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A Simple Method for the Estimation of the Axial Dispersion Coefficient in Gas Flow

M. Wójcik[1†], M. Szukiewicz[1], W. Próchniak[2] and P. Wiercioch[2]

[1] *Faculty of Chemistry, Department of Chemical and Process Engineering, Rzeszow University of Technology, al. Powstancow Warszawy 12, 35-959 Rzeszow, Poland*
[2] *New Chemical Syntheses Institute, Catalyst Department, al. Tysiaclecia Panstwa Polskiego 13a, 24-110 Pulawy, Poland*

†Corresponding Author Email: wojcik.mm@op.pl

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ABSTRACT

A simple method which is suitable for determining with reasonable precision the parameters of gas flow system has been proposed. An inverse boundary-value problem is considered. The model of gas flow with the Danckwert's boundary conditions in a real measurement system has been analyzed and solved. The tracer technique was applied to determine axial dispersion coefficient of gas phase and Pèclet number. These parameters are commonly used to characterize the flow–behavior of fluids. Axial dispersion coefficients were estimated by comparing model solution with recorded TCD signal (an inverse problem as a method for model parameter estimation) employing the Laplace transform technique. The Gaver-Stehfest algorithm for the solution of the mathematical model has been applied. The proposed model of gas show a good agreement with the experimental data. The obtained results show that under operation conditions in the studied system the flow behaviour is neither plug flow nor perfect mixing. The described method is very fast in both experimental and computational part. Simple and errorless derivation of sophisticated model formulas has been possible by application of the Computer Algebra System-type program. The program also simplifies computations. Mathematical manipulations and computations were performed using program Maple®.

Keywords: Laplace transform; Numerical inversion of Laplace transform; Non-ideal flow; Maple®.

NOMENCLATURE

c_0	inlet concentration of tracer	N	number of terms used in numerical approximation
$\bar{c}(L_n, s)$	solution of model for zone in Laplace domain, n=1..3	P	pressure
$c(L_1+L_2+L_3,t)$	outlet concentration of tracer	Pe_n	Pèclet number, n=1…3
$D_{L,n}$	axial dispersion coefficient, n=1..3	R_g	gas constant
$d_{w,n}$	diameter of the zone, n=1..3	s	laplace transform parameter
F_v	volumetric flow rate	T	temperature
$G_n(s)$	transfer function or zone, n=1…3	V_{imp}	volume of impulse of gas
L_n	length of the zone, n=1..3		

1. INTRODUCTION

The Laplace transform is applicable in many disciplines like mathematics, physics, mechanics, process control, chemical engineering and biosciences as it allows understanding the behavior of substances in many cases, e.g. in the heat transport in geothermal reservoirs, tracer transport in oil, groundwater aquifers and in porous media (Van Everdingen and Hurst 1949; Čermáková *et al.*

2006). This technique simplifies obtaining the solution of models described by the one- or more dimensional mass or heat equation. Chrysikopoulos *et al*. (1990) developed an analytical solution for solute transport through porous media for a flux-type inlet boundary condition in a semi-infinite medium. Rezaei *et al*. (2013) presented an analytical solution to the two-dimensional solute transport for an aquifer-aquitard system. Yadav *et al*. (2010) obtained analytical solutions for temporally dependent solute dispersion along a uniform flow in a semi-infinite medium. Van Genuchten and Alves (1982) presented a comprehensive set of analytical solutions for one-dimensional convective-dispersive solute transport equation. The Laplace transform is a powerful tool in solving of many engineering problems. For more complex cases an analytical inversion of problem to the time domain can be difficult or even impossible to obtain, so numerical methods have to be used. There are several methods for numerical inversion of the Laplace transform in literature. There are four main groups: (i) the Fourier series method, which is based on the Poisson summation formula, (ii) the Gaver-Stehfest algorithm, which is based on combinations of Gaver functional, (iii) the Weeks method, which is based on bilinear transformations and Laguerre expansions, (iv) the Talbot method, which is based on deforming the contour in the Bromwich inversion integral (Abate and Valkŏ 2004). According to literature reports, e.g. (Hassanzadeh and Pooladi-Darvish 2007) and authors own experience, different algorithms can be recommended for solution of a specific type of problem, e.g. the Stehfest method - see application: (Kocabas 2011; Wang and Zhan 2015); the Dubner and Abate - see application: (Kocabas 2011); the Crump method - see application: (Chen *et al*. 1996); the Zakian method and the Schapery method - see application: (Hassanzadeh and Pooladi-Darvish 2007); the de Hoog method and the Honig-Hirdes method and the Talbot method and Weeks method - see application: (Wang and Zhan 2015); the method of Juraj and Lumboir - see application: (Ali and Awais 2014); the den Iseger method - see application: (Escobar *et al*. 2014). Thus, application of proper algorithm should be preceded by thorough studies. Wang and Zhan (Wang and Zhan 2015) showed that the de Hoog method, the Talbot method and the Simon method is recommended for radial dispersion problems, whereas the Stehfest method, the Honig-Hirdes method, and the Zakian method is advised for axial dispersion problems. A comprehensive review on methods for numerical inversion of the Laplace transform based on a comparison of fourteen algorithms in terms of numerical accuracy, computational efficiency and simplicity of implementation (more precisely: simplicity to create a reasonably efficient implementation) is presented by Davies and Martin (1979).

The gas and liquid axial dispersion influence productivity of many processes usually making it worse. For this reason dispersion was investigated long time ago both theoretically and experimentally, mainly during flow heterogeneous porous media. One of the most important work reported dispersion models and different types of boundary conditions, Danckwerts (1953). Extensions of Danckwert's ideas were presented by Kreft and Zuber (1978); Van Genuchten and Alves (1982); Van Gelder and Westerterp (1990). An axial dispersion coefficient is used mathematical description of dispersion. It is estimated from theoretical or semi-empirical correlations. Several empirical correlations one can find in Gunn and Pryce (1969); Wen and Fan (1975). Experimentally, dispersion coefficients are evaluated mostly from tracer studies. Recently, most of the works were concerned axial mixing for flow through bed systems (Cho *et al.* 2000; Delgado 2006, Gigola *et al.* 2010; Fallico *et al.* 2012).

The novelty of our method consists in application of transfer function for model building, inverse Laplace transform for model solution and optimization algorithm for determining gas flow parameters. To our best knowledge the presented here method was no presented in literature.

This paper has been planned as follows. In the Section *Apparatus and experiment* the description of the measuring system and experiments is presented. The mathematical model is shown in the Section *Mathematical model*. The solution of model and the procedure for parameters estimation is described in the Section *Results*. Finally, a discussion of the results and conclusions are given in the Section *Conclusions*.

2. Apparatus and Experiment

The studied system is presented in Fig. 1.

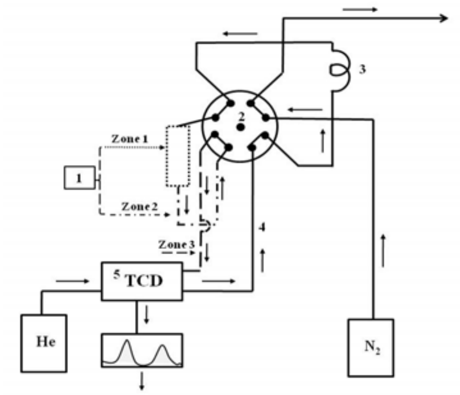

Fig. 1. Simplified schematic representation of apparatus (Micromeritics' AutoChem 2950HP).

The system consists of the following elements:

(1) – a unit called *vessel*, consisting of two steel pipes. The part of larger diameter is usually filled with porous pellets (not in experiment written below)

(2) – the 8-way valve

(3) – the sample loop

(4) – pipes

(5) – the thermal conductivity detector (TCD).

After the preliminary investigations, the unit between the valve (2) and the TCD detector was separated into three zones; they are distinguished on basis of geometry and/or its function. A volume of a fragment between the 8-way valve and *vessel* can be neglected. Geometry of the apparatus was determined on the basis of its technical data and previously made investigations.

- **Zone 1:** *vessel;*
  the length of the zone: $1.7700 \cdot 10^{-1}$m, the diameter of the zone: $7.6500 \cdot 10^{-3}$m
- **Zone 2:** the pipe connecting the *vessel* outlet and the 8-way valve;
  the length of the zone: $2.3500 \cdot 10^{-1}$m, the diameter of the zone: $1.5875 \cdot 10^{-3}$m
- **Zone 3:** the pipe connecting the 8-way valve and the TCD detector;
  the length of the zone: $5.7000 \cdot 10^{-1}$m, the diameter of the zone: $1.5875 \cdot 10^{-3}$m.

The system was flushed for 15-30 minutes with a constant flow of helium until a stable TCD signal was received. At the same time, the volume of sample loop ($2.5000 \cdot 10^{-7}$; $5.0000 \cdot 10^{-7} m^3$) was flushed also with a constant flow of nitrogen. Next, the 8-way valve was opened to allow the flow of helium with the constant volumetric flow rate (of $3.3333 \cdot 10^{-7}$ or $5.0000 \cdot 10^{-7}$ or $6.6667 \cdot 10^{-7}$ $m^3 \cdot s^{-1}$) through the sample loop, the zones and the detector TCD (see Fig. 1). After all the TCD signal was recorded.

The model solution is compared with the recorded TCD signal. If solution of inverse problem fits experimental results very closely, a model is regarded as valid and can be used to estimate the values of coefficients D_L (and next the Pèclet number). Fulfilling the presented objectives is crucial for the model parameters estimation outcomes using the inverse boundary value problem. The correct recognition of the nature of flow and selection of methods of model solution build a necessary step for the planned further research leading to determination of the diffusion coefficient in a porous sorbent.

3. MATHEMATICAL MODEL

The model is based on the following assumptions:

- the system is operated under isothermal conditions: in temperature 313.15 K and at constant pressure $1.0000 \cdot 10^5$ Pa,
- gases satisfy the equation of state of an ideal gas.

Mass balance of nitrogen in each zone can be described by the following system of partial differential equations and the initial and boundary conditions:

Zone 1:

$$\frac{\partial c(x,t)}{dt} = D_{L,1}\frac{\partial^2 c(x,t)}{\partial x^2} - \frac{4F_v}{\pi d_{w,1}^2}\cdot\frac{\partial c(x,t)}{\partial x} \tag{1}$$

$$IC: c(x,0) = 0$$

Danckwerts boundary conditions were used for the closed-closed boundaries as:

$$BC: \frac{4F_v}{\pi d_{w,1}^2}\cdot c_0 = \frac{4F_v}{\pi d_{w,1}^2}\cdot c(0^+,t) - D_{L,1}\left.\frac{\partial c(x,t)}{\partial x}\right|_{x=0^+}$$

$$\left.\frac{\partial c(x,t)}{\partial x}\right|_{x=L_1^-} = 0$$

Zone 2:

$$\frac{\partial c(x,t)}{dt} = D_{L,2}\frac{\partial^2 c(x,t)}{\partial x^2} - \frac{4F_v}{\pi d_{w,2}^2}\cdot\frac{\partial c(x,t)}{\partial x} \tag{2}$$

$$IC: c(x,0) = 0$$

$$BC: c(L_1^+,t) = c(L_1^-,t)$$

$$BC: \left.\frac{\partial c(x,t)}{\partial x}\right|_{x=(L_1+L_2)^+} = 0$$

Zone 3:

$$\frac{\partial c(x,t)}{dt} = D_{L,3}\frac{\partial^2 c(x,t)}{\partial x^2} - \frac{4F_v}{\pi d_{w,3}^2}\cdot\frac{\partial c(x,t)}{\partial x} \tag{3}$$

$$IC: c(x,0) = 0$$

$$BC: c(L_1 + L_2^+,t) = c(L_1 + L_2^-,t)$$

$$BC: \left.\frac{\partial c(x,t)}{\partial x}\right|_{x=(L_1+L_2+L_3)^+} = 0$$

where:

$c(L_1+L_2+L_3,t)$ corresponds to the concentration recorded by the TCD-detector.

We assumed that $D_{L,2} = D_{L,3}$ due the same diameter of pipes.

In this work, we used a rectangular signal pulse (the inlet concentration) which is given by

$$c_0 = \begin{cases} 0 & for \quad t < 0 \\ c_T & for \quad 0 \le t \le \dfrac{V_{imp}}{F_v} \\ 0 & for \quad t > \dfrac{V_{imp}}{F_v} \end{cases}$$

where

$$c_T = \frac{P}{R_g \cdot T \cdot 10^3} = 3.906 \cdot 10^{-2}(\text{kmol} \cdot \text{m}^{-2})$$

4. RESULTS

To obtain the outlet concentration of tracer $c(L_1+L_2+L_3,t)$, a system of partial differential equations Eqs. (1-3) has been solved with appropriate initial and boundary conditions, by applying Laplace transform technique. We obtained the following solution of the model in Laplace domain:

$$\bar{c}(L_1+L_2+L_3,s)=G_1(s)\cdot G_2(s)\cdot G_3(s)\cdot c_0 \quad (4)$$

where

$$G_1(s)=\frac{\bar{c}(L_1,s)}{c_0}=-\frac{8F_v e^{(a+b)L_1}(\pi^2 d_{w,1}^4 D_{L,1}s+F_v^2-2F_v c)}{(2F_v-g)(D_{L,1}\pi^2 d_{w,1}^4 s)e^{(a-b)L_1}+8F_v^2 e^{(a-b)L_1}-4F_v(e^{(a-b)L_1})g} \quad (4a)$$

$$G_2(s)=\frac{\bar{c}(L_1+L_2,s)}{\bar{c}(L_1,s)}=-\frac{2e^{(c+d)(L_1+L_2)}h}{2F_v e^{(c-d)(L_1+L_2)}e^{(d-c)L_1}-h(e^{(c-d)(L_1+L_2)}e^{(d-c)L_1})} \quad (4b)$$

$$G_3(s)=\frac{\bar{c}(L_1+L_2+L_3,s)}{\bar{c}(L_1+L_2,s)}=-\frac{2e^{(e+f)(L_1+L_2+L_3)}h}{2F_v e^{(e-f)(L_1+L_2+L_3)}e^{(f-e)(L_1+L_2)}-i(e^{(e-f)(L_1+L_2+L_3)}e^{(f-e)(L_1+L_2)})} \quad (4c)$$

where

$$a=\frac{2F_v-\sqrt{D_{L,1}\cdot\pi^2\cdot d_{w,1}^4\cdot s+4F_v^2}}{D_{L,1}\cdot\pi\cdot d_{w,1}^2};$$

$$b=\frac{2F_v+\sqrt{D_{L,1}\cdot\pi^2\cdot d_{w,1}^4\cdot s+4F_v^2}}{D_{L,1}\cdot\pi\cdot d_{w,1}^2}$$

$$c=\frac{2F_v-\sqrt{D_{L,2}\cdot\pi^2\cdot d_{w,2}^4\cdot s+4F_v^2}}{D_{L,2}\cdot\pi\cdot d_{w,2}^2};$$

$$d=\frac{2F_v+\sqrt{D_{L,2}\cdot\pi^2\cdot d_{w,2}^4\cdot s+4F_v^2}}{D_{L,2}\cdot\pi\cdot d_{w,2}^2}$$

$$e=\frac{2F_v-\sqrt{D_{L,3}\cdot\pi^2\cdot d_{w,3}^4\cdot s+4F_v^2}}{D_{L,3}\cdot\pi\cdot d_{w,3}^2};$$

$$f=\frac{2F_v+\sqrt{D_{L,3}\cdot\pi^2\cdot d_{w,3}^4\cdot s+4F_v^2}}{D_{L,3}\cdot\pi\cdot d_{w,3}^2}$$

$$g=\sqrt{D_{L,1}\cdot\pi^2\cdot d_{w,1}^4\cdot s+4F_v^2};$$

$$h=\sqrt{D_{L,2}\cdot\pi^2\cdot d_{w,2}^4\cdot s+4F_v^2}$$

$$i=\sqrt{D_{L,3}\cdot\pi^2\cdot d_{w,3}^4\cdot s+4F_v^2}$$

The Gaver-Stehfest numerical algorithm of inverse Laplace transform has been employed to obtain the solution of the model in the real time domain. The algorithm is briefly described at the end of this Section. As was mentioned in the *Introduction* Section this algorithm is recommended for similar mass-transfer processes. Preliminary tests that confirmed the efficiency of this algorithm were presented in Wójcik *et al.* (2015). A proper value of parameter N (number of terms used in the numerical approximation) was determined by trial and error method as it was earlier shown in Wójcik *et al.* (2015). For current calculations N=30 was accepted. The value of model parameter D_L was determined by combination of 'trial and error' procedure and inner optimization procedure (NLP Solve) of the program Maple®.

The results showed that the Gaver-Stehfest algorithm can be applied to solve the considered problem with high accuracy (an average standard deviation is equal to $7.2\cdot10^{-4}$) and quickly (an average time of calculations t=31.4 s). Typical results are presented in Figs. 2 and 3. In all cases, very good fit between numeric and experiment curves has been observed. It confirms that the presented model is correct and can be accepted for further studies. The inverse problem solution enables the determination of the proper value of the axial dispersion coefficient.

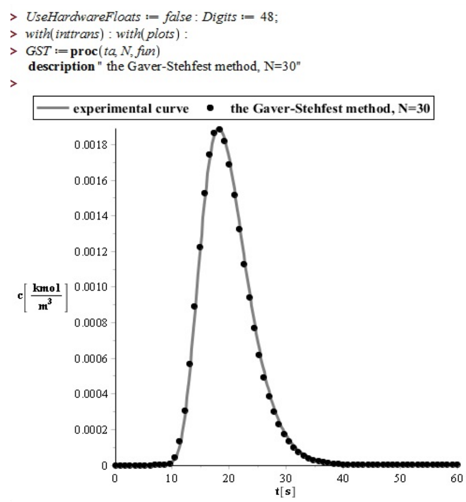

Fig. 2. Numerical (black points) and experimental (solid grey line) gas concentration profiles for the volumetric flow rate $5.0000\cdot10^{-7}$ m³/s and the volume of sample loop $2.5000\cdot10^{-7}$ m³.
Screenshot of program Maple®.

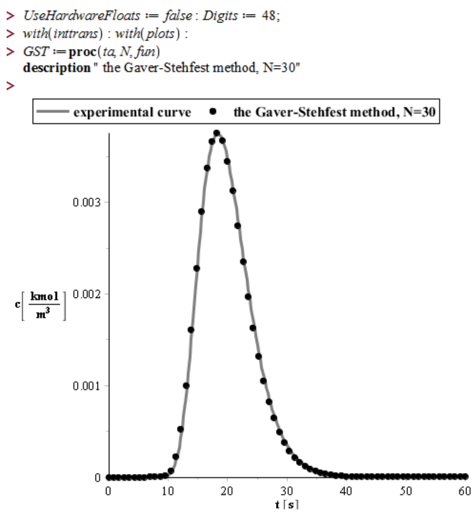

Fig. 3. Numerical (black points) and experimental (solid grey line) gas concentration profiles for the volumetric flow rate 5.0000·10⁻⁷m³/s and the volume of sample loop 5.0000·10⁻⁷m³.
Screenshot of program Maple®.

As the correct value of parameter D_L was accepted the one with the lowest value of the standard deviation (between numerical and experimental results). The appropriate results are presented in Table 1.

Table 1 Values of obtained axial dispersion coefficients and Pèclet numbers.

V_{imp}	F_v	Number of zone	$D_{L,n}$	Pe_n
2.5000·10⁻⁷	3.3333·10⁻⁷	1	6.7000·10⁻⁵	19
		2	7.7700·10⁻⁴	51
		3	7.7700·10⁻⁴	124
	5.0000·10⁻⁷	1	7.2000·10⁻⁵	27
		2	1.7826·10⁻³	33
		3	1.7826·10⁻³	81
	6.6667·10⁻⁷	1	7.4000·10⁻⁵	35
		2	3.1284·10⁻³	25
		3	3.1284·10⁻³	61
5.0000·10⁻⁷	3.3333·10⁻⁷	1	6.6000·10⁻⁵	20
		2	1.2322·10⁻³	22
		3	1.2322·10⁻³	78
	5.0000·10⁻⁷	1	7.2000·10⁻⁵	27
		2	2.6800·10⁻³	22
		3	2.6800·10⁻³	54
	6.6667·10⁻⁷	1	7.5000·10⁻⁵	34
		2	4.9390·10⁻³	16
		3	4.9390·10⁻³	39

The results show that the Laplace transform is very effective technique for solution of the model of gas flow and axial dispersion coefficients can be easily determined in this way. The values of axial dispersion coefficients indicate that the flow is neither plug flow nor perfect mixing under operation conditions applied. The presented model of gas flow is correct and it cannot be simplified.

4.1 Gaver-stehfest Method

In this paper, the Gaver-Stehfest algorithm was selected to solve dispersion model. Presented method is based on combination of Gaver functionals. This algorithm approximates the time domain solution as (Zhang 2007):

$$f(t) = \frac{\ln 2}{t} \sum_{k=1}^{N} V_k \cdot F\left(k \cdot \frac{\ln 2}{t}\right) \quad (5)$$

where V_k is described by the following equation

$$V_k = (-1)^{k+\frac{N}{2}} \sum_{j=\left(\frac{k+1}{2}\right)}^{\min\left(k,\frac{N}{2}\right)} \frac{j^{\frac{N}{2}}(2j)!}{\left(\frac{N}{2}-j\right)!\,j!\,(j-1)!\,(k-j)!\,(2j-k)!} \quad (5a)$$

The parameter N is an even integer. It is the number of terms used in Eq. (1). In practice, N should be chosen by trial and error method. The precision of calculation depends on the parameter N because the inversion is based on a summation of N weighted values. Thus, a suitable choice of value N is important to achieve the most accurate solution. Theoretically, the large value of parameter N determines the more accurate solution but if N is too large the results may be worsened due to round-off errors. Many authors propose a different value of the parameter N to obtain the most accurate solution (Cheng and Sidauruk 1994).

5. Conclusions

On the basis of the performed calculations the following conclusions can be drawn:

I. The numerical solution of the presented model fits experimental results very well indicating the correctness of the model identification
II. The axial dispersion coefficient can be easily determined.
III. The Laplace transform is very effective technique for solution of the model of gas flow. Its advantages are particularly visible for the discussed inverse boundary value problem.
IV. The Gaver-Stehfest algorithm for numerical inversion of Laplace transform, although it was developed in the late 1960s, is fast and precise for the considered problem. Additional advantage is its simplicity.
V. Computer Algebra System Program was very helpful for solution of considered problem both at the stage of model building (fast and errorless conversion of differential equations into Laplace domains and further rearrangement) and on the stage of solution obtaining (built-in procedures simplify development of users' own procedures and optimization).

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