DEVELOPMENT OF DYNAMIC, SPACE DISTRIBUTED MATHEMATICAL MODEL OF DCT OF PRODUCTION URANIUM HEXAFLUORIDE AND THE FURTHER MODELING OF PROCESS

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Annotation

The publication deals with two major hydrodynamic model, which is used in the simulation of mass transfer processes. This model of an ideal mixing and model of ideal displacement. Job pokkazyvaet their application in industry, namely the use of the device-combined typeWork shows their application in industry, in part the use of the device-combined type.

1. Mathematical reactor model of ideal mixing

Mathematical description of the ideal mixing reactor (Figure 1.1) characterizes the change in concentration in the reaction medium in a time that is due to traffic flow (hydrodynamic factor) and chemical conversion (kinetic factor). Therefore, the model of ideal mixing reactor can be built on the basis of a standard model of ideal mixing considering the chemical reaction rate.

Ideal mixing model is idealized flow and provides the theoretical model. According to this model it is assumed that the flow entering the unit immediately distributed throughout the volume due to complete (ideal) mixing the particles of the medium. The concentration of the substance distributed at all points in the flow system and the output thereof is the same:

$$Cin \rightarrow C = Cout.$$

Differential equation model of ideal mixing will have the form:

$$\frac{dc}{dt} = \frac{\upsilon}{V} \cdot \left(C_{in} - C\right), \quad (1.1)$$

Where $\tau = \frac{V}{\upsilon}$ - the contact time, which characterizes the average residence time of the particles in the reactor, s;

V - volume of the reactor, m3;

υ - Volumetric flow material m3 / h.

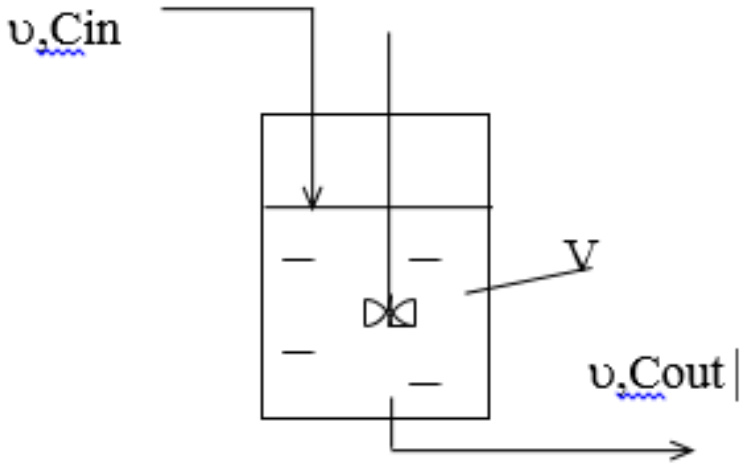

Fig. 1.1. Scheme of the reactor of ideal mixing

Equation (1.1) describes the change in concentration of a substance in an area ideal mixing due to flow.

Then, taking into account the kinetic factor, the dynamic model of an isothermal reactor with ideal mixing continuous action will have the form

$$\frac{dC_i}{dt} = \frac{1}{\tau}\cdot\left(C_{in} - C_{out}\right) \pm w_i \qquad (1.2)$$

This equation is written for each of the components involved in the reaction. Then:

Ci - concentration of the i-th substance, kmol/m3;

wi - the reaction rate of i-th substance kmol/m3.

The system of the above equations is a mathematical model of ideal mixing reactor taking into account changing concentrations over time (dynamic model).

For example, reaction $A \xrightarrow{k} B$ in equation (3.2) can be written:

$C_{in} = C_{A0}$; $C_{out} = C_A$; $w_A = -k \cdot C_A$;

$$\frac{dC_A}{dt} = \frac{1}{\tau_0}\cdot\left(C_{A0} - C_A\right) - w_A. \qquad (1.3)$$

In the steady (stationary) operation of the reactor $\frac{dC_i}{dt} = 0$, then the equation (3.3) can be written as :

$$\frac{1}{\tau}\cdot\left(C_{AO} - C_A\right) = w_A,$$

$$\tau = \frac{C_{AO} - C_A}{w_A}, \qquad (1.4)$$

$$x_A = \frac{C_{A0} - C_A}{C_{A0}}.$$

Using expressions (1.3), (1.4), we can find the main parameters characterizing the operation of the apparatus:

1) τ - residence time in the reactor of the starting material, the magnitude of which depends on the volume of the apparatus (the lower τ, the smaller V);

2) changing the concentration of the reactants, as a function f(τ), and hence to calculate the degree of conversion and selectivity.

Similarly, the material balance equation of ideal mixing reactor (3.2) The equation of heat balance. Thus, we obtain for the adiabatic reactor

$$C_p^{\text{mix}} \frac{\text{dT}}{\text{dt}} = \frac{C_{\text{p}}^{\text{mix}}}{\tau} \cdot \left(T_{\text{in}} - T\right) + \sum_{\text{j=1}}^{\text{N}} \left(-\Delta \text{H}_{\text{j}}\right) \cdot \text{W}_{\text{j}} , \quad (1.5)$$

where :

W_{j} - the speed of the j-th chemical reaction, 1 / s;

$\Delta \text{H}_{\text{j}}$ - The thermal effect of the j-th of the chemical reaction, Joule / mol;

$C_{\text{p}}^{\text{mix}}$ - Heat capacity of the reaction mixture, J / mol K □;

T_{in} - Temperature at the reactor inlet, K;

T - The current temperature, K.

Heat capacity i - substance as a function of temperature is described by the following equation:

$$C_{\text{P}_\text{i}} = (\text{a}_\text{i} + \text{b}_\text{i} \cdot \text{T} + \text{c}_\text{i} \cdot \text{T}^2 + \text{d}_\text{i} \cdot \text{T}^3) \cdot 4.1887 . \quad (1.6)$$

Heat of the mixture is calculated by the additivity rule:

$$\text{C}_\text{P}^{\text{см}} = \sum_{\text{i=1}}^{\text{N}} \text{Cp}_\text{i} \cdot \text{C}_\text{i} , \quad (1.7)$$

where Ci - the concentration of i-th substance mixture mole share.

The dependence of the rate constant on a chemical reaction temperature is expressed by the Arrhenius equation

$$\text{k}_\text{i} = \text{k}_{\text{i,0}} \cdot \text{e}^{-\text{E}_\text{i}/\text{R}\cdot\text{T}} , \quad (1.8)$$

Where:

k_i - the rate constant i-th chemical reactions (for a first order reaction, 1/s);

$\text{k}_{\text{i,0}}$- pre-exponential factor , s-1 ;

E_i - activation energy of the i-th reaction, Joule / mole ;

R- universal gas constant , R = 8,314 J / mole * K.

In order to investigate the dynamic behavior of the reactor ideal mixing , i.e. tracking changes in concentrations of reactants and temperature over time at the exit of the reactor , it is necessary to solve the system of differential equations for each material balance of the components and the heat balance equation .

2. Mathematical reactor model of ideal displacement

Mathematical models of chemical reactors are based on the principle of using a block model of hydrodynamic models that take into account the motion of matter flows.

In accordance with a model of ideal displacement piston taken along flow without stirring for a uniform flow distribution of the concentration of a substance in a direction perpendicular to the movement (Fig. 3-2).

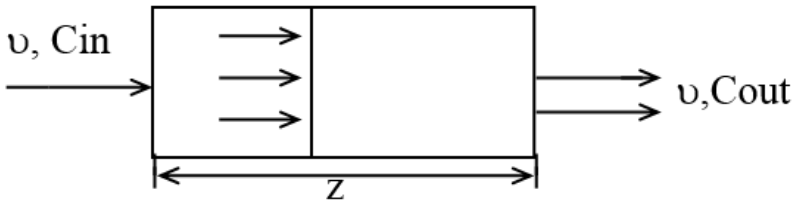

Fig. 3.2. Scheme of ideal displacement

Differential equation model of ideal displacement has the following form:

$$\frac{\partial C_i}{\partial t} = -u \cdot \frac{\partial C_i}{\partial l}, \qquad (1.9)$$

Where:

C - concentration substance mole/l;

t- time , seconds;

u- linear flow velocity, m / s;

l- coordinate (length unit) , m

Mathematical model of ideal displacement is a differential equation in partial derivatives, since the concentration varies in time and space. Such a model is called a model with distributed parameters.

Model of ideal displacement corresponds to a first approximation process in tubular devices for which the ratio of length to diameter of the pipe is more than 20 or diffusion Peclet number is set to ≈ 100 .

If we substitute the linear flow velocity u for the value $u = \upsilon / S$, in the equation (1.9), we obtain :

$$S\frac{dC_i}{dt} = -\upsilon\frac{dC_i}{dl}, \qquad (1.10)$$

Where:

S - the cross section area of ideal displacement, m^2;

υ - Volumetric flow rate (flow) of the substance, m^3 / s.

If the mathematical model of ideal displacement is considered as changing the concentration of power at the expense of chemical reaction, the material balance of a plug flow reactor can be written as

$$\frac{\partial C_i}{\partial t} = -u\frac{\partial C_i}{\partial l} \pm W_i, \qquad (1.11)$$

Where:

C_i - the concentration of the corresponding i-th material;

W_i - Reaction rate of i-th substance.

Heat balance equation adiabatic flow reactor

$$\rho^{\text{mix}} \cdot C_p^{\text{mix}} \cdot \frac{\partial \text{T}}{\partial \text{t}} = -\text{U} \cdot \rho^{\text{mix}} \cdot \text{C}_p^{\text{mix}} \cdot \frac{\partial \text{T}}{\partial \text{l}} + \sum_{\text{j}=1}^{\text{N}} \left(\pm \Delta \text{H}_{\text{j}} \right) \cdot \text{W}_{\text{j}} \,. \tag{1.12}$$

Hence, the mathematical description of a plug flow reactor is characterized by changing the concentration and temperature of the reaction medium in time and space due to movement of the flow (hydrodynamic factor) and chemical conversion (kinetic factor).

Equation (3.11) is written for each of the components involved in the reaction. For example, for the reaction in an isothermal plug flow reactor, mathematical model (dynamic mode) will have the form

$$\frac{\partial \text{C}_\text{A}}{\partial \text{t}} = -\text{u} \cdot \frac{\partial \text{C}_\text{A}}{\partial \text{l}} - \text{k} \cdot \text{C}_\text{A}, \tag{1.13}$$

$$\frac{\partial \text{C}_\text{B}}{\partial \text{t}} = -\text{u} \cdot \frac{\partial \text{C}_\text{B}}{\partial \text{l}} + \text{k} \cdot \text{C}_\text{A}.$$

In the steady (stationary) operation of the reactor

$$\frac{\partial \text{C}_\text{A}}{\partial \text{t}} = 0; \quad \frac{\partial C_\text{B}}{\partial \text{t}} = 0, \tag{1.14}$$

When

$$\text{u} \frac{\text{dC}_\text{A}}{\text{dl}} = -\text{k} \cdot \text{C}_\text{A}, \tag{1.15}$$

$$\text{u} \frac{\text{dC}_e}{\text{dl}} = \text{k} \cdot \text{C}_\text{A}.$$

since the $\frac{\text{l}}{\text{u}} = \tau$, equations (1.15) take the form

$$\frac{\text{dC}_\text{A}}{\text{d}\tau} = -\text{k} \cdot \text{C}_\text{A}, \tag{1.16}$$

$$\frac{\text{dC}_\text{B}}{\text{d}\tau} = \text{k} \cdot \text{C}_\text{A},$$

Where τ - the residence time of reactants in the reactor core (contact time), sec.

In order to investigate the variation of the concentrations of reactants and temperature of the chemical reactor, it is necessary to solve the system of differential equations of (1.11, 1.12).

At this moment my work on modeling of processes occurring in the DCT, represents basic equations describing the behavior of the system under different assumptions, which are accounted for in the modeling of the system by various methods, namely a model of ideal mixing and plug flow model. Further work will go towards the unification of the models described above into one. It will be able to show the work of the unit in an

environment closest to the real, and can use it in the future to the real production process.

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