

## Evaluation of Gas Solid Reactions in Packed Bed Applying Differential Transformation Method

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### Abstract

Differential transformation method (DTM), followed by Laplace transformation, has been used to solve the governing mass balance equations through a packed bed of solid reactants. The principle of this method is briefly introduced and is then applied to the nonlinear mass balance equations. Conversion and dimensionless gas concentration has been achieved and plotted with different values of  $D_z$ . Results show that conversion increases with a high rate initially, and the rate of increasing will decrease dramatically in infinity. All obtained results have been compared with the experimental results, which represent the high accuracy of the presented method. DTM is an efficient analytical technique which is used to solve the nonlinear differential equations, governing the problem in the form of series with easily computable terms.

**Keywords:** Gas solid reactions, packed bed, differential transformation method (DTM), Laplace transform, analytical methods

### Introduction

Non-catalytic gas solid reactions are very important in chemical and metallurgical industries, such as reduction of metal oxides, roasting of sulfides, calcination of limestone, etc. These reactions are processed in packed bed reactors, which are more flexible and efficient, and also have lower costs compared to the other types of reactors because of their low amounts of heat generation and consumption. Due to the transient nature of gas-solid reactions in comparison with catalytic reactions, the complexity of governing mass and energy balance equations are higher. As a result, analytical solutions have not yet been used for solving coupled series of mass and energy balance equations in the bed and in the pellets. Despite using modern computers, solving these equations consumes much time and energy. The models describing gas solid reactions and transport phenomena in packed bed reactors have been grouped in 2 broad categories by Froment and Bischoff [1]. The 2 categories are the pseudo homogeneous model (which ignores the presence of catalyst pellets) and the heterogeneous model (which accounts for the changes occurring inside the pellet). The non-catalytic gas solid reactions in packed beds stand in the second group.

Numerical solution of packed bed equations for non-catalytic gas solid reactions has been followed by numerous researchers. Sampath, Ramachandran and Hughes [2] solved a set of one dimensional coupled mass and energy balance equations in the axial direction using orthogonal collocation, and accounted for the wall heat transfer by introducing the corresponding term into the heat balance equation. Hastaoglu and Jibril [3] proposed an extensive 2 dimensional non-isothermal model, and solved the equations using the finite difference method. Furthermore, the finite volume method, with uniform and

non-uniform mesh size, has frequently been used for the numerical solution of governing equations of mass and energy in gas solid reactions [4-8]. As mentioned before, analytical methods have not yet been applied to solve these equations. Differential transformation method, as an analytical method, was first applied in the engineering domain by Zhou [9]. The DTM obtains an analytical solution in the form of a polynomial. It is different from the traditional higher order Taylor series method. The traditional higher order Taylor series method requires symbolic computation. So, the Taylor series method is computationally expensive for large orders. However, the DTM obtains a polynomial series solution by means of an iterative procedure. The DTM is an alternative procedure for obtaining an analytic Taylor series solution of the differential equations. With this method, it is possible to obtain highly accurate results or exact solutions for differential equations. This method is well addressed in [10-19]. Chiou [20] applied the Taylor transformation to solve non-linear vibration problems. Furthermore, the method may be employed for the solution of both ordinary and partial differential equations. Jang *et al.* [21] applied the 2-dimensional differential transformation method to the solution of partial differential equations. Hassan [22] adopted the differential transformation method to solve some problems. Finally Joneidi *et al.* [23] solved fin efficiency of convective straight fins with temperature-dependent thermal conductivity. Analytical methods were successfully applied to various application problems [24-30]. In the present study, the one dimensional differential transformation method is applied to the Laplace transformed governing equations. The run time and CPU usage of the computer is considerably reduced in comparison with the numerical methods.

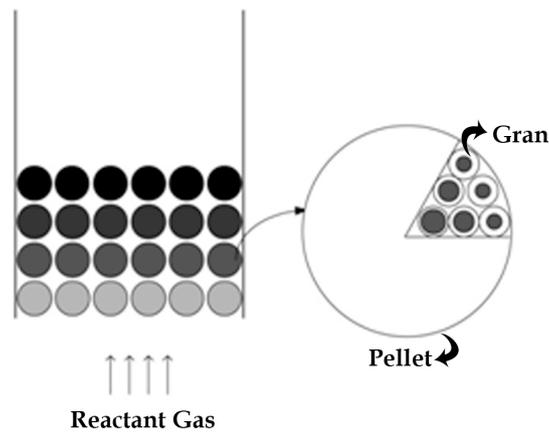
### Description of the problem

A general form of non-catalytic gas solid reaction has been considered as;



where  $A$  and  $B$  are the reacting gas and solid, respectively and,  $a$  and  $b$  are the stoichiometric coefficients.

The products include both the gas and the solid phases. The grain model [8] has been considered to describe what is happening in the pellet. In the grain model, it is assumed that the pellet consists of small particles or grains which are nonporous and react according to the shrinking core model. The reacting gas penetrates through the interstices between the grains and reacts with each grain. If the chemical reaction presents a high resistance to the progress of reaction compared to the diffusion through the pellet, the concentration profile through the pellet will have a smooth shape. The other possibility is that the diffusion through the pellet plays the main role for the resistance to the progress of reaction which results in a steep profile for the concentration through the pellet. In this case, the whole pellet can be divided into 2 separate zones during the reaction time as the reacted and unreacted zones. On the other hand, in a packed bed reactor (a schema of which has been shown in **Figure 1**), the gaseous reactant is charged through the reactor and flows through the interstices formed between the pellets. As is seen in **Figure 1**, each pellet consists of finer particles or grains which react with the gaseous reactant and are converted to the reaction products. The pellets near the reactor inlet, due to their access to higher concentrations of unreacted gas compared to the pellets in higher heights, have higher conversions. Depending on the rate of reaction, rate of diffusion, and flow rate, the concentration profile of reacting gas can take various shapes in the bed and through the pellets.



**Figure 1** Packed bed reactor, pellets and grains.

**Assumptions**

To reduce the complexity of the physical and chemical phenomena of the flow and chemical reaction through the bed and the pellets, the following assumptions have been considered:

- The chemical reaction is irreversible and first order with respect to the gas reactant.
- There is a counter-diffusion flow inside the pellets, so fluxes due to the bulk flow and viscous flow are ignored.
- The pellets and their grains are spherical and their sizes do not change during the course of chemical reaction.
- The isothermal condition is assumed through the whole bed and pellets.
- The gas concentration through the bed changes in an axial direction only.
- There is no diffusion resistance in the product layer formed around each grain.

**Governing equations**

Using the simplifying assumptions considered for the bed and the pellets, the governing equations through the bed and the pellets can be written.

**Mass balance equation in the bed**

The mass balance equation in the bed is written as follows;

$$D_d \frac{\partial^2 C_b}{\partial Z^2} - U_s \frac{\partial C_b}{\partial Z} - k_m a_s (C_b - C_p|_{r=R}) = \frac{\partial C_b}{\partial t} \tag{2}$$

where  $C_b$  is the concentration of the reacting gas through the bed and  $C_p$  is the concentration of the reacting gas through the pellet in the considered axial position,  $U_s$  is the superficial velocity of the reacting gas,  $D_d$  and  $k_m$  are the axial mass dispersion coefficient and the convective mass transfer coefficient, respectively.  $r$  is the radial coordinate through the pellet and  $R$  is the radius of the pellet.  $Z$  and  $t$  are the independent parameters of distance and time coordinates in the bed, respectively, and  $a_s$  is the surface area of the solid per unit volume of the bed which is defined as;

$$a_s = \frac{3(1 - \varepsilon_b)}{R} \quad (3)$$

where  $\varepsilon_b$  is the porosity of the bed. The boundary condition for (2) at the reactor inlet is;

$$D_d \frac{\partial C_b}{\partial Z} = U_s (C_b - C_{in}) \quad \text{at} \quad z = 0 \quad (4)$$

where  $C_{in}$  is the concentration of the gaseous reactant at the reactor inlet. Mass transfer at the reactor inlet has been considered to include convection and dispersion, while, outside of the reactor, convection is the only mechanism of mass transfer. The boundary condition at the end of the bed is as follows;

$$\frac{\partial C_b}{\partial Z} = 0 \quad \text{at} \quad Z = L_b \quad (5)$$

where  $L_b$  is the height of the bed. In (5), it is assumed that there is no change for the concentration of the gaseous reactant out of the bed. The initial condition for (2) throughout the bed is;

$$C_b = 0 \quad \text{at} \quad t = 0 \quad \text{for} \quad 0 \leq Z \leq L_b \quad (6)$$

Defining;

$$\bar{Z} = \frac{Z}{L_b} \quad (7)$$

as the dimensionless axial coordinate and;

$$\bar{C} = \frac{C_b}{C_{in}} \quad (8)$$

as the dimensionless concentration of the reacting gas through the bed, and considering the following dimensionless form for the concentration of the gaseous reactant through the pellet;

$$C = \frac{C_p}{C_{in}} \quad (9)$$

Eq. (2) can be rewritten in a dimensionless form as follows;

$$D_z \frac{\partial^2 \bar{C}}{\partial \bar{Z}^2} - \frac{\partial \bar{C}}{\partial \bar{Z}} - \alpha(\bar{C} - C|_{\zeta=1}) = \frac{\partial \bar{C}}{\partial \tau} \quad (10)$$

where  $D_z$  is the axial dispersion coefficient.  $D_z$ ,  $\tau$  and  $\alpha$  are defined as;

$$D_z = \frac{D_d U_s}{L_b} \quad (11)$$

$$\tau = \frac{U_s t}{L_b} \quad (12)$$

$$\alpha = \frac{a_s k_m L_b}{U_s} \quad (13)$$

Eqs. (4), (5) and (6) can be rewritten in dimensionless forms as follows;

$$D_z \frac{\partial \bar{C}}{\partial \bar{Z}} = (\bar{C} - 1) \quad \text{at} \quad \bar{Z} = 0 \quad (14)$$

$$\frac{\partial \bar{C}}{\partial \bar{Z}} = 0 \quad \text{at} \quad \bar{Z} = 1 \quad (15)$$

$$\bar{C} = 0 \quad \text{at} \quad \tau = 0 \quad \text{for} \quad 0 \leq \bar{Z} \leq 1 \quad (16)$$

#### Mass balance equation in the pellet

The mass balance equation for the pellet is written as follows;

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D_e \frac{\partial C_p}{\partial r} \right) - \frac{3k_r (1 - \varepsilon_p)}{r_g} \left( \frac{r_c}{r_g} \right)^2 C_p = \varepsilon_p \frac{\partial C_p}{\partial t} \quad (17)$$

where  $\varepsilon_p$  is the porosity of the pellet, and  $r_g$  and  $r_c$  are the radius of the grains and the radius of the reaction front through each grain, respectively.  $k_r$  is the chemical reaction rate coefficient and  $D_e$  is the effective diffusivity of the gaseous reactant through the pellet. The boundary condition for (17) at the pellet surface is;

$$D_e \frac{\partial C_p}{\partial r} = k_m (C_b - C_p) \Big|_{r=R} \quad \text{at} \quad r = R \quad (18)$$

where the mass transfer of the gaseous reactant from the bulk flow to the surface of the pellet is considered to be equal to the diffusion of gaseous reactant through the pellet on its surface. The boundary condition in the center of the pellet is;

$$\frac{\partial C_p}{\partial r} = 0 \quad \text{at} \quad r = 0 \quad (19)$$

where it is assumed that, due to the symmetry of the pellet, there is no concentration gradient for the gaseous reactant in the center of the pellet. The initial condition for the concentration of the gaseous reactant throughout the pellet is;

$$C_p = 0 \quad \text{at} \quad t = 0 \quad \text{for} \quad 0 \leq r \leq R \quad (20)$$

The local rate of reaction through the pellet is;

$$\rho_s \frac{\partial r_c}{\partial t} = -bk_r C_p \quad (21)$$

where  $\rho_s$  is the molar density of the solid reactant. The initial condition for (21) is;

$$r_c = 1 \quad \text{at} \quad t = 0 \quad \text{for} \quad 0 \leq r \leq R \quad (22)$$

Defining;

$$\zeta = \frac{r}{R} \quad (23)$$

as the dimensionless time, (17) can be rewritten in a dimensionless form as follows;

$$\frac{1}{\zeta^2} \frac{\partial}{\partial \zeta} \left( \zeta^2 \frac{\partial C}{\partial \zeta} \right) - \phi^2 \rho^2 C = N \frac{\partial C}{\partial \tau} \quad (24)$$

where  $N$  is a constant which matches the dimensionless time for (33) and (25).  $\phi$  is the Thiele modulus for the non-catalytic gas solid reaction through the pellet. These are defined as follows;

$$\phi = r_p \sqrt{\frac{3k_r (1 - \varepsilon_p)}{D_e r_g}} \quad (25)$$

$$N = \frac{\varepsilon_p R^2 U_s}{D_e L_b} \quad (26)$$

The dimensionless form of (18) is;

$$\frac{\partial C}{\partial \zeta} = Nsh^* (\bar{C} - C) \Big|_{\zeta=1} \quad \text{at} \quad \zeta = 1 \quad (27)$$

where  $Nsh^*$  is the modified Sherwood number which is defined as follows;

$$Nsh^* = \frac{k_m R}{D_e} \quad (28)$$

The dimensionless forms of (19) and (20) are;

$$\frac{\partial C}{\partial \zeta} = 0 \quad \text{at} \quad \zeta = 0 \quad (29)$$

$$C = 0 \quad \text{at} \quad \tau = 0 \quad \text{for} \quad 0 \leq \zeta \leq 1 \quad (30)$$

Defining;

$$\rho = \frac{r_c}{r_g} \tag{31}$$

as the dimensionless reaction front radius, (21) can be written in a dimensionless form as;

$$\frac{\partial \rho}{\partial \tau} = -N^* \cdot C \tag{32}$$

where  $N^*$  is defined as follows;

$$N^* = \frac{C_{in} b k_r L_b}{r_g \rho_s U_s} \tag{33}$$

and its initial condition in a dimensionless form is;

$$\rho = 1 \quad \text{at} \quad \tau = 0 \quad \text{for} \quad 0 \leq \zeta \leq 1 \tag{34}$$

#### Fundamentals of differential transformation method (DTM)

We suppose  $x(t)$  to be analytic function in a domain  $D$  and  $t = t_i$  represents any point in  $D$ . The function  $x(t)$  is then represented by one power series whose center is located at  $t_i$ . The Taylor series expansion function of  $x(t)$  is of the form [31-33];

$$x(t) = \sum_{k=0}^{\infty} \frac{(t-t_i)^k}{k!} \left[ \frac{d^k x(t)}{dt^k} \right]_{t=t_i} \quad \forall t \in D \tag{35}$$

The particular case of Eq. (35) when  $t_i = 0$  is referred to as the Maclaurin series of  $x(t)$  and is expressed as;

$$x(t) = \sum_{k=0}^{\infty} \frac{t^k}{k!} \left[ \frac{d^k x(t)}{dt^k} \right]_{t=0} \quad \forall t \in D \tag{36}$$

As explained in [13] the differential transformation of the function  $x(t)$  is defined as follows;

$$X(k) = \sum_{k=0}^{\infty} \frac{H^k}{k!} \left[ \frac{d^k x(t)}{dt^k} \right]_{t=0} \tag{37}$$

where  $x(t)$  is the original function and  $X(k)$  is the transformed function. The differential spectrum of  $X(k)$  is confined within the interval  $t \in [0, H]$ , where  $H$  is a constant. The differential inverse transform of  $X(k)$  is defined as follows;

$$x(t) = \sum_{k=0}^{\infty} \left(\frac{t}{H}\right)^k X(k) \tag{38}$$

It is clear that the concept of differential transformation is based upon the Taylor series expansion. The values of function  $X(k)$  at values of argument  $k$  are referred to as Discrete, i.e.  $X(0)$  is known as the zero discrete,  $X(1)$  as the first discrete, etc. The more discrete available, the more precisely it is possible to restore the unknown function. The function  $x(t)$  consists of the  $T$ -function  $X(k)$ , and its value is given by the sum of the  $T$ -function with  $\left(\frac{t}{H}\right)^k$  as its coefficient. In real applications with the right choice of constant  $H$ , the larger values of argument  $k$  lead to the rapid reduction in the discrete number. The function  $x(t)$  is expressed by a finite series, and Eq. (38) can be written as;

$$x(t) = \sum_{k=0}^n \left(\frac{t}{H}\right)^k X(k) \tag{39}$$

Mathematical operations performed by differential transformation method are listed in **Table 1**.

**Application of the coupled Laplace and differential transformation methods**

Considering that Eqs. (10), (25) and (33) are partial differential equations, we try to convert them to ordinary differential equations using Laplace transformation. Eq. (10) is linear, whereas Eq. (25) is nonlinear due to existence of the term  $\rho^2$ . Therefore, Laplace transformation cannot be applied to Eq. (25) in its present form. Rectifying this problem, here, it is assumed that  $\rho = 1$ . Considering this assumption, Eq. (33) will be omitted and we can apply Laplace transform to the Eqs. (10) and (25) as follows;

$$D_z \frac{d^2 \bar{C}(\bar{Z}, S)}{d\bar{Z}^2} - \frac{d\bar{C}(\bar{Z}, S)}{d\bar{Z}} - \alpha \left( \bar{C}(\bar{Z}, S) - C(\zeta, S) \Big|_{\zeta=1} \right) = S\bar{C}(\bar{Z}, S) - \underbrace{\bar{C}(\bar{Z}, 0)}_{=0, \text{ initial cond.}} \tag{40}$$

$$D_z \frac{d\bar{C}(\bar{Z}, S)}{d\bar{Z}} = \bar{C}(\bar{Z}, S) - \frac{1}{S} \quad \text{at} \quad \bar{Z} = 0 \tag{41}$$

$$\frac{d\bar{C}(\bar{Z}, S)}{d\bar{Z}} = 0 \quad \text{at} \quad \bar{Z} = 1 \tag{42}$$

And Eq. (25) will convert as follows;

$$\frac{1}{\zeta^2} \frac{d}{d\zeta} \left( \zeta^2 \frac{dC(\zeta, S)}{d\zeta} \right) - \phi^2 C(\zeta, S) = N \left( SC(\zeta, S) - \underbrace{C(\zeta, 0)}_{=0, \text{ initial cond.}} \right) \tag{43}$$

$$\frac{dC(\zeta, S)}{d\zeta} = Nsh^* (\bar{C}(\bar{Z}, S) - C(\zeta, S)) \quad \text{at} \quad \zeta = 1 \tag{44}$$

$$\frac{dC(\zeta, S)}{d\zeta} = 0 \quad \text{at} \quad \zeta = 0 \tag{45}$$

Considering differential transformation method,  $\bar{C}(\bar{Z}, S)$  and  $C(\zeta, S)$  are assumed as follows;

$$\bar{C}(\bar{Z}, S) = \sum_{k=0}^n \bar{c}_k(S) \cdot \bar{Z}^k \tag{46}$$

$$C(\zeta, S) = \sum_{k=0}^n c_k(S) \cdot \zeta^k \tag{47}$$

Substituting Eq. (46) into Eqs. (40), (47) into Eq. (43), considering the boundary conditions and assuming  $n = 2$ , the initial results for  $\bar{c}_k(S)$  and  $c_k(S)$  will be as follows;

$$\begin{aligned} \bar{c}_0(s) = & (3.333333333(2.29560242510^{30} + 2.52087535310^{28} s \\ & + 1.04544888710^{25} s^2 - 1.00803745910^{32} z \\ & - 1.10690542710^{30} z s + 5.04018729510^{31} z^2 \\ & + 5.53452713610^{29} z^2 s + 2.29256721310^{26} z^2 s^2 \\ & - 4.58513442510^{26} z s^2)) / ((9.96880775610^{20} \\ & + 2.03771528210^{19} s + 8.61056910510^{15} s^2 \\ & - 4.36011606610^{22} z - 1.87990511510^{19} z s \\ & + 2.18005806010^{22} z^2 + 9.39952837410^{18} z^2 s \\ & + 1.15615320710^9 z^2 s^2) s (7.70650325010^9 \\ & + 8.130081310^7 s)) \end{aligned} \tag{48}$$

$$\begin{aligned} \bar{c}_1(s) = & -(16.26000000(9.13705574710^{28} + 4.62163900510^{29} s \\ & + 5.06456452010^{27} s^2 - 1.06007639810^{23} z \\ & - 6.53666372710^{21} z s + 6.27956646110^{24} z^2 \\ & + 1.31646514910^{23} z^2 s + 7.09383685210^{20} z^2 s^2 \\ & - 1.81076491210^{18} z s^2 + 2.10013880610^{24} s^3 \\ & + 2.81988587010^{17} z^2 s^3)) / ((9.96880775610^{20} \\ & + 2.03771528210^{19} s + 8.61056910510^{15} s^2 \\ & - 4.36011606610^{22} z - 1.87990511510^{19} z s \\ & + 2.18005806010^{22} z^2 + 9.39952837410^{18} z^2 s \\ & + 1.15615320710^9 z^2 s^2) s (7.70650325010^9 \\ & + 8.130081310^7 s)) \end{aligned} \tag{49}$$

$$\bar{c}_2(s) = - (1.0000000010^{-8} (-9.99419037810^{33} z - 3.75739246310^{38} s - 6.51002382110^{31} z^2 - 4.11749092910^{36} s^2 - 2.06179981010^{32} z s - 1.28147228410^{30} z^2 s - 1.70741283910^{33} s^3 - 3.50550317910^{26} z^2 s^2 - 7.42840336610^{37} - 1.15128461910^{30} z s^2 - 4.58513442510^{26} z s^3 + 5.38692997610^{16} z^2 s^3)) / ((9.96880775610^{20} + 2.03771528210^{19} s + 8.61056910510^{15} s^2 - 4.36011606610^{22} z - 1.87990511510^{19} z s + 2.18005806010^{22} z^2 + 9.39952837410^{18} z^2 s + 1.15615320710^9 z^2 s^2) s (7.70650325010^9 + 8.130081310^7 s)) \tag{50}$$

$$c_0(s) = (1.77000000010^7 (-5.35509219510^{19} z - 1.18975609710^{18} z s + 1.21414609710^{18} + 2.67754606110^{19} z^2 + 5.94878045110^{17} z^2 s)) / (s (9.96880775610^{25} + 2.03771528210^{24} s + 8.61056910510^{20} s^2 - 4.36011606610^{27} z - 1.87990511510^{24} z s + 2.18005806010^{27} z^2 + 9.39952837410^{23} z^2 s + 1.15615320710^{14} z^2 s^2)) \tag{51}$$

$$c_1(s) = 0 \tag{52}$$

$$c_2(s) = (2.95000000010^6 (21.6 + 0.0119s) (-5.35509219510^{19} z - 1.18975609710^{18} z s + 1.21414609710^{18} + 2.67754606110^{19} z^2 + 5.94878045110^{17} z^2 s)) / (s (9.96880775610^{25} + 2.03771528210^{24} s + 8.61056910510^{20} s^2 - 4.36011606610^{27} z - 1.87990511510^{24} z s + 2.18005806010^{27} z^2 + 9.39952837410^{23} z^2 s + 1.15615320710^{14} z^2 s^2)) \tag{53}$$

Regarding to the definition of the differential transformation method,  $\bar{c}_k(S)$  terms should not be functions of  $z$ ; therefore, with respect to the obtained results for  $C_k(S)$  terms, Differential transformation has been applied to Eq. (40) for the second test. The new results have been achieved as follows;

$$\bar{c}_{0,N}(s) = (3.333333333(4.59120485110^{23} + 5.04175070610^{21} s + 2.09089777410^{18} s^2)) / (s (1.99376155110^{14} + 4.07543056410^{12} s + 1.72211382110^9 s^2) (7.70650325010^9 + 8.13008130010^7 s)) \tag{54}$$

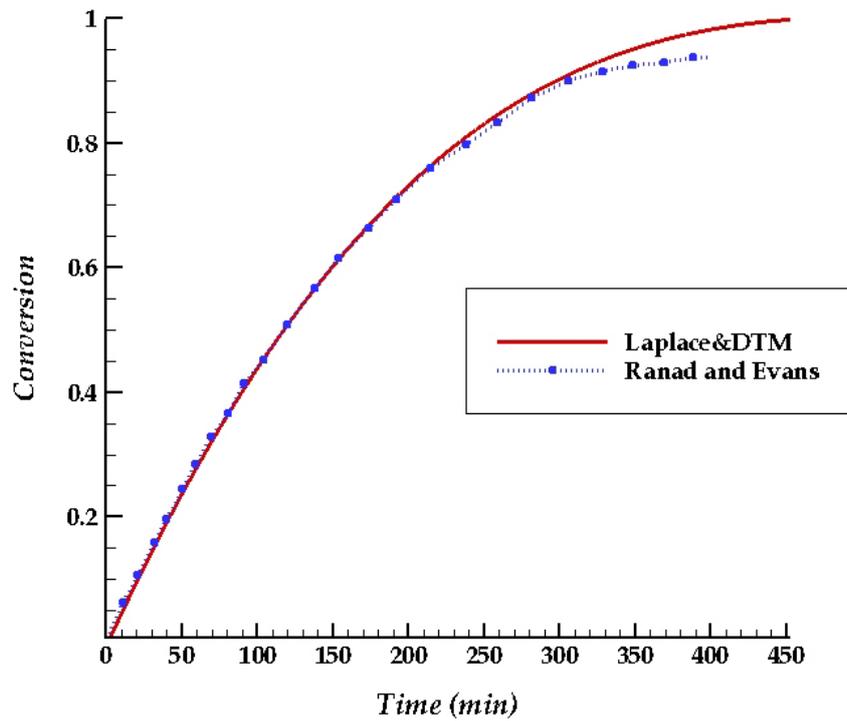
$$\bar{c}_{1,N}(s) = (162.6000000(4.59120485110^{23} + 5.04175070610^{21} s + 2.09089777410^{18} s^2)) / (s (1.99376155110^{14} + 4.07543056410^{12} s + 1.72211382110^9 s^2) (7.70650325010^9 + 8.13008130010^7 s)) \quad (55)$$

$$\begin{aligned} \bar{c}_{2,N}(s) = & (7625.203249(4.59120485110^{23} + 5.04175070610^{21} s + 2.09089777410^{18} s^2)) / (s (1.99376155110^{14} + 4.07543056410^{12} s + 1.72211382110^9 s^2) (7.70650325010^9 + 8.13008130010^7 s)) - \frac{1189.756097}{s} \\ & - (5489.024390(3.95423100910^{13} + 1.70490394910^{10} s)) / (s (1.99376155110^{14} + 4.07543056410^{12} s + 1.72211382110^9 s^2)) \\ & + (81.30081299(4.59120485110^{23} + 5.04175070610^{21} s + 2.09 + 1.72211382110^9 s^2) (7.70650325010^9 + 8.13008130010^7 s)) \end{aligned} \quad (56)$$

At this step,  $\bar{C}_1(\bar{Z}, \tau)$ , regarding to the new results, and  $C_1(\zeta, \tau)$  have been achieved after applying Laplace inversion. Substituting  $C_1(\zeta, \tau)$  into Eq. (32), and considering Eqs. (33) and (34),  $\rho_1(\zeta, \tau)$  has been obtained. The obtained results can be seen in **Figure 2**. **Figure 2** shows the conversion with respect to the time variation, where conversion is defined as follows;

$$conversion = 1 - \rho^3 \quad (57)$$

It can be observed from the second figure that the achieved results for conversion are very close to the results represented by Ranade and Evans [34]. **Table 1** shows error of the obtained conversion in comparison with Ranade and Evans' results. It is obvious from both **Figure 2** and **Table 1** that the present work is considerably accurate.

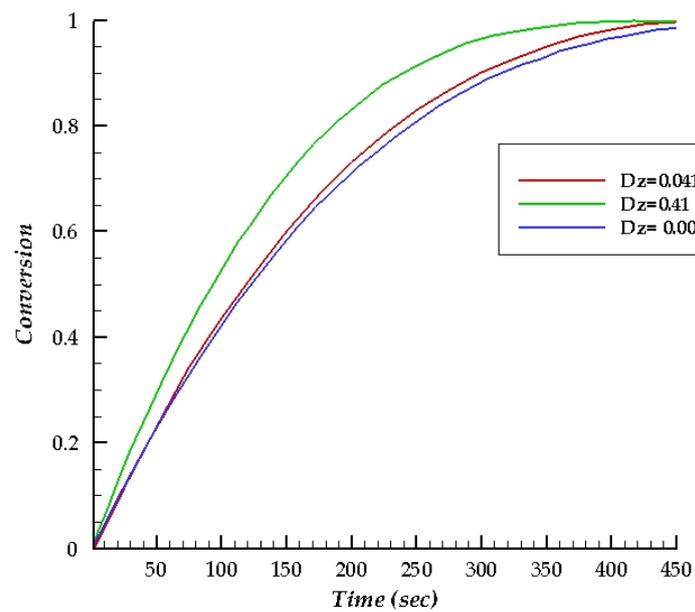


**Figure 2** Diagram of conversion versus time.

In order to be more accurate, this procedure should be continued, meaning that obtained  $C_1(\zeta, \tau)$  and  $\rho_1(\zeta, \tau)$  have to be used in the Eqs. (10) and (24), respectively, to obtain  $\bar{C}_2(\bar{Z}, \tau)$ ,  $C_2(\zeta, \tau)$  and  $\rho_2(\zeta, \tau)$ . As the obtained results represented in **Table 1** show a very good convergence, we stop at this step. **Figures 3, 4** and **5** represent Conversion,  $\bar{C}_2(\bar{Z}, \tau)$  and  $C_1(\zeta, \tau)$  for different values of  $D_z$ , respectively.

**Table 1** Error of present work in comparison with Ranade and Evans' results [34].

Time	Ranade's results	Present work	Error, %
0	0.0021097046	0.0021097046	0.00
25	0.1244725738	0.1160337553	6.78
50	0.2447257384	0.2320675105	5.17
75	0.3459915612	0.3417721519	1.22
100	0.4388185654	0.4345991561	0.96
125	0.5253164557	0.5210970464	0.80
150	0.6054852321	0.6012658228	0.70
175	0.6687763713	0.6708860759	0.32
200	0.7278481013	0.7320675105	0.58
225	0.7742616034	0.7827004219	1.09
250	0.8164556962	0.8291139241	1.55
275	0.8607594937	0.8670886076	0.74
300	0.8924050633	0.9008438819	0.95
325	0.9135021097	0.9282700422	1.62
350	0.9261603376	0.9514767932	2.73
375	0.9324894515	0.9704641350	4.07
400	0.9388185654	0.9831223629	4.72



**Figure 3** Conversion with respect to different values of  $D_z$ .

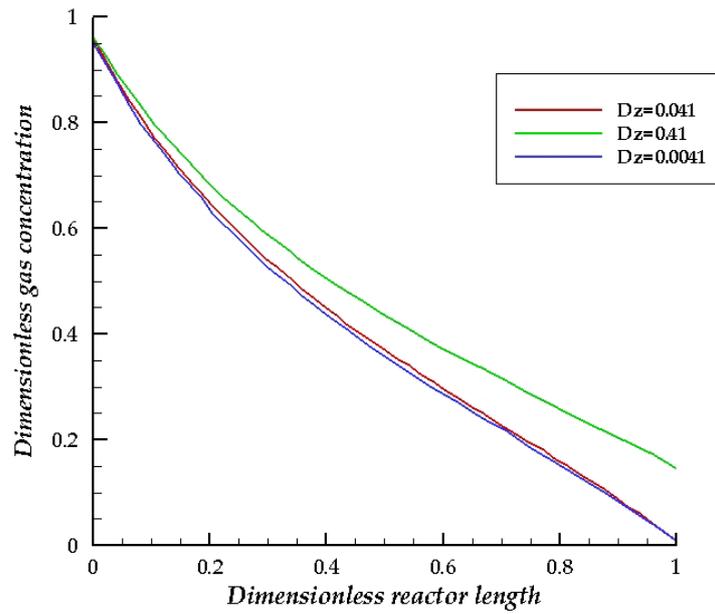


Figure 4  $\bar{C}_2(\bar{Z}, \tau)$  achieved in the present work for different values of  $D_z$ .

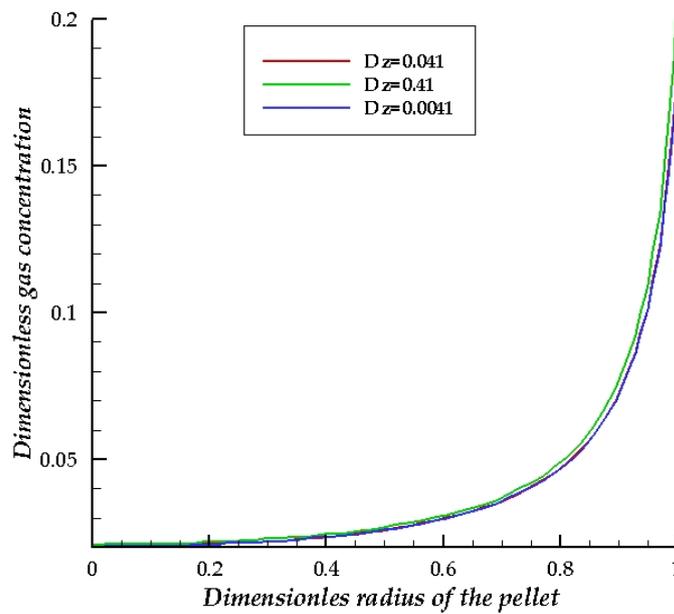


Figure 5  $C_1(\zeta, \tau)$  achieved in the present work for different values of  $D_z$ .

## Conclusions

The differential transformation method, coupled with the Laplace transformation, is successfully applied to the governing mass balance equations through the packed bed of solid reactants. A symbolic calculation software package, MATLAB, is used for all calculations. All the computations show that the approximate solutions are perfectly identical to the solutions presented in the previous relevant literatures. Also, the work emphasizes our belief that this method is a reliable technique to handle these types of problems. It provides solutions in terms of convergent series with easily computable components in a direct way. This method saves time and energy, in comparison to numerical works, to a great extent.

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