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Generalized semi-opened axial dispersion model

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The axial dispersion model (ADM) is studied and then generalized by a new form of the left boundary condition of semi-open flow system. The resulting parameter driven model covers the traditional axial models: axial closed-opened dispersion model with enforced input concentration (AEO), axial closed-opened dispersion model with input Danckwerts' condition (ACO), and axial opened-opened model (AOO). It also enables development of the degraded axial model (ADO). The research is concerned with both modeling and mathematical solution. Also, many numerical aspects of computer realization are discussed.

Key words: axial dispersion, flow models, analytical solution, generalization, limit cases, numerical aspects

1. Introduction

The study of axial dispersion flow models is the subject of our research because of their applications in both industry (chemical apparatuses, pipe-lines, reactors, etc.) [1, 4, 7, 8, 12, 13] and natural sciences (medicine, ecology, metrology, etc.). All the applications are based on the following simple presumptions: the first and the second Fick's diffusion laws in one-dimensional system; absence of radial mixing; inclusion of turbulent behavior into diffusion process; constant diffusion coefficient and flow velocity; and idealized mathematical expression of boundary conditions. These result in the linear system with distributed parameters, i.e. two independent variables: time and spatial coordinate.

An example of biomedical application can be the model of blood vessel system identified via radio-markers or treatment via pharmaceuticals. Another application in chemical engineering is the hydrodynamic model of column or tube apparatuses (e.g. flow of multi-component mixtures in pipe-lines, tubular reactors, absorbers and distillation columns).

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The other reason for our research is in the chance of analytical solubility of any individual model.

The traditional approach to modeling of semi-opened flow canals is based on the choice out of three axial models:

- axial closed-opened dispersion model with enforced input concentration (AEO),
- axial closed-opened dispersion model with input Danckwerts' condition (ACO),
- axial opened-opened model (AOO).

The novelty of this paper is in the generalization of the left boundary condition which is physically motivated having only one new positive parameter (w). This parameter is the ratio of the diffusion coefficients in the input zone and in the internal canal.

The paper is devoted especially to the original generalized closed-opened axial model (AGO) and namely its

- detailed description with physical motivation,
- analytical solution in complex and time domains,
- dynamic properties study,
- special cases and their relation to traditional ADM,
- advantage in interpolation ability among traditional models.

2. Model description

The one-dimensional axial flow dispersion model [1, 7, 8] is considered. The traditional mathematical expression of such a model is [7]

$$D_{\mathrm{L}} \frac{\partial^2 \mathrm{c}\,(x,t)}{\partial x^2} - u \frac{\partial \mathrm{c}\,(x,t)}{\partial x} = \frac{\partial \mathrm{c}\,(x,t)}{\partial t} \tag{1}$$

with the initial condition in the form

$$\forall x \geqslant 0 : \lim_{t \to 0+} \mathrm{c}(x,t) = 0 \tag{2}$$

and the boundary conditions

$$\forall t \geqslant 0 : \mathrm{c}_{\mathrm{in}}(t) = \mathrm{c}(0,t), \tag{3}$$

$$\forall t \geqslant 0 : \lim_{x \to +\infty} \mathrm{c}(x,t) = 0 \tag{4}$$

where D_L is the coefficient of axial dispersion, x the length coordinate, t the time, $c(x,t)$ the concentration profile in a given canal, u the positive flow velocity in the direction of the x–coordinate.

The left boundary condition (3) means that the input concentration is enforced (E) and the right one (4) is the so-called open one (O, the pipe line is open to infinity). According to the notation for the purpose of the paper, the model will be referred to as AEO (axial enforced-opened model). The output definition is also necessary for in several applications. The output is define as

$$y(t) = \mathrm{c}(H,t) \tag{5}$$

where H is the real canal length. References [9] also present forms for the so called mean residence time τ and Peclet criterion Pe as

$$\tau = \frac{H}{u} \tag{6}$$

$$Pe = \frac{uH}{D_\mathrm{L}}. \tag{7}$$

It is useful to consider the solutions in a dimensionless form which is simpler to understand and analyze. We obtain the dimensionless model AEO as

$$\frac{1}{Pe}\frac{\partial^2 \mathrm{c}(\xi,\theta)}{\partial \xi^2} - \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \xi} = \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \theta}, \tag{8}$$

$$\forall \xi \geqslant 0 : \lim_{\theta \to 0+} \mathrm{c}(\xi,\theta) = 0, \tag{9}$$

$$\forall \theta \geqslant 0 : \mathrm{c_{in}}(\theta) = \mathrm{c}(0,\theta), \tag{10}$$

$$\forall \theta \geqslant 0 : \lim_{\xi \to +\infty} \mathrm{c}(\xi,\theta) = 0, \tag{11}$$

$$y(\theta) = \mathrm{c}(1,\theta) \tag{12}$$

where $\xi = x/H$ and $\theta = t/\tau$ are the dimensionless length coordinate and dimensionless time respectively.

The other semi-opened axial dispersion models (ADM) are also included in this paper. These models differ in the left boundary condition according to [7].

When the left side of the canal is closed (C), the adequate boundary condition (in dimensionless form) has the following form

$$\mathrm{c_{in}}(\theta) = \mathrm{c}(0,\theta) - \frac{1}{Pe}\lim_{\xi \to 0+} \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \xi} \tag{13}$$

So, the model with the boundaries (13), (4) is indicated as axial closed-opened (ACO).

The last traditional case included in this paper is the called axial opened-opened (AOO) with the left boundary corresponding to (4)

$$\forall t \geqslant 0: \lim_{x \to -\infty} \mathrm{c}(x,t) = 0. \tag{14}$$

The input condition for this model can be expressed as

$$\mathrm{c_{in}}(\theta) = \frac{1}{Pe}\left(\lim_{\xi \to 0-} \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \xi} - \lim_{\xi \to 0+} \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \xi}\right). \tag{15}$$

3. Basic characteristics of the traditional models

The transfer function is the most important basic characteristic of the given models. It will be presented in a dimensionless form, where $q = s\tau$ is a complex variable for one-sided Laplace transform [5, 10] and

$$a = \sqrt{1 + \frac{4q}{Pe}} \tag{16}$$

which is a traditional term [12, 14, 15] for expressing the transfer function.

The resulting transfer functions of all the studied ADMs have general form

$$\mathrm{G}(q) = \mathrm{D}(Pe,q)\exp\left(\frac{Pe}{2}(1-a)\right) \tag{17}$$

where:

- $\mathrm{D}(Pe,q) = 1$ for AEO, [12, 14, 15, 16],
- $\mathrm{D}(Pe,q) = 2/(1+a)$ for ACO, [12, 15, 16],
- $\mathrm{D}(Pe,q) = 1/a$ for AOO, [12, 15, 16].

Therefore, (17) is the well decomposed formula which covers all three traditional models.

Similarity of the transfer functions is inspiring for finding a general axial model (AGO), whose transfer function can be expected as the next special form of (17).

The impulse responses of ADMs are important for the simulation and identification purposes. The dimensionless impulse response of AEO [12, 14, 15, 16] has the form

$$\mathrm{g}(\theta) = \frac{1}{2\theta}\sqrt{\frac{Pe}{\pi\theta}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right). \tag{18}$$

For ACO [12, 14], the dimensionless impulse function is presented as

$$g(\theta) = \sqrt{\frac{Pe}{\pi\theta}} \exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right) - \frac{Pe}{2} \exp(Pe) \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1+\theta}{2}\right), \tag{19}$$

and, finally for AOO [12, 14] the dimensionless impulse characteristic is

$$g(\theta) = \frac{1}{2}\sqrt{\frac{Pe}{\pi\theta}} \exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right). \tag{20}$$

The last important characteristic to be studied in the paper is the dimensionless step response for given ADMs. For AEO [12, 14, 15, 16] it has the form

$$h(\theta) = \frac{1}{2} \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1-\theta}{2}\right) + \frac{\exp(Pe)}{2} \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1+\theta}{2}\right), \tag{21}$$

for ACO [12, 14] it is expressed as

$$\begin{aligned} h(\theta) = & \sqrt{\frac{Pe\theta}{\pi}} \exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right) + \frac{1}{2} \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1-\theta}{2}\right) \\ & - \frac{(1+Pe+Pe\theta)\exp(Pe)}{2} \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1+\theta}{2}\right), \end{aligned} \tag{22}$$

and, finally, for AOO [12, 14] the dimensionless step function is

$$h(\theta) = \frac{1}{2} \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1-\theta}{2}\right) - \frac{\exp(Pe)}{2} \operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}} \frac{1+\theta}{2}\right). \tag{23}$$

4. Physical generalization of semi-opened axial model

The similarities of transfer functions, impulse responses, and step responses for various ADMs are good motivation for physical generalization of the semi-opened axial model. The main goal is to find a general form of the left boundary condition, which enables interpolation among the following models: AEO, ACO and AOO.

The main physical presumption is that the coefficient of axial dispersion in the input zone D_L^* could be different from the internal coefficient of axial dispersion D_L. The length and thus the volume of input zone approach a zero value. In the same way as traditional Peclet criterion Pe was defined above (7), we define the Peclet criterion for the input zone as

$$Pe^* = \frac{uH}{D_{\mathrm{L}}^*}. \tag{24}$$

It is also useful to introduce the dimensionless ratio

$$w = \frac{D_L^*}{D_L} > 0, \tag{25}$$

which enables the consequent parametric study. The relationship between both the Peclet criteria Pe, Pe^* is clearly

$$Pe^* = \frac{uH}{wD_\mathrm{L}} = \frac{Pe}{w}. \tag{26}$$

The new model is obtained in the dimensionless form if we substitute Pe with Pe^* in the left boundary condition of ACO model. The resulting equations of AGO model are

$$\frac{1}{Pe}\frac{\partial^2 \mathrm{c}(\xi,\theta)}{\partial \xi^2} - \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \xi} = \frac{\partial \mathrm{c}(\xi,\theta)}{\partial \theta}, \tag{27}$$

$$\forall \xi \geqslant 0 : \lim_{\theta \to 0+} \mathrm{c}(\xi,\theta) = 0, \tag{28}$$

$$\mathrm{c}_{\mathrm{in}}(\theta) = \mathrm{c}(0,\theta) - \frac{w}{Pe}\lim_{\xi \to 0+}\frac{\partial \mathrm{c}(\xi,\theta)}{\partial \xi}, \tag{29}$$

$$\forall \theta \geqslant 0 : \lim_{\xi \to +\infty} \mathrm{c}(\xi,\theta) = 0, \tag{30}$$

$$y(\theta) = \mathrm{c}(1,\theta). \tag{31}$$

5. Analytical solution of AGO model

Due to the fact that time is dimensionless, we also have to establish the dimensionless complex variable $q = s\tau$ for Laplace transform. Then the dimensionless Laplace transform can be defined as

$$\mathrm{F}(q) = \mathcal{L}\{\mathrm{f}(\theta)\} = \int_0^{+\infty} \mathrm{f}(\theta)\exp(-q\theta)\mathrm{d}\theta. \tag{32}$$

Applying it, we obtain the model (27, 28, 29, 30, 31) in Laplace domain as

$$q\mathrm{C}(\xi,q) = \frac{1}{Pe}\frac{\partial^2 \mathrm{C}(\xi,q)}{\partial \xi^2} - \frac{\partial \mathrm{C}(\xi,q)}{\partial \xi}, \tag{33}$$

$$\mathrm{C}_{\mathrm{in}}(q) = \mathrm{C}(0,q) - \frac{w}{Pe}\lim_{\xi \to 0+}\frac{\partial \mathrm{C}(\xi,q)}{\partial \xi}, \tag{34}$$

$$\lim_{\xi \to +\infty} \mathrm{C}(\xi, q) = 0, \tag{35}$$

$$\mathrm{Y}(q) = \mathrm{C}(1, q). \tag{36}$$

The general solution of (33) is

$$\mathrm{C}(\xi, q) = \mathrm{A}(q) \exp\left(\frac{Pe}{2}(1-a)\xi\right) + \mathrm{B}(q) \exp\left(\frac{Pe}{2}(1+a)\xi\right), \tag{37}$$

where a is given as (16).

Applying the left and right boundary conditions (34, 35) it is possible to express the unknown functions $A(q)$ and $B(q)$ as

$$\mathrm{A}(q) = \frac{\mathrm{C_{in}}(q)}{1 - \frac{w}{2}(1-a)}, \tag{38}$$

$$\mathrm{B}(q) = 0. \tag{39}$$

The particular solution of AGO model is then

$$\mathrm{C}(\xi, q) = \frac{\mathrm{C_{in}}(q)}{1 - \frac{w}{2}(1-a)} \exp\left(\frac{Pe}{2}(1-a)\xi\right). \tag{40}$$

The aim is to express the dimensionless transfer function of the given system defined as

$$\mathrm{G}(q) = \frac{\mathrm{Y}(q)}{\mathrm{C_{in}}(q)} = \frac{\mathrm{C}(1, q)}{\mathrm{C_{in}}(q)}. \tag{41}$$

The resulting form of AGO transfer function is

$$\mathrm{G}(q) = \frac{1}{1 - \frac{w}{2}(1-a)} \exp\left(\frac{Pe}{2}(1-a)\right), \tag{42}$$

which is a special case of (17).

6. Properties of AGO model

The first aim is to obtain the dimensionless impulse response. The formal way to the result is by Bromwich formula [5, 10]

$$\mathrm{g}(\theta) = \mathcal{L}^{-1}\{\mathrm{G}(q)\} = \frac{1}{2\pi \mathrm{j}} \int_{a-\mathrm{j}\infty}^{a+\mathrm{j}\infty} \mathrm{G}(q) \exp(q\theta) \mathrm{d}q. \tag{43}$$

The dictionary of Laplace transform [3] contains the formula

$$\mathcal{L}^{-1}\left\{\frac{\exp\left(-\sqrt{\alpha}\sqrt{s+A}\right)}{B+\sqrt{s+A}}\right\}= \tag{44}$$
$$=\exp\left(-At\right)\ \left(\frac{A}{\sqrt{\pi t}}\exp\left(-\frac{\alpha}{4t}\right)-B\exp\left(B\sqrt{\alpha}+B^2t\right)\ \mathrm{erfc}\left(\frac{1}{2}\sqrt{\frac{\alpha}{t}}+B\sqrt{t}\right)\right).$$

Applying the Laplace transform grammar [5, 10], we obtain the expression for the dimensionless impulse function

$$\begin{aligned}\mathrm{g}\left(\theta\right)=&\frac{1}{w}\sqrt{\frac{Pe}{\pi\theta}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right)\\&+\frac{Pe(w-2)}{2w^2}\exp\left(\frac{Pe}{w^2}\left(w+\theta-w\theta\right)\right)\mathrm{erfc}\left(v\right)\end{aligned} \tag{45}$$

where

$$v=\sqrt{\frac{Pe}{\theta}}\frac{w+\left(2-w\right)\theta}{2w}. \tag{46}$$

The dimensionless step response is defined [5, 6] as

$$\mathrm{h}(\theta)=\int_0^{\theta}\mathrm{g}(\theta)\mathrm{d}\theta. \tag{47}$$

To integrate such a function is not trivial. Therefore, we use the method of undetermined coefficients [10] combined with intuition based on the responses of traditional ADMs. The following form was assumed

$$\begin{aligned}\mathrm{h}\left(\theta\right)=&A_1\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1-\theta}{2}\right)+A_2\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right)\\&+A_3\exp\left(\frac{Pe}{w^2}\left(w+\theta-w\theta\right)\right)\mathrm{erfc}\left(v\right)\end{aligned} \tag{48}$$

and after determining the unknown coefficients we obtained the resulting dimensionless step response function

$$\begin{aligned}\mathrm{h}\left(\theta\right)=&\frac{1}{2}\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1-\theta}{2}\right)+\frac{\exp\left(Pe\right)}{2\left(1-w\right)}\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right)+\\&+\frac{w-2}{2\left(1-w\right)}\exp\left(\frac{Pe}{w^2}\left(w+\theta-w\theta\right)\right)\mathrm{erfc}\left(v\right)\ .\end{aligned} \tag{49}$$

The next useful characteristics are the dimensionless moments of impulse function $g(\theta)$ which are also used to identify the system. The central dimensionless moment is defined [10] as

$$\mu_k^\theta = \int_0^\infty \left(\theta - M_1^\theta\right)^k g(\theta) \mathrm{d}\theta, \tag{50}$$

where

$$M_1^\theta = \int_0^\infty \theta g(\theta) \mathrm{d}\theta \tag{51}$$

is the first dimensionless raw moment.

The moments can be expressed via the cumulant method [10] which, in this case, is extremely efficient. The relationship between the dimensionless transfer function and the cumulants is expressed by

$$\ln \mathrm{G}(q) = \sum_{n=0}^{\infty} (-1)^n K_n \frac{q^k}{k!}. \tag{52}$$

The dimensionless cumulants can be calculated by the differentiating

$$K_n = (-1)^n \lim_{q \to 0+} \frac{\mathrm{d}^n \ln \mathrm{G}(q)}{\mathrm{d}q^n}. \tag{53}$$

The formulas for cumulants and adequate dimensionless moments were calculated as

$$K_0 = 0 \tag{54}$$

$$K_1 = 1 + w/Pe = M_1^\theta \tag{55}$$

$$K_2 = 2/Pe + w\,(w+2)\,/Pe^2 = \mu_2^\theta \tag{56}$$

$$K_3 = 12/Pe^2 + 2w\left(6 + 3w + w^2\right)/Pe^3 = \mu_3^\theta \tag{57}$$

$$K_4 = 120/Pe^3 + 6w\left(20 + 10w + 4w^2 + w^3\right)/Pe^4 = \mu_4^\theta - 3\left(\mu_2^\theta\right)^2. \tag{58}$$

The way to traditional characteristics - mean residence time, variance, coefficient of variation, skewness and kurtosis - is straightforward.

The dimensionless mean residence time is

$$M_1^\theta = K_1 = 1 + w/Pe. \tag{59}$$

The dimensionless variance (dispersion) is

$$\sigma^2 = K_2 = 2/Pe + w\,(w+2)\,/Pe^2. \tag{60}$$

The coefficient of variation, skewness, and kurtosis are defined as

$$\gamma = \sqrt{K_2}/K_1 \tag{61}$$

$$\gamma_1 = K_3/{K_2}^{3/2} \tag{62}$$

$$\gamma_2 = K_4/{K_2}^2. \tag{63}$$

The next and last useful characteristics of the AGO model is its frequency response. The direct substitution $q = j\omega\tau$ in the dimensionless transfer function (42) does not cause any difficulties. Thus, the way to obtain the Nyquist plot and frequency spectrum is quite clear.

7. Numeric difficulties with AGO model

Nevertheless, all the properties were expressed in explicit forms. There are several circumstances where the numerical difficulties increase. The numerical problems occur for the impulse and step responses if $\theta > 0$; $Pe > 0$; $w > 0$; $v > 0$.

If the value of v (46) is large $(v > 3)$, the value of $\mathrm{erfc}(v)$ approaches zero while the value of multiplying term

$$\exp\left[\frac{Pe}{w^2}\,(w+\theta-w\theta)\right] \tag{64}$$

reaches very high values. Therefore, the round-off error of $\mathrm{erfc}(v)$ is magnified to an unacceptable value. This event can be eliminated using the well-known asymptotic formula [10]

$$\mathrm{erfc}\,(v) \approx \frac{1}{\sqrt{\pi}v}\exp\left(-v^2\right)\sum_{n=0}^{N}(-1)^n\frac{(2n)\,!}{n\,!\,(2v)^{2n}} \tag{65}$$

After substitution the multiplicative term is approximated as

$$\begin{aligned}\exp\left(\frac{Pe}{w^2}\,(w+\theta-w\theta)\right)\mathrm{erfc}\,(v) \approx \\ \approx \frac{1}{\sqrt{\pi}v}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right)\sum_{n=0}^{N}(-1)^n\frac{(2n)\,!}{n\,!\,(2v)^{2n}}\end{aligned} \tag{66}$$

and we obtain the approximate formulas for response functions

$$g(\theta) \approx \frac{1}{w}\sqrt{\frac{Pe}{\pi\theta}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right)\left(1-\frac{(2-w)\,\theta}{w+\theta\,(2-w)}\sum_{n=0}^{N}(-1)^n\frac{(2n)\,!}{n\,!\,(2v)^{2n}}\right) \quad (67)$$

$$\begin{aligned} h(\theta) \approx\; & \frac{1}{2}\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1-\theta}{2}\right)+\frac{\exp(Pe)}{2(1-w)}\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right)+ \\ & +\frac{w-2}{2(1-w)\sqrt{\pi v}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right)\sum_{n=0}^{N}(-1)^n\frac{(2n)\,!}{n\,!\,(2v)^{2n}}\,, \end{aligned} \quad (68)$$

which are valid for $v > 3$ and $N = 3$. These formulas will also be useful in the following parts where several limit cases will be discussed for $v \to \infty$.

8. Five special cases of AGO model

The generalized model has been described above. Now, we will discuss five special cases. There are three main reasons for focusing on them:

- Physical meaning of every individual case.
- Comparison with the traditional models.
- Several special cases of AGO unobtainable via direct substitution in w but approaching them is possible by calculation of limits.

Case 1

In the first case suppressed dispersion in the input part of the pipe-line is considered. Then $D_L^* \to 0+$, which implies that $w \to 0+$. The dimensionless transfer function is obtained via direct evaluation of (42) as

$$\lim_{w\to 0+} G(q) = \exp\left(\frac{Pe}{2}(1-a)\right). \quad (69)$$

The dimensionless impulse response function was obtained by application of l'Hospital rule to (67) as

$$\lim_{w\to 0+} g(\theta) = \frac{1}{2\theta}\sqrt{\frac{Pe}{\pi\theta}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right). \quad (70)$$

The dimensionless step response function was derived from (49) as

$$\lim_{w\to 0+} \mathrm{h}(\theta) = \frac{1}{2}\operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1-\theta}{2}\right) + \frac{\exp(Pe)}{2}\operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right). \tag{71}$$

The resulting formulas correspond with AEO model (17, 18, 21).

Case 2

In the second case the constant coefficient of axial dispersion in the whole pipe-line is considered. Then $D_L^* = D_L$, which implies that $w \to 1$. The dimensionless transfer function is derived from (42) via direct evaluation as

$$\lim_{w\to 1} \mathrm{G}(q) = \frac{2\exp\left(\frac{Pe}{2}(1-a)\right)}{1+a}. \tag{72}$$

The dimensionless impulse response function was also obtained via direct evaluation of (45) as

$$\lim_{w\to 1} \mathrm{g}(\theta) = \sqrt{\frac{Pe}{\pi\theta}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right) - \frac{Pe}{2}\exp(Pe)\operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right). \tag{73}$$

The dimensionless step response function was derived from (68) by application of l'Hospital rule as

$$\begin{aligned}\lim_{w\to 1} \mathrm{h}(\theta) = {}& \sqrt{\frac{Pe\theta}{\pi}}\exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right) + \frac{1}{2}\operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1-\theta}{2}\right) - \\ & -\frac{(1+Pe+Pe\theta)\exp(Pe)}{2}\operatorname{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right).\end{aligned} \tag{74}$$

The resulting formulas correspond with ACO model (17, 19, 22).

Case 3

In the third case the doubled value of the coefficient of axial dispersion in the input part of the pipe-line is considered. Then $D_L^* = 2D_L$, which implies that $w \to 2$. The dimensionless transfer function is derived from (42) via direct evaluation as

$$\lim_{w\to 2} \mathrm{G}(q) = \frac{1}{a}\exp\left(\frac{Pe}{2}(1-a)\right). \tag{75}$$

Both the dimensionless impulse response function and the dimensionless step response function were also obtained via direct evaluation and they produce the following formulas

$$\lim_{w\to 2} \mathrm{g}(\theta) = \frac{1}{2}\sqrt{\frac{Pe}{\pi\theta}} \exp\left(-\frac{Pe}{4\theta}(1-\theta)^2\right) \tag{76}$$

$$\lim_{w\to 2} \mathrm{h}(\theta) = \frac{1}{2}\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1-\theta}{2}\right) - \frac{\exp(Pe)}{2}\mathrm{erfc}\left(\sqrt{\frac{Pe}{\theta}}\frac{1+\theta}{2}\right) \tag{77}$$

The great advantage of AGO model is the fact that the resulting formulas correspond with AOO model (17, 20, 23). The conformity of the external behavior is guaranteed despite the distinct physical formulation of the left boundary condition.

The previous cases have demonstrated the mutual relationships between the traditional models (AEO, ACO, AOO) and AGO model.

Case 4

The coefficient of axial dispersion in the input part should be constant but positive, e.g. $D_L^* = \text{const}$, while dispersion inside the pipe-line is suppressed, e.g. $D_L \to 0+$. This means that $w \to +\infty$, respecting the condition

$$Pe = wPe^*. \tag{78}$$

The following results are easy to express via auxiliary variables

$$a^* = \sqrt{1 + \frac{4q}{wPe^*}} \tag{79}$$

$$v^* = \sqrt{\frac{wPe^*}{\theta}}\frac{w + (2-w)\,\theta}{2w}. \tag{80}$$

The dimensionless transfer response function is expressed via l'Hospital rule as

$$\lim_{\substack{w\to+\infty \\ Pe=wPe^*}} \mathrm{G}(q) = \lim_{w\to+\infty} \frac{\exp\left(\frac{wPe^*}{2}(1-a^*)\right)}{1-\frac{w}{2}(1-a^*)} = \frac{\exp(-q)}{1+\frac{q}{Pe^*}}. \tag{81}$$

The dimensionless impulse response function is defined as

$$\begin{aligned} \lim_{\substack{w\to+\infty \\ Pe=wPe^*}} \mathrm{g}(\theta) = \lim_{w\to+\infty} & \frac{1}{w}\sqrt{\frac{wPe^*}{\pi\theta}} \exp\left(-\frac{wPe^*}{4\theta}(1-\theta)^2\right) + \\ & + \frac{wPe^*(w-2)}{2w^2} \exp\left(\frac{wPe^*}{w^2}(w+\theta-w\theta)\right) \mathrm{erfc}(v^*) \;. \end{aligned} \tag{82}$$

After a formal discussion concerning the dimensionless time, we again use l'Hospital rule and obtain

$$\lim_{\substack{w\to+\infty \\ Pe=wPe^*}} \mathrm{g}(\theta) = \begin{cases} 0 & \text{for } \theta < 1 \\ Pe^* \exp\left(-Pe^*(\theta-1)\right) & \text{for } \theta \geqslant 1 \, . \end{cases} \tag{83}$$

Analogically, the dimensionless step response function is defined as

$$\begin{aligned} \lim_{\substack{w\to+\infty \\ Pe=wPe^*}} \mathrm{h}(\theta) = \lim_{w\to+\infty} & \frac{1}{2}\mathrm{erfc}\left(\sqrt{\frac{wPe^*}{\theta}}\frac{1-\theta}{2}\right) \\ & + \frac{\exp\left(wPe^*\right)}{2\left(1-w\right)}\mathrm{erfc}\left(\sqrt{\frac{wPe^*}{\theta}}\frac{1+\theta}{2}\right) + \\ & + \frac{w-2}{2\left(1-w\right)}\exp\left(\frac{wPe^*}{w^2}\left(w+\theta-w\theta\right)\right)\mathrm{erfc}\left(v^*\right) \, , \end{aligned} \tag{84}$$

which produces the resulting formula

$$\lim_{\substack{w\to+\infty \\ Pe=wPe^*}} \mathrm{h}(\theta) = \begin{cases} 0 & \text{for } \theta < 1 \\ 1-\exp\left(-Pe^*(\theta-1)\right) & \text{for } \theta \geqslant 1 \, . \end{cases} \tag{85}$$

It is easy to see that the fourth case is equivalent to the first order linear lumped-parameter dynamical model with the time-delay. This model will be referred to as ADO (axial degraded closed-opened model) with the dimensionless time-delay equal to 1 and the dimensionless time constant equal to $1/Pe^*$.

Case 5

The last special case does not offer new possibilities but verifies the properties of AGO model. When $D_L \to 0+$ and $w = \text{const} < +\infty$, then $Pe \to +\infty$. This corresponds with the piston flow. The dimensionless transfer function is obtained via l'Hospital rule as

$$\lim_{Pe\to+\infty} \mathrm{G}(q) = \exp\left(-q\right). \tag{86}$$

The previous form corresponds with pure transfer delay. Analogically, it is possible to obtain the dimensionless impulse response function as

$$\lim_{Pe\to+\infty} \mathrm{g}\left(\theta\right) = \delta\left(\theta-1\right) \tag{87}$$

and dimensionless step response function as

$$\lim_{Pe \to +\infty} \mathrm{h}(\theta) = \begin{cases} 0 & \text{for } \theta < 1 \\ 1 & \text{for } \theta \geqslant 1\,. \end{cases} \tag{88}$$

This is nothing more than the zero order linear system with dimensionless time-delay equal to 1.

9. Conclusions

A suitable axial dispersion model was selected out of the references related to axial dispersion flow. The traditional modeling approach starts the fixed left boundary condition which is physically well motivated. The result is then one individual model (e.g. AEO) suitable for one special type of flow. Previous researchers concentrated on expanding the number of models describing the particular flow types. This paper develops the opposite strategy. Therefore, a single generalized semi-opened model (AGO) covering a variety of known models was created and then studied.

The resulting generalized model of axial dispersion flow is designed to have a good physical interpretation. The second useful property of AGO is its analytical solubility, which means that it is possible to obtain explicit forms of transfer function, impulse response, step response, and moments. This given model covers the traditional axial models (AEO, ACO, AOO, and piston flow). Sequential passage from model to model is realized only via changing parameter w. This enables interpolation between model pairs (AEO - ACO; ACO - AOO). The next advantage of the proposed model is the fourth particular case (ADO) which corresponds with AGO model for infinite value of w. A variety of other models can be created via interpolation between AOO and ADO models.

The new AGO model is relatively simple (only one parameter w is added) and analytically soluble but it significantly shifts the border line between the systems which are explicitly soluble and not. The behavior of many real systems is close to ACO model. The new model enables to gently analyze the state in the neighborhood of ACO which is split into AEO or AOO influence domain.

The main effect of AGO model is in the area of parametric identification and optimization. The paper provides a background for an analysis in time and frequency domains. The moment method and impulse, or step response identification are supported in the case of the time domain identification. The transfer function can be directly used to identify system in the frequency domain.

The derived formulas are widely applicable both in industrial and biomedical areas. They were directly used for trickle-bed reactor identification [14] from impulse response via both LSQ and robust estimation methods.

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