

MODELING OF PROCESS FOR MASS TRANSFER AT CONDITIONS ELECTROLYSIS OF IONIC FUSIONS

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It is built and decided system of equations of the connected task for transfer of the charged particles in ionic fusion. The eventual formulas of distribution of ions are got on volume fusion. Speeds of renewal of ions are certain with formation of atoms and condition of diffusion of the recovered atoms in the volume of cathode. The conditions of formation of new phase and motion of her front are set. Distribution of diffusible atoms is described after front of new phase.

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One of methods for perfection of structure and properties of material surface is an electrolysis of ionic fusions, in the process of which the recovered atoms diffuse in the volume of cathode material and its form a new phase the border of which is displaced from the cathode surface in a depth material.

Mass transfer electrolytically active particles in the volume of ionic fusion can be described by equation:

$$\frac{\partial C_i}{\partial \tau} = D_i \cdot \nabla^2 C_i + \frac{z_i \cdot F \cdot D_i}{R \cdot T} \cdot \nabla(C_i \cdot \Delta \phi) - \vec{\vartheta} \cdot \nabla C_i, \quad (1)$$

where C_i , D_i , z_i are accordingly concentration of particles, coefficient of diffusion and charge of particles of sort i ; $\Delta \phi$ is a gradient of potential; $\vec{\vartheta}$ is a speed of movement for hydrodynamic stream; F is a Faraday number; ∇ is a sign of divergence; τ , T are time and temperature of process of electrolysis.

Common equation (1) can be simplified for every concrete technological scheme. So, in the case of flat cathode with an area S_K and flat anode with an area S_A at distance between the electrodes L , it can be presented as

$$\frac{\partial C_i}{\partial \tau} = D_i \frac{\partial^2 C_i}{\partial x^2} + \frac{z_i \cdot F \cdot D_i}{R \cdot T} \cdot \frac{\partial(C_i \cdot \Delta \phi)}{\partial x} - \vec{\vartheta} \cdot \frac{\partial C_i}{\partial x}, \quad (2)$$

where x is a co-ordinate, perpendicular to the plane of electrodes with a zero value in the center of electrolysis cell.

In the case when $\Delta \phi = \text{const}$ equation (1) will look like:

$$\frac{\partial C_i}{\partial \tau} = D_i \frac{\partial^2 C_i}{\partial x^2} + \left(\frac{z_i \cdot F \cdot D_i \cdot \Delta \phi}{R \cdot T} - \vec{\vartheta} \right) \frac{\partial C_i}{\partial x}. \quad (3)$$

At the set mode equation (3) looks like

$$\frac{\partial^2 C_i}{\partial x^2} + \left(\frac{z_i \cdot F \cdot \Delta \phi}{R \cdot T} - \frac{\vec{\vartheta}}{D_i} \right) \frac{\partial C_i}{\partial x} = 0. \quad (4)$$

Values of concentration in the center of electrolysis cell must obey a condition

$$C_i \big|_{x=0} = C_i^0, \quad (5)$$

where C_i^0 is a concentration of particles for sort i in the center of electrolysis cell.

The decision of equation (6) taking into account a condition (7) appears in a kind

$$C_i = C_i^0 \cdot \exp \left[\left(\frac{\vec{\partial}}{D_i} - \frac{z_i \cdot F \cdot \Delta \phi}{R \cdot T} \right) \cdot x \right] . \quad (6)$$

A decision (6) describes the process of transfer for the charged particles of sort i in the volume of electrolysis cell in stationary terms at $\Delta \phi = \text{const}$.

The appearing atoms of sort i are diffused in the volume of electrode, and the new phase of sort i appears after achievement of some maximum concentration $C_i^{i\phi}$.

Within the limits of new phase equation of diffusive mass transfer for a flat electrode can be written in a kind

$$\frac{\partial C_i}{\partial \tau} = D_i \cdot \frac{\partial^2 C_i}{\partial x^2} , \quad (7)$$

where D_i is a coefficient of diffusion for atoms of sort i in material of electrodes.

Regional conditions it is possible to write down for equation (7)

$$\left. \frac{\partial C_i}{\partial \tau} \right|_{\substack{x=0 \\ \tau=0}} = V_i^0 ; \quad (8)$$

$$C_i \Big|_{\substack{x=0 \\ \tau=0}} = C_i^{0II} ; \quad (9)$$

$$C_i \Big|_{\substack{x \rightarrow \infty \\ \tau=0}} = 0 , \quad (10)$$

where V_i^0 is speed of formation of atoms of sort i on the border of electrode; C_i^{0I} is a concentration of atoms of sort i on the border of electrode.

After a border the phase transition of equation for transference of atoms of sort i looks like

$$\frac{\partial C_i}{\partial \tau} = \frac{\partial}{\partial x} \left(D_i^2 \frac{\partial C_i}{\partial x} \right) , \quad (11)$$

where D_i^2 is a coefficient of diffusion for atoms of sort i in material of electrodes.

After a border a phase transition equation of atoms of sort i transfer looks like

$$\frac{\partial C_i}{\partial \tau} = \frac{n \cdot D_i^0}{(C_i^0)^n} \cdot C_i^{n-1} \frac{\partial C_i}{\partial x} + D_i^0 \cdot \frac{C_i^n}{(C_i^0)^n} \frac{\partial^2 C_i}{\partial x^2} . \quad (12)$$

At the subzero values of concentration for new phase $C_i^{i\phi}$ a relation C_i/C_i^0 will be near enough to unit and equation (12) will correspond to the record of equation (7).

The decision of equation (7) can be presented in a kind

$$C_i = f(x) \cdot \exp(\alpha \cdot \tau) , \quad (13)$$

where $f(x)$ is a function which depends only on the co-ordinate x ; α is an unknown parameter.

Putting a decision (13) in equation (7), will have

$$D \frac{d^2 f}{dx^2} - \alpha \cdot f = 0 . \quad (14)$$

The decision of equation (14) can be written down as

$$f = G_1 \cdot \exp [-(\alpha/D)^{0.5} \cdot x] + G_2 \cdot \exp [(\alpha/D)^{0.5} \cdot x] , \quad (15)$$

where G_1, G_2 are permanent integrations.

Taking into account correlation (15) a common decision (13) will look like:

A common decision (15) can be written down in a kind

$$C_i(x, \tau) = C_i^{0\Pi} \cdot \exp \left[\frac{V_i^0 \cdot \tau}{C_i^{0\Pi}} - \left(\frac{V_i^0}{C_i^0 \cdot D_i} \right)^{0.5} \cdot x \right]. \quad (16)$$

For equation (12), describing diffusion of atoms of sort i after a border a phase transition, regional conditions can be written down as

$$C_i \Big|_{\substack{x=\xi \\ \tau=\tau_\xi}} = C_i^{\Pi\Phi}; \quad (17)$$

$$C_i \Big|_{\substack{x \rightarrow \infty \\ \tau=0}} = 0; \quad (18)$$

$$\frac{\partial C_i}{\partial x} \Big|_{\substack{x=\xi \\ \tau=\tau_\xi}} = \Delta C_{i,npun}, \quad (19)$$

where $\Delta C_{i,npun}$ is a possible gradient of concentration for atoms of sort i on the border of phase transition.

Common decision of equation (12) taking into account regional conditions (17), (18) and (19) looks like:

$$C_i = \frac{(\Delta C_{i,\partial on})^2}{C_i^{\Pi\Phi}} \cdot \exp \left[\frac{C_i^{\Pi\Phi}}{\Delta C_{i,\partial on}} \cdot (x - \xi) + D_i \cdot \frac{(C_i^{\Pi\Phi})^2}{(\Delta C_{i,\partial on})^2} \cdot (\tau - \tau_\xi) \right]. \quad (20)$$

A decision (20) describes distribution of concentration for atoms of sort i after border of the formed new phase.

Conclusions. The got decisions describe mass transfer of ions of sort i in the volume of electrolyte at influence of gradient of potential $\Delta\phi$ at the temperature of T [equation (6)], transfer of atoms of sort i from the border of electrode in it volume to the border of phase transition $C_i^{I\phi}$ in the distance ξ from a border for a time τ_ξ [equation (16)], and also transfer of atoms of sort i from the border of the phase passing to the volume of electrode [equation (20)].