Rheological model of mixing and transformation processes in multiphase medium

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Abstract
Theory of rheological transitions and transformations was used in multiphase medium for description of mixing and transformation processes. In the article there presented models of irreversible rheological transitions and shown that such transitions are described by integrated impulse Dirac delta function. Rheological model of process with the usage of zero gradient method is obtained.
Key words: MULTIPHASE MEDIUM, RHEOLOGICAL TRANSITION, TRANSFORMATION, MIXING, MASS TRANSFER, MODELING

Introduction

Modeling of control objects is complicated by multiphase character of the medium during development of control systems for operational procedures in beneficating and metallurgical production and also at petrochemical enterprises, where the processes of mixing of various substances and phases are applied [1-6].

Researches use various approaches for modeling of multiple-phase process. Microbalance models allow to consider interphasal activity [7]. There also known the experience of their application to the devices with fluid bed. Use of disordered flow dynamics [8] allows to model multiphase systems. Anyhow the most effective from the point of view of synthesis of control systems is rheological approach [9]. Application of rheological theories during construction of models of such multiphase objects allows to consider dispersive character and physical peculiarities of technological processes. This in its turn gives the opportunity to create adequate mathematical models, which allow to apply modern means of optimal control [10].

The objective of this article is development of mass transfer model in conditions of ideal mixing and transformation of multiphase medium taking into account diffusion and convection.

Statement of basic materials

For most of the devices, where there occurs mixing in conditions of multiphase medium, it is characteristic randomness of discontinuous phase motion in the volume of device and intensive fluctuations of various types [11, 12]. Such behavior may be considered when applying rheological theories.

We will consider the processes as rheological transitions, in the base of which there is transfer of mass, energy and motion amount [13, 14]. As it is shown in [9, 15, 16] the presence of one or another rheological transition leads to the change of response time of transition processes and according to the change of manufacturing efficiency.

Hereafter for development of mathematical model of mass transfer let us accept the following assumptions:

1. We consider the device of ideal mixing, where there is fulfilled continuous mechanical activation and crushing of hard phase (e.g. catalytic agent).
2. We consider the particle, which is formed in result of crushing, to be identical to all the others.
3. Formed particle is of spherical shape.

Hereafter we will consider no all the instrument at large, but only one simple connecting piece, which is half-full with dispersing material. Substances forming multiphase medium are fed into it.

Transfer of material flow in some considered volume of machinery consists of transfer of substances due to molecular diffusion and convectional transfer (Q concentration) and is characterized by field of velocities $\bar{v}(\bar{r}, \theta)$, where $\bar{r}$ is vector of directivity of transfer motion; θ - transfer time. In such a way equation for total flow of *F* transfer may be written as follows

$$\bar{F} = Q\bar{v} + \bar{q}. \qquad (1)$$

Integral form of storage conditions for this volume *V* will be

$$\int_V \frac{\partial Q}{\partial \theta} dV = -\oint_S F df + \int_V \gamma dV, \qquad (2)$$

where $df = nd\nabla$ - surface element; *n* - unit vector of the element $d\nabla$; γ - runoff vector.

As in considered volume there takes place interaction of various substances, then, having defined v – linear speed of mass transfer; Q_i - concentration of the *i-th* substance; D_i - effective coefficient of mass transfer of the *i-th* substance; γ_i - runoff of the *i-th* substance per one unit of time *t*, equation of transfer looks as follows

$$\frac{\partial Q_i}{\partial \theta} + \mathrm{div}(Q_i \mathrm{v}) = \mathrm{div}(D_i \nabla Q_i) + \gamma_i, \qquad (3)$$

During investigation of diffusion processes in many cases [17-20] one may introduce a notion of diffusion region, which formally is integrated impulse Dirac delta function. Usage of linear grade laws during description of processes of mass transfer leads to antinomy about unlimited speed of disturbance of concentration fields. In real situation on the basis of theory of presence of nominal film on the boundary of two substances [21], unlimited in value concentration gradients may take place only under the condition if film thickness equals $\delta = 0$. This means that the boundary represents step Dirac delta both at the right and at the left of the boundary (fig.1).

If the process is characterized by that the transmutation products are constantly derived from reaction zone, one may consider that the process of transitions stops when the runoff of created substance is absent [22].

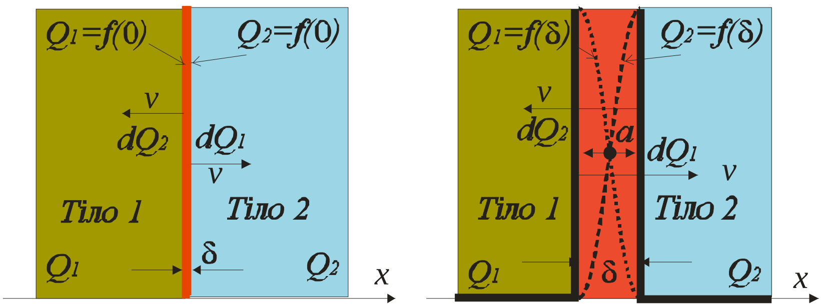

Figure 1. Principle of mass transfer at the boundary of two phases

In general case transformation equation when runoff of created substance is present looks as follows

$$\frac{\partial Q_i(\delta,\theta)}{\partial\theta}+D_i\frac{\partial^2 Q_i(\delta,\theta)}{\partial\delta^2}+v\frac{\partial Q_i(\delta,\theta)}{\partial\delta}=\gamma_{iP}(\delta,\theta)-\gamma_C(x,t), \qquad (4)$$

where $y_C(x,t)$ - runoff of created substance from reaction zone, $y_{iP}(\delta,\theta)=k_{P0}f[Q_i(\delta,\theta)]$ - runoff of reaction components in reaction zone.

If reacting components are fed in call-off quantity with concentrations Q_1 and Q_2, then one may consider that runoff of these components is fulfilled according to exponential rule and runoff rate is described by such differential equation

$$\gamma_{iP}(\delta,\theta)=\tau_{2P}^2\frac{d^3Q_i(\delta,\theta)}{d\theta^3}+\tau_{1P}\frac{d^2Q_i(\delta,\theta)}{d\theta^2}+\frac{dQ_i(\delta,\theta)}{d\theta} \qquad (5)$$

where τ_{1P}, τ_{2P} - response time of runoff of the i-th components.

Then according to each component we may write

$$\gamma_{1P}(\delta,\theta)=\tau'\frac{d^2Q_1(\delta,\theta)}{d\theta^2}+\frac{dQ_1(\delta,\theta)}{d\theta}+Q_2(\delta,\theta); \qquad (6)$$

$$\gamma_{2P}(\delta,\theta)=\tau''\frac{d^2Q_2(\delta,\theta)}{d\theta^2}+\frac{dQ_2(\delta,\theta)}{d\theta}, \qquad (7)$$

where τ' and τ'' - response time of transfer of components with concentration Q_1 and Q_2 respectively.

In such a way time response in equation (5) is equal to $\tau_{1P}=\tau'+\tau''$ and $\tau_{2P}^2=\tau'\tau''$. Runoff of produced substance is constant and in dynamic relation is an element of the second-order [21]

$$\gamma_C(x,t)=\tau_C\frac{d^2Q_P(x,t)}{dt^2}+\frac{dQ_P(x,t)}{dt}, \qquad (8)$$

where τ_C - response time of created substance.

Having substituted (5) and (8) into equation (4), we will obtain the following nonlinear differential equation

$$\frac{\partial Q_i(\delta,\theta)}{\partial\theta}+D_i\frac{\partial^2 Q_i(\delta,\theta)}{\partial\delta^2}+v\frac{\partial Q_i(\delta,\theta)}{\partial\delta}= \\ =\tau_{2P}^2\frac{d^3Q_i(\delta,\theta)}{d\theta^3}+\tau_{1P}\frac{d^2Q_i(\delta,\theta)}{d\theta^2}+\frac{dQ_i(\delta,\theta)}{d\theta}-\tau_C\frac{d^2Q_P(x,t)}{dt^2}-\frac{dQ_P(x,t)}{dt}. \qquad (9)$$

In the equation (9) let us accept that $\tau_{2P}^2=0$ and diffusion process occurs in one direction $x(x=\delta)$, then the equation (9) looks as follows

$$\frac{\partial Q(x,\tau)}{\partial\theta}+D_i\frac{\partial^2Q(x,\tau)}{\partial x^2}+v\frac{\partial Q(x,\tau)}{\partial x}=\tau_c\frac{d^2Q_{gas}}{dt^2}+\frac{dQ_{gas}}{dt}. \qquad (10)$$

Let us accept that average speed of phase motion is $v=\frac{\partial x}{\partial\theta}$ and $\partial x=v\partial\theta$, then the equation (10) looks as follows:

$$\frac{D_i}{v^2}\cdot\frac{\partial^2Q(\theta)}{\partial\theta^2}+2\frac{\partial Q(\theta)}{\partial x}=\tau_c\frac{d^2Q_{gas}}{dt^2}+\frac{dQ_{gas}}{dt}. \qquad (11)$$

Equation (11) is nonlinear mathematical model of processes of mixing and transformation in multiphase medium. According to zero gradient method [11] this equation characterizes the core of integrated impulse delta-Dirac function, for which boundary of gradient is equal to zero. Let us write the equation (11) in the following form

$$\frac{\partial}{\partial\theta}\left[\frac{D_i}{v^2}\cdot\frac{\partial Q(\theta)}{\partial\theta}+2Q(\theta)\right]=\frac{d}{dt}\left[\tau_c\frac{dQ_{gas}(t)}{dt}+Q_{gas}(t)\right]. \qquad (12)$$

Taking into account zero gradient method we will obtain the following system of linear deferential equations:

$$\frac{D_i}{2v^2}\cdot\frac{\partial Q(\theta)}{\partial\theta}+Q(\theta)=0 \qquad (13)$$

$$\tau_c\frac{dQ_{gas}(t)}{dt}+Q_{gas}(t)=0. \qquad (14)$$

Equation (13) describes the process of simultaneous carry of reacting components mass, and equation (14) – runoff process of ready product.

Conclusions

For modeling of multi phase objects there used theory of rheological transitions and transformations, which allowed to consider dispersive character and physical peculiarities of technological processes. Rheological transitions are described by integrated impulsive delta-Dirac function, cores of which are connected with nonlinear differential equations of mass transfer.

Rheological model of mass transfer in conditions of ideal mixing and transformation of multiphase medium with the usage of zero gradient method is obtained. The results of researches may be used for solution of check problems, control and optimization of this process.

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