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Unsteady Mass Transfer into a Sphere under Equilibrium Condition $y = Ax + B$

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Abstract—We obtained an analytical solution of a problem of unsteady mass transfer under the equilibrium condition $y = Ax + B$ to compare results with a problem solution in the case of equilibrium condition looking as $y = Ax$.

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As follows from an universal experience of a softened water treatment there exist large companies manufacturing ion exchange continuous operation plants and apparatus in each industrial country.

Advantages of this equipment are undoubted: countercurrent phase interaction upon all stages of an apparatus, a high rate of filtration, a small operation volume, a low consumption of a regenerant, and of wash-water.

An implementation of a three phase vortex layer (TVL) [1–3] in a sectional pneumatic apparatus for a ion exchanger regeneration and washing results in further improvement of indices of the latter [4].

Nonlinearity of equilibrium curves is an exclusive character of the ion exchange only except for the curves of the Na^+–NH_4^+ that causes difficulties at simulation of this process [5].

Development of a step circulation model whose determinism in the case of ideal conditions exhibits true residence time of an ion exchanger particle on each step of the process, promotes a more correct simulation of the step process in comparison with calculations developed earlier.

Only process models with a linear equilibrium dependence can be analytically solved therefore let us take the equilibrium dependence as a strength line that does not pass through an origin.

We consider unsteady mass transfer with an equilibrium function $y = Ax + B$ where A and B are constants, y determines a concentration of a target constituent in the solid phase (wt %), x, in the liquid phase (wt %) .

In a start time a spherical body of a radius R with a some given initially distributed concentration y is placed into the liquid medium of the constant concentration x_c. Under an interaction of the sphere and environmental a concentration field of the constituent changes into the particle both along a coordinate r and over the time τ.

In this case the simulation of the unsteady mass transfer for the sphere under the constant concentration of the environment looks as

$$\frac{\partial y(r,\tau)}{\partial \tau} = D\left[\frac{\partial^2 y(r,\tau)}{\partial \tau^2} + \frac{2}{r}\frac{\partial y(r,\tau)}{\partial \tau}\right], \quad (1)$$

$$0 < r < R,\ \tau > 0;$$

$$y(r,\ 0) = y_0,\ 0 < r < R; \quad (2)$$

$$x(r,\ \tau)\big|_{\tau=0} = x_0,\ r > R; \quad (3)$$

$$-D\left.\frac{\partial y(r,\tau)}{\partial \tau}\right|_{r=R} = -\ k\,[x_c - x\,(R,\tau)]; \quad (4)$$

$$\frac{\partial y(0,\tau)}{\partial \tau} = 0 \quad \text{(the symmetry condition);} \quad (5)$$

$$y(0,\ \tau) \neq \infty; \quad (6)$$

$$\frac{G}{L}(y_0 - \bar{y}) = (x_0 - x); \tag{7}$$

$$y^* = Ax + B; \tag{8}$$

$$\bar{y} = y^*, \quad \tau \longrightarrow \infty, \tag{9}$$

where D, G/L, A, R, k are constants.

In this paper we present mathematical transformations which lead to the relation for computation of an average concentration $\bar{y}$. We use dimensionless variables

$$R' = \frac{r}{R}, \ T = \frac{D\tau}{R^2}, \ \mathrm{Bi} = \frac{kR}{D}.$$

Then set (1)–(9) look as

$$\frac{\partial y(R',T)}{\partial T} = \frac{\partial^2 y(R',T)}{\partial R'^2} + \frac{2}{R'}\frac{\partial y(R',T)}{\partial R'}, \tag{10}$$

$$0 < R' < 1, \ T > 0;$$

$$y(R', 0) = y_0, \quad 0 < R' < 1; \tag{11}$$

$$x(R', T)\big|_{T=0} = x_0, \quad R' > 1 \tag{12}$$

$$\left.\frac{\partial y(R',T)}{\partial R'}\right|_{R'=1} = \mathrm{Bi}[y^* - y\ (1,T)]; \tag{13}$$

$$\frac{\partial y(0,T)}{\partial R'} = 0 \quad \text{(the symmetry condition)}; \tag{14}$$

$$y(0, T) \neq \infty; \tag{15}$$

$$\frac{G}{L}(y_0 - \bar{y}) = (x_0 - x); \tag{16}$$

$$y^* = Ax + B; \tag{17}$$

$$\bar{y} = y^*, \quad T \longrightarrow \infty. \tag{18}$$

We used Laplace transform that was performed with respect to a variable T to solve equations (10)–(18). The value of T changed in the range from 0 to $\propto$ in which is taken Laplace integral. It was assumed that variable R' was unchangeable in the course of the transformation. Therefore an image depends on s (a transformation parameter) as well as on R':

$$F(R', s) = \int_0^\infty y(R',T)e^{-sT}dT.$$

Subjecting partial derivatives with respect to T to Laplace transform we have

$$\frac{\partial y(R',T)}{\partial T} \longrightarrow sF(R',s) - y(R',0) \longrightarrow \frac{\partial y(R',T)}{\partial T} \longrightarrow sF - y_0.$$

Relative to partial derivatives with respect to R', an assumption, that operations for composition of such derivatives and Laplace integral can change places, should be made in order to use Laplace transform for a solution of the equation. For example:

$$\frac{\partial y(R',T)}{\partial R'} \to \frac{\partial F}{\partial R'}, \quad \frac{\partial^2 y(R',T)}{\partial R'^2} \to \frac{\partial^2 F}{\partial R'^2}.$$

Thus, an application of Laplace transform to equation (10) leads to the following equation

$$sF - y_0 = \frac{\partial^2 F}{\partial R'^2} + \frac{2}{R'}\frac{\partial F}{\partial R'} \quad \text{or} \quad \frac{\partial^2 F}{\partial R'^2} + \frac{2}{R'}\frac{\partial F}{\partial R'} - sF + y_0 = 0. \tag{19}$$

Let us take $F \to z$, $R' \to x$, then we write the last equation according to new significations:

$$z'' + (2/x)z' - sz + y_0 = 0.$$

As $\frac{\partial^2 y}{\partial r^2} + \frac{2}{r}\frac{\partial y}{\partial r} = \frac{1}{r}\frac{\partial^2}{\partial r^2}(ry)$, then we have $z'' + (2/x)z' = (1/x)(xz)''$. The equation reduces to $(xz)'' - s(xz) + y_0 x = 0$. In the case of $xz \to \tilde{z}$, we get an ordinary differential equation

$$(\tilde{z})'' - s(\tilde{z}) + y_0 x = 0. \tag{20}$$

Let us write a characteristic equation for (20): $\lambda^2 - s = 0$. Then $z_{\mathrm{odn}} = c_1 e^{x\sqrt{s}} + c_2 e^{-x\sqrt{s}}$. After computation of constant $\tilde{z}$ in a partial solution $z_{\mathrm{p}} = cx$, where c = const we substitute $\tilde{z}$ in equation (20) that results in $c = y_0/s$. A general solution of equation (20) looks as $\tilde{z}_{\mathrm{gen}} = c_1 e^{x\sqrt{s}} + c_2 e^{-x\sqrt{s}} + y_0 x/s$. Solution for equation (19) looks as the following relation:

$$R'F = c_1 e^{R'\sqrt{s}} + c_2 e^{-R'\sqrt{s}} + y_0 R'/s. \tag{21}$$

Now we determine an image of a function $\bar{y}$:

$$\overline{F} = 3\int_0^1 R'^2 F\,\mathrm{d}R' = 3\int_0^1 R'^2 \left(\frac{c_1}{R'}\mathrm{e}^{R'\sqrt{s}} + \frac{c_2}{R'}\mathrm{e}^{R'\sqrt{s}} + \frac{y_0}{s}\right)\mathrm{d}R' = \frac{y_0}{s} + 3\int_0^1 R'\,(c_1\mathrm{e}^{R'\sqrt{s}})\,\mathrm{d}R'$$

$$+ 3\int_0^1 R'\,(c_2\mathrm{e}^{-R'\sqrt{s}})\,\mathrm{d}R' = \frac{y_0}{s} + 3c_1\left(\frac{\mathrm{e}^{\sqrt{s}}}{\sqrt{s}} - \frac{\mathrm{e}^{\sqrt{s}}}{s} + \frac{1}{s}\right) + 3c_2\left(-\frac{\mathrm{e}^{-\sqrt{s}}}{\sqrt{s}} - \frac{\mathrm{e}^{-\sqrt{s}}}{s} + \frac{1}{s}\right). \quad (22)$$

From conditions $G/L(y_0 - y\_) = (x_0 - s)$, $y^* = Ax + B$ the following relation results

$$y^* = y_0{}^* - A\beta(y_0 - \overline{y}). \quad (23)$$

If relation (23) is substituted in condition $\left.\frac{\partial y(R',T)}{\partial R'}\right|_{R'=1} = \mathrm{Bi}[y^* - y(1,\,T)]$, and the derivative is subjected to Laplace transform we obtain

$$\left.\frac{\partial F(R',s)}{\partial R'}\right|_{R'=1} = \mathrm{Bi}\left[\frac{y_0^*}{s} - A\beta\left(\frac{y_0}{s} - \overline{F}\right) - F(1,s)\right].$$

We write taking into account equation (21)

$$F(1,s) = c_1\mathrm{e}^{\sqrt{s}} + c_2\mathrm{e}^{-\sqrt{s}} + \frac{y_0}{s}. \quad (24)$$

Now we differentiate equation (21) after preliminary division of both its terms into R'.

$$\frac{\partial F(R',s)}{\partial R'} = c_1\frac{R'\sqrt{s}\,\mathrm{e}^{R'\sqrt{s}} - \mathrm{e}^{R'\sqrt{s}}}{R'^2} + c_2\frac{-R'\sqrt{s}\,\mathrm{e}^{-R'\sqrt{s}} - \mathrm{e}^{R'\sqrt{s}}}{R'^2}. \quad (25)$$

Then

$$\left.\frac{\partial F(R',s)}{\partial R'}\right|_{R'=1} = c_1(\sqrt{s}\,\mathrm{e}^{\sqrt{s}} - \mathrm{e}^{\sqrt{s}}) - c_2(\sqrt{s}\,\mathrm{e}^{-\sqrt{s}} + \mathrm{e}^{-\sqrt{s}}). \quad (26)$$

After substituting relatives (22), (25), and (26) in equation (24) we get

$$c_1(\sqrt{s}\,\mathrm{e}^{\sqrt{s}} - \mathrm{e}^{\sqrt{s}}) - c_2(\sqrt{s}\,\mathrm{e}^{-\sqrt{s}} + \mathrm{e}^{-\sqrt{s}}) = \mathrm{Bi}\left\{\frac{y_0^*}{s} - A\beta\frac{y_0}{s} + A\beta\left[\frac{y_0}{s} + 3c_1\left(\frac{\mathrm{e}^{\sqrt{s}}}{\sqrt{s}}\frac{\mathrm{e}^{\sqrt{s}}}{s} + \frac{1}{s}\right) + 3c_2\left(\frac{\mathrm{e}^{-\sqrt{s}}}{\sqrt{s}}\frac{\mathrm{e}^{-\sqrt{s}}}{s} + \frac{1}{s}\right)\right] - \left(c_1\mathrm{e}^{\sqrt{s}} + c_2\mathrm{e}^{-\sqrt{s}} + \frac{y_0}{s}\right)\right\}. \quad (27)$$

In solution of equation (21) the constants c_1, c_2 are unknown. As $\frac{\partial y(0\,,T)}{\partial R'} = 0$ (the symmetry condition) then $y(0, T) = \mathrm{const}$ in any time and according to Laplace transform $F(0, s) = \mathrm{const}$. Accounting for this condition in equation (21) we obtain $c_1 = -c_2$. Hence we rewrite equation (27):

$$c_1 = \frac{\mathrm{Bi}\left(\frac{y_0^*}{s} - \frac{y_0}{s}\right)}{2\left[\sinh(\sqrt{s})\left(-1 + \mathrm{Bi} + 3A\beta\mathrm{Bi}\,\frac{1}{s}\right) + \cosh(\sqrt{s})\left(\sqrt{s} - 3A\beta\mathrm{Bi}\,\frac{1}{\sqrt{s}}\right)\right]}. \quad (28)$$

and equation (23)

$$\overline{\mathrm{F}} - \frac{y_0}{s} = 6c_1\left[\frac{\cosh(\sqrt{s})}{(\sqrt{s})} - \frac{\sinh(\sqrt{s})}{s}\right]. \quad (29)$$

After substitution of equation (28) in (29) and transformations we have

$$\frac{\overline{\mathrm{F}} - \frac{y_0}{s}}{y_0^* - y_0} = \frac{3\,\mathrm{Bi}\left[\frac{\cosh(\sqrt{s})}{(\sqrt{s})} - \frac{\sinh(\sqrt{s})}{s}\right]}{\mathrm{s}\left[\sinh(\sqrt{s})\left(-1 + \mathrm{Bi} + 3A\beta\mathrm{Bi}\,\frac{1}{s}\right) + \cosh(\sqrt{s})\left(\sqrt{s} - 3A\beta\mathrm{Bi}\,\frac{1}{\sqrt{s}}\right)\right]}. \quad (30)$$

We multiply by s both nominator and denominator in equation (30) in the right term. Thus a ratio of two polynoms forms equation (30). We denote them:

$$\Psi(s) = s^2\left[\sinh(\sqrt{s})\left(-1+\mathrm{Bi}+3A\beta\mathrm{Bi}\frac{1}{s}\right) + \cosh(\sqrt{s})\left(\sqrt{s}-3A\beta\mathrm{Bi}\frac{1}{\sqrt{s}}\right)\right],$$

$$\Phi(s) = 3\mathrm{Bi}\,[\sqrt{s}\cosh(\sqrt{s}) - \cosh(\sqrt{s})]\,.$$

According to a method of integral transformation we took into account all conditions of the expansion theorem that can be applied in the case of transition of the solution for equation (30) to the solution for the origin equation. The expansion theorem is written as the following expression $L^{-1}\left|\frac{\Phi(s)}{\Psi(s)}\right| = \sum_{n=1}^{\infty}\frac{\Phi(s_n)}{\Psi(s_n)}\,e^{s_n\tau}$, where s_n is roots of polynom $\Psi(s)$.

$s = 0$, and set μ_n, $n = \overline{1, \infty}$, are function $\Psi(s)$ zeros computed from relation:

$$\coth(\mu_n) = \frac{\mu_n^2(\mathrm{Bi}-1)+3A\beta\mathrm{Bi}}{3\mu_n A\beta\mathrm{Bi} - \mu_n^3}. \tag{31}$$

We determine $\Psi'(s)$:

$$\Psi'(s) = \sqrt{s}\cosh(\sqrt{s})\left(\frac{\mathrm{Bi}\,s}{2} - 3A\beta\mathrm{Bi} + 2s\right) + \sinh(\sqrt{s})\left[3A\beta\mathrm{Bi} + \frac{s^2}{2} - \frac{3A\beta\mathrm{Bi}\,s}{2} + 2s(\mathrm{Bi}-1)\right].$$

Thus:

$$\lim_{s\to 0}\frac{\Phi(s)}{\Psi'(s)} = -\frac{1}{A\beta}\,.$$

Then a limit at $s \to s_n$ should be found. We use equation (31) , preliminary dividing both nominator and denominator by $\sinh(\sqrt{s})$ in relation $\frac{\Phi(s)}{\Psi'(s)}$, and we obtain:

$$\lim_{s\to s_n}\frac{\Phi(s)}{\Psi'(s)} = \frac{3\mathrm{Bi}^2\sqrt{s}}{\frac{\mathrm{Bi}^2 s\sqrt{s}}{2} + \frac{9A\beta\mathrm{Bi}^2\sqrt{s}}{2} - \frac{\mathrm{Bi}\,s\sqrt{s}}{2} + 3A\beta\mathrm{Bi}\,s\sqrt{s} - \frac{s^2\sqrt{s}}{2} - \frac{9(A\beta\mathrm{Bi})^2\sqrt{s}}{2}}\,.$$

After multiplication of both nominator and denominator by value $\frac{2}{\mathrm{Bi}^2\sqrt{s}}$ and assuming that $s \to s_n$, we have

$$\lim_{s\to s_n}\frac{\Phi(s)}{\Psi'(s)} = \frac{6}{\mu_n^2 + 9A\beta - \frac{\mu_n^2}{\mathrm{Bi}} + \frac{6A\beta\mu_n^2}{\mathrm{Bi}} - \frac{\mu_n^4}{\mathrm{Bi}^2} - 9(A\beta)^2}\,.$$

As a result of the performed transformations the original of the general solution looks like

$$\frac{\bar{y}-y_0}{y_0^*-y_0} = -\frac{1}{A\beta} + \sum_{n=1}^{\infty}\frac{6}{\mu_n^2\left(\frac{2}{\mathrm{Bi}}+1\right) + 3\left(3A\beta - \frac{\mu_n^2}{\mathrm{Bi}}\right) - \left(3A\beta - \frac{\mu_n^2}{\mathrm{Bi}}\right)}\,e^{-\mu_n^2 T}. \tag{32}$$

Thus we got analytical solution of the presented problem of the unsteady mass transfer at $y^* = Ax + B$.

Known solution for the unsteady mass transfer into the sphere with an equilibrium function $y = Ax$:

$$\frac{\bar{y}-y_0}{y_0^*-y_0} = \sum_{n=1}^{\infty}\frac{6\mathrm{Bi}^2}{\mu_n^2(\mathrm{Bi}^2+\mu_n^2-\mathrm{Bi})}\,e^{-\mu_n^2 T}.$$

Unfortunately the initially accepted equilibrium function approximates only first step of a target line in contrast to the equation $y^* = Ax + B$. The latter function in dependence on the coefficient B can approximate a certain part of the equilibrium line that is required to be determined. Therefore an introduction of coefficient B increases significance of the obtained solution.

CONCLUSIONS

Simulation and computation of the mass transfer at unsteady equilibrium $y^* = Ax + B$ were performed. An introduction of the coefficient B increases the possibility of the approximation of the equilibrium line in comparison with approximation by equation $y = Ax$.

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