{J}/(\text{kg}\cdot\text{K})$ ;  $W_1$  and  $W_g$  are average liquid and gas velocities over entire cross-sectional area of column,  $\text{m}/\text{sec}$ ;  $T_1$  and  $T_g$  are liquid and gas temperatures,  $^\circ\text{C}$ ;  $z$  is vertical coordinate;  $D_{m.l}$  and  $D_{m.g}$  are coefficients of reverse mixing of liquid and gas phases,  $\text{m}^2/\text{sec}$ ;  $Q(z)$  heat is flux,  $\text{W}$ ;  $V_b$  is volume of packed bed,  $\text{m}^3$ ;  $I_g$  is enthalpy of gas,  $\text{J}/\text{kg}$ ;  $x$  is moisture concentration in gas phase,  $\text{kg}/\text{kg}$ ;  $(\beta_g a_v)$  is volume coefficient of mass transfer of moisture in gas phase,  $\text{sec}^{-1}$ ;  $\beta_g$  is average mass transfer coefficient,  $\text{m}/\text{sec}$ ;  $a_v$  is specific phase contact surface,  $\text{m}^2/\text{m}^3$ ;  $x_{if}$  is moisture concentration at phase interface;  $x^*$  is equilibrium moisture concentration.

The expressions for heat and mass sources in equations (1)–(3) are written proceeding from the fact that the main resistance to heat and mass transfer is concentrated in the gas phase.

In comparison with condensation of clean vapor, the process of heat transfer from a vapor-gas mixture is characterized by diffusional resistance of vapor-gas interlayer formed near the phase interface [7, 8]. The heat flux transferred from the vapor-gas mixture to the phase interface consists of the heat transferred by convection and the heat transferred by the condensing vapor. Then,

$$Q(z) = F(z) \left[ \alpha_g (T_g - T_1) + I_{v,i} \rho_g \beta_g (x_{if} - x^*) \right], \quad (4)$$

where  $F(z)$  is phase contact area,  $\text{m}^2$ ;  $\alpha_g$  is heat transfer coefficient,  $\text{W}/(\text{m}^2 \cdot \text{K})$ ;  $I_v$  is enthalpy of water vapor at water temperature  $T_1$ ,  $\text{J}/\text{kg}$ .

Let us solve equations (1)–(3) for the following boundary conditions:

– at  $z = H$  (entry of liquid and exit of gas)

$$T_{1,i} = T_1 + \frac{1}{\text{Pe}_1} \frac{dT_1}{dz}, \quad \frac{dT_g}{dz} = 0, \quad \frac{dx}{dz} = 0,$$

– at  $z = 0$  (entry of gas and exit of liquid)

$$T_{g,i} = T_g - \frac{1}{Pe_g} \frac{dT_g}{dz}, \quad \frac{dT_l}{dz} = 0,$$

$$x_i = x - \frac{1}{Pe_g} \frac{dx_g}{dz}$$

(Danckwerts condition), where  $T_{l,i}$ ,  $T_{g,i}$ ,  $x_i$  are initial liquid temperature, gas temperature, and moisture concentration, respectively;  $Pe_l$  and  $Pe_g$  are modified Peclet diffusion numbers characterized by reverse mixing of liquid and gas streams (at  $Pe \rightarrow 0$  mixing is ideal and at  $Pe \rightarrow \infty$  displacement is ideal);  $Pe_l = W_l l / D_{m,l}$  and  $Pe_g = W_g l / D_{m,g}$ ;  $l$  is characteristic dimension, m.

Let us determine the enthalpy of the gas at the inlet by the familiar expression

$$I_{g,i} = (c_{d,g} + c_v x_i) T_{g,i} + R_0 x_i$$

where  $c_{d,g}$  and  $c_v$  are the specific heats of the dry gas and water vapor, J/(kg·K);  $R_0$  is the specific liquid vaporization heat, J/kg;  $x_i$  is the moisture content of the gas at the inlet, kg (vapor)/kg (dry gas).

The proposed equations system can be used to determine the liquid and gas temperature fields (indicating temperature distribution along the column height) and the thermal efficiency in conditions of uniform delivery of the phases to the packed bed.

### Cellular Model

For transition from diffusion model to cellular (Fig. 1), we can use the equivalence relationship  $n \approx Pe_g / 2$ , where  $Pe_g = W_g H / D_{m,g}$ ;  $H$  is the height of the packed bed. Then, Eq. (2) can be written for the  $i$  th cell as follows:

$$\rho_g W_g \frac{I_{g,i-1} - I_{g,i}}{\Delta z} = \frac{Q_i}{V_i}, \quad (5)$$

where  $i = 1, 2, \dots, n$ ;  $n$  is the number of cells of the packed column;  $Q_i$  is the heat flux into the  $i$  th cell, W;  $V_i$  is the volume ( $m^3$ ) of the  $i$  th cell,  $V_i = \Delta z S$ ;  $\Delta z$  is the solution step;  $\Delta z = H/n$ ;  $S$  is the area of the column cross-section,  $m^2$ .

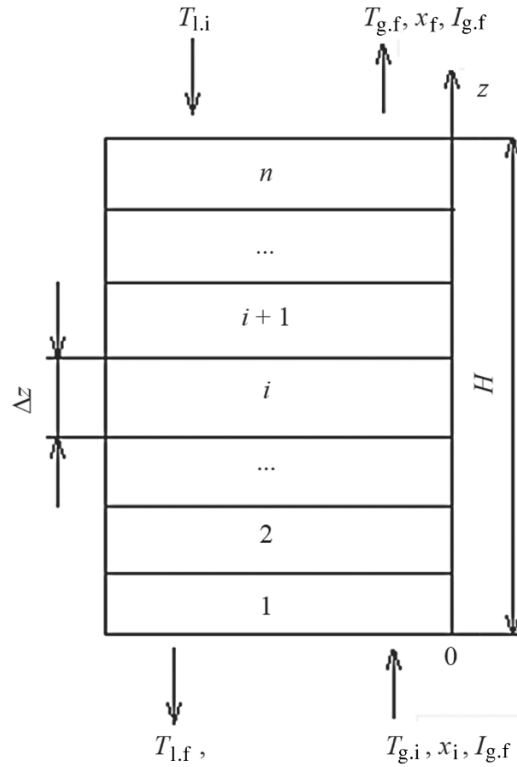
From Eq. (5) we can find the enthalpy of the gas:

$$I_{g,i} = I_{g,i-1} - \frac{\Delta z Q_i}{\rho_g W_g V_i} = I_{g,i-1} - \frac{Q_i}{G}, \quad (6)$$

where  $G$  is the gas mass flow rate (kg/sec),  $G = \rho_g S W_g$ .

From the heat balance equation

$$L c_l (T_{l,i-1} - T_{l,i}) = G (I_{g,i-1} - I_{g,i}) \quad (7)$$



**Fig. 1.** Notional division of packed bed into cells.

we can determine the liquid temperature in the  $i$  th cell:

$$T_{l,i} = T_{l,i-1} - \frac{G}{L} \frac{(I_{g,i-1} - I_{g,i})}{c_l}, \tag{8}$$

where the liquid and gas mass flow rates  $L$  and  $G$  can be taken as constant across the packed bed height.

Performing similar transformations using the cellular model for equation of evaporating moisture mass transfer we can determine the moisture concentration in the  $i$  th cell:

$$x_i = \frac{x_{i-1} + (\beta_g a_v) \Delta z x^* / W_g}{1 + (\beta_g a_v) \Delta z / W_g}. \tag{9}$$

Let us solve the system of equations (6), (8), and (9) from  $i = 0$  to  $i = n + 1$ .

From the expression for the final enthalpy of the gas

$$I_{g,f} = (c_{d,g} + c_v x_f) T_{g,f} + R_0 x_f,$$

we can determine its final temperature (at known values of  $T_{g,f}$  and  $x_f$ ):

$$T_{g,f} = \frac{I_{g,f} + R_0 x_f}{c_{d,g} + c_v x_f}.$$

Note that the number of cells of the packed column is linked with the modified Peclet number [6] ( $Pe > 10$ ) by the following equation:

$$n = 0.5Pe^2 [Pe - 1 + \exp(-Pe)]^{-1}. \quad (10)$$

At  $Pe = 2-10$ , it is advisable to take  $Pe = 1.25(2n - 1)$  [6].

The modified Peclet number of reverse mixing is generally determined experimentally or by using semiempirical equations [5, 6, 9].

The system of equations (6), (8), and (9) can be solved in iteration cycle by the successive approximation method. The obtained solution must satisfy the heat balance equation in the integral form.

In the case of transition from the ideal displacement model ( $Pe \rightarrow \infty$ ) to the ideal mixing model ( $Pe \rightarrow 0$ ), the heat transfer efficiency declines by 20–35%.

### Parameters of Models

The coefficients of reverse mixing in irregular and regular packed beds are calculated by empirical equations derived by treatment of S-curve of the function of response to pulse disturbance at the apparatus inlet [5, 6]. For new packings, we can use the expression obtained by using Taylor's model [9] (Reynolds number  $Re_g > 3000$ ):

$$Pe_g = \frac{W_g H}{D_{m.g}} = 0.43 \frac{H}{d_e \sqrt{\xi_{ir}}}, \quad (11)$$

where  $d_e$  is the equivalent diameter of the packing, m;  $\xi_{ir}$  is the coefficient of hydraulic resistance of irrigated packings.

For irregular packings [9] ( $40 < Re_g < 10^4$ )

$$Pe_g = 0.52H \left( \frac{Re_g}{\xi_{ir}} \right)^{0.25} d_e^{-1}, \quad (12)$$

where  $Re_g = W_g d_e / \nu_g$ ;  $\nu_g$  is the coefficient of kinematic viscosity of the gas,  $m^2/sec$ .

The coefficient of heat transfer in the gas phase  $\alpha_g$  for irregular packings can be determined from the expression [10]

$$Nu_g = \frac{\alpha_g d_e}{\lambda_g} = 0.175 Re_g^{0.75} \left( \frac{\xi_{ir}}{2} \right)^{0.25} Pr_g^{0.33}, \quad (13)$$

where  $Nu_g$  is the Nusselt number;  $\lambda_g$  is the coefficient of thermal conductivity of the gas,  $W/m \cdot K$ ;  $Pr_g$  is the Prandtl number.

A similar expression was obtained for the Sherwood number  $Sh_g$  [10];

$$Sh_g = \frac{\beta_g d_e}{D_g} = 0.175 Re_g^{0.75} \left( \frac{\xi_{ir}}{2} \right)^{0.25} Sc_g^{0.33}, \quad (14)$$

where  $D_g$  is the coefficient of moisture diffusion into the gas phase,  $m^2/sec$ ;  $Sc_g$  is the Schmidt number.

For regular packings we can use the equation [11]:

$$\text{Nu}_g = 0.158 \text{Re}_g^{0.857} \left( \frac{\xi_{\text{ir}}}{2} \right)^{0.429} \text{Pr}_g^{0.33}, \quad (15)$$

$$\text{Sh}_g = 0.158 \text{Re}_g^{0.857} \left( \frac{\xi_{\text{ir}}}{2} \right)^{0.429} \text{Sc}_g^{0.33}. \quad (16)$$

Expressions (11)–(16) can be used to calculate the  $\text{Pe}_g$ ,  $\text{Nu}_g$ , and  $\text{Sh}_g$  values in each cell, taking account of the variation of thermophysical properties of the cooled gas and hydraulic resistance, which is an advantage over the known methods of calculation of cooling of gases by contact with liquids.

Calculation of air cooling with water at atmospheric pressure in a column having ceramic Raschig rings of 25 mm diameter was performed as an example.

Air velocity  $W_g = 1$  m/sec, irrigation density  $q = 10 \text{ m}^3/(\text{m}^2 \cdot \text{h})$  (film flow), initial temperature of water  $T_{l,i} = 20^\circ\text{C}$  and of air  $T_{g,i} = 40^\circ\text{C}$ , and initial moisture concentration  $x_i \approx 0$ .

The following were obtained by the calculations: air temperature at the exit of the bed with a height of 1 m  $T_{g,f} = 22^\circ\text{C}$  and water temperature  $T_{l,f} = 22.5^\circ\text{C}$ . The thermal balance is maintained with a relative error of about 3%.

The authors use the cited equations of the mathematical model to calculate the parameters of packed column performance in various oil and gas processing enterprises. The obtained data satisfactorily match the real parameters of operation of industrial apparatuses.

### Updating of Pyrogas Cooling Column

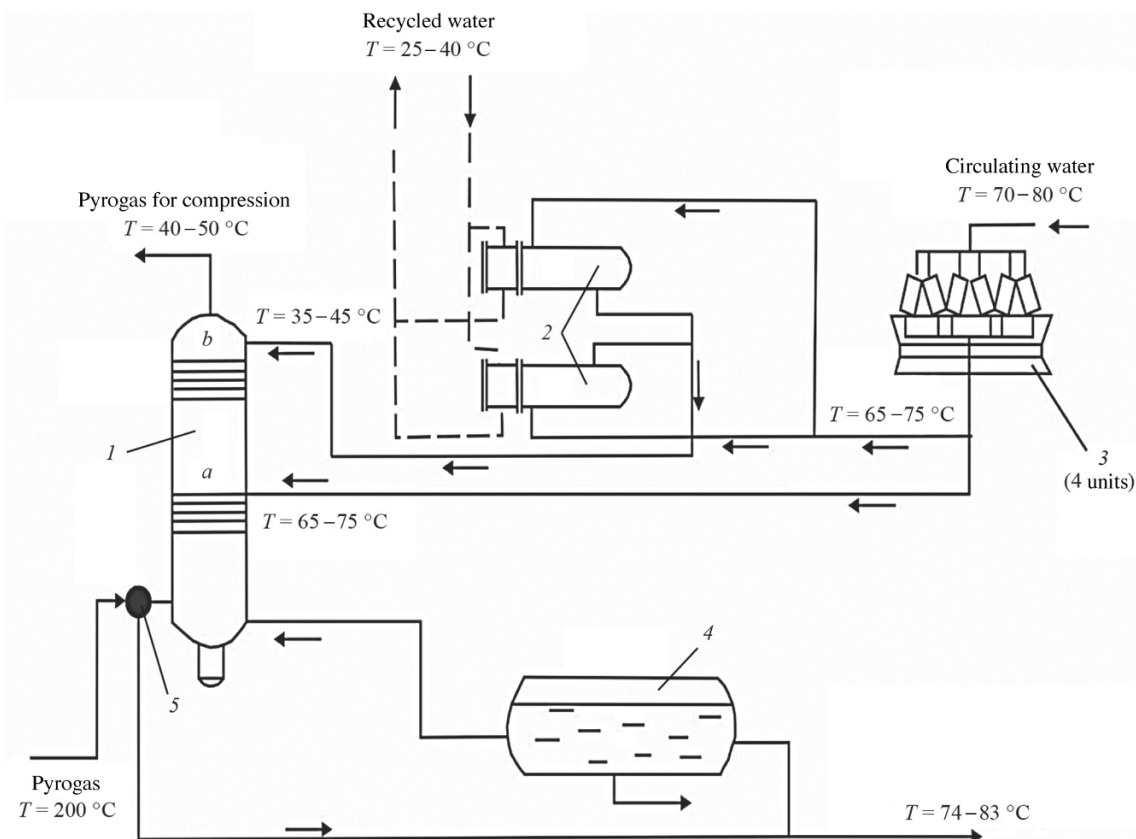
Let us consider the example of updating of an industrial pyrogas cooling scrubber in a gas separation unit employed at an ethylene production plant.

The unit for pyrogas washing with water is designed for cooling and scrubbing of pyrogas from coke and tar and for settling and separating chemically polluted water from pyrolysis tars, followed by its cooling before delivering back to the pyrogas scrubbing column.

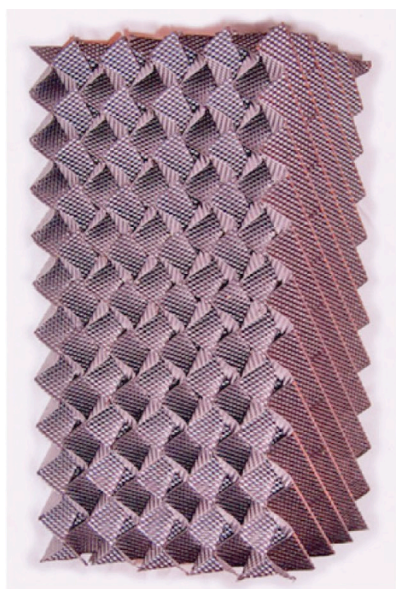
In the E-200 unit at the ‘Ethylene’ plant of the PAO Kazanorgsintez (Kazan Organic Synthesis PJSC), the pyrogas coming from the pyrolysis ovens and the evaporative-quenching apparatuses has, after water spraying into the pipeline, a temperature  $T_g = 80\text{--}105^\circ\text{C}$  and a pressure  $p_g = 60\text{--}80$  kPa. Thereafter, the pyrogas flows into a K-201 water-scrubbing column and moves countercurrent with the cooled water (Fig. 2).

Before updating, the column contained seven angle and seven valve plates in the lower and upper sections of the column, respectively. The plates are intended for additional washing of the pyrogas from tars and coke and cooling to a fixed temperature of the circulating water flowing into the top and mid sections of the column. After cleaning and cooling, the gas flows into the pyrogas compressors of the gas separation department. The specified temperatures and pressures of the cleaned and cooled pyrogas are  $T_{g,f} = 40\text{--}45^\circ\text{C}$  and  $p_g = 50\text{--}60$  kPa, respectively. Before updating, the column did not ensure the fixed pyrogas cooling temperature.

Technical solutions were developed to update the column by replacing plates with regular IRG packings (OOO IVTs Inzhekhim) ( $a_v = 162 \text{ m}^2/\text{m}^3$ ) and Inzhekhim-2000 irregular packing ( $a_v = 70 \text{ m}^2/\text{m}^3$ ) [12] (Fig. 3).



**Fig. 2.** Flow diagram of pyrogas cooling in K-201 column before updating: 1 – K-201 column; 2 – T-203 circulating water cooler; 3 – T-201 circulating water cooler; 4 – E-203 circulating water settler; 5 – device for water spraying into pyrogas stream; a and b – lower and upper sections of the column.



(a)



(b)

**Fig. 3.** Packet of plates of IRG regular packing (a) and Inzhekhim-2000 irregular packing (b).

After updating, the temperature of the cooled pyrogas was calculated by the proposed method. The obtained data satisfactorily (with an error of  $\pm 6\text{--}8\%$ ) agree with the actual industrial column performance parameters. Thus, for example, while the initial pyrogas temperature was  $T_{g,i} = 80^\circ\text{C}$ , the temperature at the exit of the upper section of the column with the packing was  $T_{g,f} = 40.5^\circ\text{C}$  as a result of the calculation. According to the industrial performance data, this temperature is  $T_{g,f} = 43^\circ\text{C}$  (at cooling water temperature  $T_{g,i} = 35^\circ\text{C}$ ).

Thus, the adequacy of the mathematical model and the efficacy of updating of the column using packings are validated.

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