DE GRUYTER OPEN

JACSM 2014, Vol. 6, No. 1, pp. 43 - 53

DOI 10.2478/jacsm-2014-0003

THE APPLICATION OF THE LAPLACE TRANSFORM FOR MODELING OF GAS FLOW USING MAPLE®

Małgorzata Wójcik[1], Mirosław Szukiewicz[1], Paweł Kowalik[2]

[1] Department of Chemical and Process Engineering
Rzeszow University of Technology, Rzeszow, Poland
wojcik.m@aol.com,ichms@prz.edu.pl

[2] Institute of New Chemical Synthesis, Pulawy, Poland
pawel.kowalik@ins.pulawy.pl

Abstract

The Laplace transform is powerful method for solving differential equations. This paper presents the application of Laplace transform to solve the mathematical model of gas flow through the measuring system. The basis of the mathematical model used to describe and simulate the analyzed process is a system of ordinary differential equations. As a result is obtained a single algebraic equation in terms of the complex variable *s*. In order to study the dynamics of the system these equation should be reverted to the time domain by performing an inverse Laplace transform. Calculations were performed in the environment of Maple®. Determining of mixing in a u-shape vessel is aim of presented calculations.

Key words: Laplace transform, mathematical model, differential equations, Maple program

1 Introduction

The Laplace transform is an important integral transform with many applications in mathematics, physics, engineering etc. The Laplace transform is powerful tool of solving computational problems. For example, this method can be used for solution and analysis of time – invariant systems such as electrical circuits, mechanical systems, optical devices and harmonic oscillators. Primarily, this transform is very attractive in solving differential equations and therefore play important role in automatics and control theory.

Mathematical modeling is an important theoretical approach in studying problems. Generally, it involves finding the solutions to the mathematical model constructed to investigate the problem of interest. Usually, a mathematical model consists of a set of differential equations mathematically describing the physical conditions of the problem and a set of boundary and initial conditions appropriately prescribed. Many analytical solutions for various mathematical models of chemical process have been obtained using the Laplace transform technique.

The Laplace transform has been studied by many authors over the years due to the wide array of applications of the Laplace transform technique to different areas of science. There have now been many publications, for example the book written by Widder (1941) [1] about the Laplace transform and inversion formulas, the book written by Jaeger in 1961 [2] describes applied the Laplace transform with engineering applications. A nice review of this transform applied to Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs) is given in Poularikas [3]. There are also articles describing the use of the Laplace transform in chemical engineering, e.g. articles written by Kolev and Linden [4], Ahmed and Batin [5], Ahmed and Kalita [6], Membrez and others [7]. Kolev and Linden [4] used Laplace transform for the solution of partial equations describing the transient mass-transfer in laminar flow systems and heat-transfer in single and multi-stream flow systems. The papers [5] and [6] describe the use of the Laplace transform for analysis the transient convection-radiation magnetohydrodynamic viscous flow in a porous medium and study hydromagnetic flow in chemical reactors. Membrez and others [7] used the Laplace transform technique of find the kinetic parameters for the adsorption of a protein on porous beads. A bibliography of a great many papers are available on the WEB.

In this paper, application of Laplace transform technique for analysis of the process of two gases mixing on the basis of signal given by TCD-type detector is presented. The actual investigation have two main aims. The first one is determination of gas mixing in the continuous flow vessel. And the second one is checking out the hypothesis that the Laplace transform makes easier solution finding and the analysis of the answer of the analytic system.

2 Definition and notation of the Laplace transform

The Laplace transform of a function f(t) is formally defined as

$$\mathcal{L}\{f(t)\} = F(s) = \int_0^\infty f(t)e^{-st}dt \tag{1}$$

where s is a complex variable corresponding to time. In the above formula (1), the function e^{-st} is defined as the kernel of the integral of Laplace. The integral $\int_0^\infty f(t)e^{-st}dt$ is called the Laplace integral of the function *f(t)*. The symbol $\mathcal{L}$ is the Laplace transformation, which generates a new function $F(s) = \mathcal{L}\{f(t)\}$.

Applications of the Laplace transform to the mathematical models simplifies the models by reducing the degree of freedom of the independent variable. The various types of problems that can be treated with the Laplace transform include ordinary and partial differential equations as well as integral equations. A differential equation of the model for a physical system can be subjected to the Laplace transform in order to produce an algebraic form of model in the transform variable s. The solutions for the transformed models in the Laplace domain can be easier obtained. The most difficult step is inverse Laplace transform finding. The Laplace transform method requires usually much less work than classical methods. Computer Algebra Systems (CAS) programs usually operate the method.

3 Model

Presented here investigations are the part of larger research task and it seems to be purposeful to present main problem of the task. Presented in Figure 1 research unit was developed to determine a value of effective diffusion coefficient in a catalyst pellet. The idea of the experiment is new, it has not been described in literature. The procedure of main experiment will be the same as described below, in the point 3.2 with the only difference namely the column will be filled with catalyst pellets. Under experimental conditions two crucial factors will determine a shape of recording signal. They are: (i) effective diffusion coefficient in the catalyst pellets and (ii) mixing in the zones 1, 3 and 4. The proper evaluation of effective diffusion coefficient needs separating of influence of mixing. To determine it were made investigations described below, carrying on without catalyst. It was the main goal of the described experiments. The second aim was finding easy and effective method of the model analysis and solution.

The influence of mixing in the unit can be determined in the following way. Each zone is divided into n cells, a fluent is perfectly mixed in each cell. Cells are placed in series. The more cells in a zone, the flow better approaches plug flow. Matching the model solution for chosen number of the cells with curves obtained as a results of experiments one can determine mixing in the unit. Presented way is very convenient, moreover the number of cells the best fitting experimental results can take into consideration also parameters or factors with no reflection in model equations.

3.1 Measuring system

Scheme of the measuring system is presented in Figure 1.

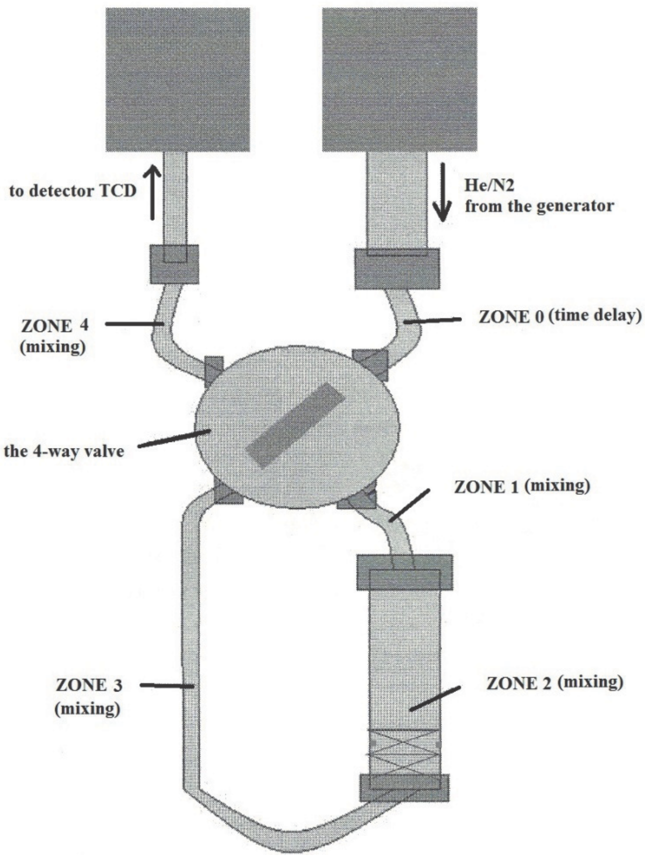

Figure 1. The scheme of the measuring system with u-shape vessel.

The unit consists of the following elements, the 4-way valve, u-shape vessel (empty in the actual investigations), thermal conductivity detector (TCD) and pipes connected the mentioned elements. The system was divided onto five zones; they are distinguished on basis of geometry and/or its the function.

Zone 0: the pipe connected inlet of gas and the 4-way valve;
the length of the zone: 0.75dm, the diameter of the zone: 0.0125dm
Zone 1: the pipe connected the 4-way valve and a column inlet;
the length of the zone: 1.8 dm, the diameter of the zone: 0.0125 dm

Zone 2: empty vessel;
the length of the zone: 1.0 dm, the diameter of the zone: 0.056 dm
Zone 3: the pipe connected a column outlet and the 4-way valve;
the length of the zone: 4.0 dm, the diameter of the zone: 0.0125dm
Zone 4: the pipe connected the 4-way valve and TCD detector;
the length of the zone: 0.75dm, the diameter of the zone: 0.0125dm.

In order to identify the type of mixing, each zone were divided into *n* cells. Number of cells in each zone may be different. One cell in the zone corresponds to the ideal mixing in this zone. Infinite number of cells in the zone corresponds to the plug flow.

3.2 Description of the experiments

The study was conducted as follows. The system was flushed for 10 minutes with a constant flow of helium (flow rate of 0.04 dm^3/min). Then the valve was closed the 4-way valve leading to shut off the flow of the gas through the vessel (Zone 1, 2, 3). For the next 15 minutes the system (beside the vessel) was purged with a nitrogen (flow rate of 0.01dm^3/min) until a stable base TCD signal was reached. After about seven minutes of stabilizing the system again turned over the 4-way valve to allow a constant flow of nitrogen with the volumetric flow rate of 0.01dm^3/min or 0.04 dm^3/min through the vessel. In result ' trapped ' helium was removed and TCD signal was generated and recorded.

3.3 Assumptions of the model

Model describing the process is based on the following assumptions:
- The system is operated under isothermal conditions at constant pressure.
- Gases satisfy the equation of state of an ideal gas.

3.4 Mass balance of the process

Mass balance of the nitrogen in the individual zones and for the number of cells of *n* leads to the following equations:

Zone 0: $c_0(t) = c_{in}(t - t_d)$ (2)

Zone 1: $V_{c1}\frac{dc_{1,1}}{dt} = q(c_0 - c_{1,1}); V_{c1}\frac{dc_{1,k}}{dt} = q(c_{1,k-1} - c_{1,k})$; k=2..n1 (3)

Zone 2: $V_{c2}\frac{dc_{2,1}}{dt} = q(c_{1,n_1} - c_{2,1})$; $V_{c2}\frac{dc_{2,k}}{dt} = q(c_{2,k-1} - c_{2,k})$; k=2..n2 (4)

Zone 3: $V_{c3}\frac{dc_{3,1}}{dt} = q(c_{2,n_2} - c_{3,1})$; $V_{c3}\frac{dc_{3,k}}{dt} = q(c_{3,k-1} - c_{3,k})$; k=2..n3 (5)

Zone 4: $V_{c4}\frac{dc_{4,1}}{dt} = q(c_{3,n_3} - c_{4,1})$; $V_{c4}\frac{dc_{4,k}}{dt} = q(c_{4,k-1} - c_{4,k})$; k=2..n4 (6)

The He/N_2 mixture outlet concentration from the previous cell is the inlet concentration for the next (excluding the first and the last cell in the system). Concentration $c_{4,n4}$ is outlet concentration and is measured by TCD detector. n1, n2, n3 n4 are the numbers of cells in each of zones.
The number of cells in the zones determine the number of equations. Transforming the system of equations into a one equation is difficult and even is not impossible.

For each zone were formulated accordingly initial and boundary conditions:

Zone 1: $c_{1,1}(0) = c_T$; k=1..n1; (7)

Zone 2: $c_{2,1}(0) = c_T$; k=1..n2; (8)

Zone 3: $c_{3,1}(0) = c_T$; k=1..n3; (9)

Zone 4: $c_{4,1}(0) = 0$; k=1..n4; (10)

where:
q - gas flow [dm^3/min]
c_{in} - gas concentration in inlet to zone 0 [mol/dm^3]
V_{ck} - volume of a single cell in *k*-th cell [dm^3]
$c_{j,k}$ - gas concentration in *j*-th zone, in cell *k* [mol/dm^3]
t – time [min]
$c_T = \frac{P}{R_g \cdot T \cdot 10^3}$ = 0.03906 [mol/dm^3]
P – pressure [Pa]
R_g – gas constant [$J \cdot mol^{-1} \cdot K^{-1}$]
T – temperature [K]

And finally inlet concentration is described by

$$c_{in} = \begin{cases} 0 \text{ for } t < 0 \\ c_T \text{ for } t \geq 0 \end{cases} \quad (11)$$

and time delay by

$$t_d = \frac{V_0}{q} \tag{12}$$

where:
V_0 is the volume of zone 0.

3.5 Analysis of the model and its solution

Presented in previous section model is simple, but obtaining a solution can be a little difficult. The variable of interest is $c_{4,n4}$ as measurable concentration. For different values of n1, n2, n3 and n4 the model consist various number of equations. Moreover the values of n1 – n4 have to be determined using trial and error method to obtain the best fit between model solution and experiments. For this reason it is necessary to solve the system repeatedly, the system can contain large number of equations, and finally the number of equations changes for each try. It is very inconvenient situation. One can try to eliminate variables out of interest from the system, but as a result high order differential equation will be obtained and the order of equation will changes for each try. Due to mentioned reasons we paid our attention on well-known tool of analysis and solution of non-stationary models namely Laplace transform. Model transformed into algebraic equations model one can easily solve with respect to variable $c_{4,n4}$, see equation (13)

$$c_{4,n4} = \frac{1}{s} \cdot \left[\left(\frac{q}{n4 \cdot V_{c4} \cdot s + q}\right)^{n4} \left(\frac{q}{n3 \cdot V_{c3} \cdot s + q}\right)^{n3} \left(\frac{q}{n2 \cdot V_{c2} \cdot s + q}\right)^{n2} \left(\frac{q}{n1 \cdot V_{c1} \cdot s + q}\right)^{n1} \cdot c_{in} + \left(\frac{q}{n4 \cdot V_{c4} \cdot s + q}\right)^{n4} \cdot c_{in} \right] \cdot e^{-t_d s} \tag{13}$$

It is noteworthy, that initial conditions and time delay are considered in the equation (13),
where:
s – complex variable (Laplace variable).

It is expected, that Eq. (13) for real conditions will be of high order. In that case a solution will contain many terms and its obtaining would arduous. But currently there exists computer programs, usually called Computer Algebra Systems which can help to obtain model solution. We are use one of this type program, namely Maple®. Maple® operates Laplace transform. Finding the general, valid for any values of n1 .. n4 coefficients, solution was impossible using Maple®. Despite this fact the program was very helpful. Trial and error method calculations were made fast and evaluation of n1..n4 coefficients and thereby evaluation of the mixing did not cause problems. In Figure 2 is presented screenshot with a single calculation by Maple (data introduction are omitted). It is worth paying attention on scary amount of the lines of Maple code. Presented lines concern model equation, its inversion, error calculation and visualization of results. Data input and "answers" of the program was omitted, excluding visualization of the solution. Average time spent for calculation is equal to 0.06s.

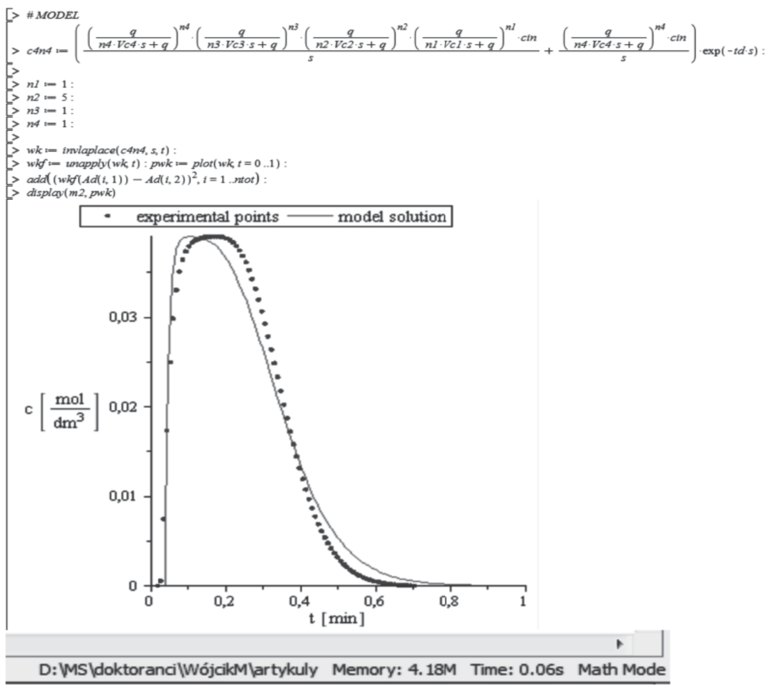

Figure 2. Screenshot of program Maple.

4 Results

On the basis of presented model the following results were obtained. The best fit the smaller gas flow is presented on Figure 3 and for the larger gas flow in Figure 4. the model solution is presented by red solid line while the blue points show the results of experiment. The best fit was determined on the basis of minimal value of sum of squares of differences between calculations and experiments.

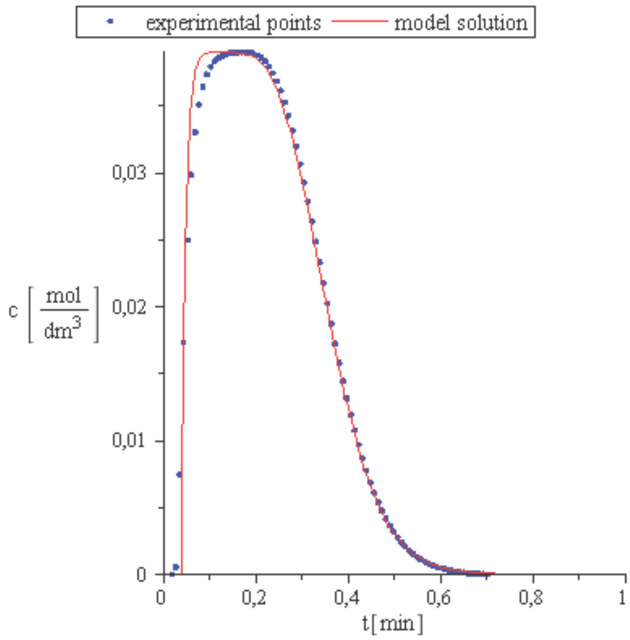

Figure 3. Experimental and theoretical profiles gas concentrations for 0.01dm^3/min and n1=1, n2=12, n3=1, n4=1.

In both cases the obtained fits are very good, differences are small. The best fit for smaller gas flow was obtained for smaller number of cells in the zone 2. This result agrees with the flow theory – the higher velocity of gas the more similar to the plug flow is a real flow. Numbers of cells in zones 1, 3 and 4 are the same and equal to 1. This means that gas in the pipes is perfectly mixed.

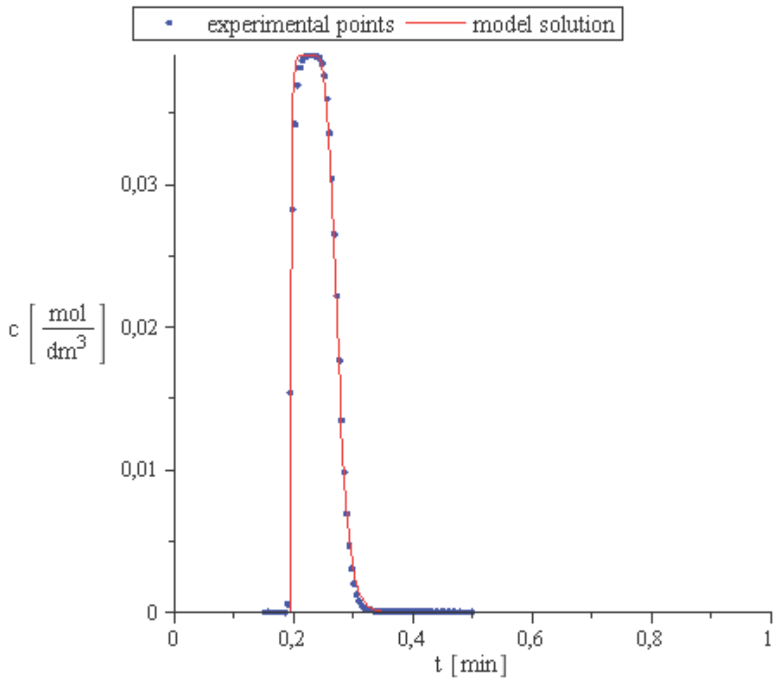

Figure 4. Experimental and theoretical profiles gas concentrations for 0.04dm^3/min and n1=1, n2=40, n3=1, n4=1.

In both cases one can observe similar differences between theoretical and experimental curves. Sloping down part of experimental curve is much better fitted than their sloping up part. In theory sloping up part of the curve is almost vertical in contrast to experimental, especially for the smaller gas flow. It results from the simplicity of the used model which do not consider all theoretically predicted phenomena. In the unit occurs dispersion, phenomenon causing migration of compound from high to low concentration region (analogously to diffusion). As a result of dispersion a slope of a recorded curve is not as sharp as theoretical one. In our opinion precision of the presented model is satisfactory, especially for the higher gas flow. Consideration of dispersion phenomenon in model results in much complicated system of equations, more difficult for solution. Expected in this case improvement of fit is rather not large. Presented result show that further investigations should be conducted for larger values of gas flow, probably larger than used here.

5 Conclusions

Following conclusion can be drawn on the basis presented investigations:
1. The theoretical model fits experimental results very well. It shows that the presented model of the process is correct. The fitting is better for larger gas velocity.
2. Gas in the pipes is perfectly mixed; in the column the flow approaches the plug, especially for larger gas velocity.
3. The main advancement of Laplace transform method application for solving such class of problems is its higher efficiency and convenience of calculations comparing to classical methods.
4. Using of CAS-type program (Maple®) significantly makes calculations simpler and faster.

Appendices

This work was supported by The National Centre for Research and Development (Poland) under a grant PBS1/A1/6/2012.

References

1. Widder D. V., 1946, *The Laplace transform,* Princeton University Press, USA.
2. Jaeger J. C., 1961, *An introduction to the Laplace transformation with engineering applications,* Methuen, London.
3. Poularikas A. D., 1996, *The transforms and applications handbook,* CRC Press, USA.
4. Kolev. S. D., Linden W. E., 1993, *Application of Laplace transforms for the solution of transient mass- and heat- transfer problems in flow systems,* International Journal of Heat and Mass Transfer, vol. 36, pp.135-139
5. Ahmed S., Batin A., 2013, *Convective laminar radiating flow over an accelerated vertical plate embedded in a porous medium with an external magnetic field,* International Journal of Engineering and Technology, vol. 3, pp. 66-72.
6. Ahmed S., Kalita D., 2012, *Laplace technique on magnetohydrodynamic radiating and chemically reacting fluid over an infinite vertical surface,* International Journal of Engineering and Technology, vol. 2, pp. 684-693.
7. Memberez J., Infelta P. P., Renken A., 1996, *Use of the Laplace transform technique for simple kinetic parameters evaluation. Application to the adsorption of a protein on porous beads,* Chemical Engineering Science, vol. 51, pp. 4489-4498.