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ANALYTICAL SOLUTION OF THE CONCENTRATION OF SPECIES USING MODIFIED ADOMIAN DECOMPOSITION METHOD

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ABSTRACT

A mathematical model of bioreduction of acetophenone in an up-flow packed bed reactor is discussed. In this paper an approximate analytical method (Modified Adomian decomposition method) is used to solve the non-linear differential equations for a spherical catalyst. A single catalyst pellet of radius R can be treated as a porous medium through which reactants diffuses. A simple and closed-form of analytical expressions pertaining to substrate concentration and effectiveness factor are presented for all values of diffusion parameters. These analytical results are compared with numerical results and they are found to be in good agreement.

Keywords*: Chemical and biological systems, Modified Adomian decomposition method, Nonlinear reaction diffusion equation.*

1. INTRODUCTION

The reaction rate in a porous catalyst is affected by intraparticle mass and heat transfer in addition to the intrinsic kinetics. Except for an isothermal first-order reaction and a zero-order reaction, the balance equations are non-linear and are usually solved numerically to calculate the effectiveness factor. Since the numerical solution of the problem is regarded as tedious and time consuming, approximation of the effectiveness factor has been extensively investigated in the past and various simple approximate formulae are available in textbooks (for example, [1-5]).

The usual numerical methods for the boundary-value problem are the finite-difference methods, the shooting methods [6] and the orthogonal collocation methods [7]. When the problem is non-linear, the methods become necessarily iterative ones, finding an improved solution based on the results of the previous iterations with a prospect that the iterative procedure will lead to the desired solution. The finite-difference method converts the boundary-value problem to a system of non-linear algebraic equations, the solution of which can be very difficult to obtain, especially when many base points are used in the method. The collocation methods are efficient when successful, but they are often unstable when many collocation points are used and the Thiele modulus is large [8]. The shooting methods convert the boundary-value problem into an initial-value problem, in which the missing boundary condition at the initial point is assumed. Through an iterative procedure, the methods try to produce a solution that agrees with all the given boundary conditions [9].

An interval method [10], continuation method [11], a branch and bound algorithm [12], simulated annealing [13], genetic algorithms [14], a terrain-following method [15, 16] are also used to solve the non-linear equations. Currently, both trial-and-error shooting method [17, 18] and a direct method that combines numerical integration and interval analysis [19] are available to find all solutions. Angelo Lucia [20] and co-workers present the two different collocation methods for the classical reaction –transport problems in spherical catalyst pellet. However, to the best of our knowledge, there was no rigorous solution for the concentration of reactant A at the surface of catalyst has been reported. The purpose of this communication is to derive simple analytical expression for concentration and effectiveness factor for all possible values of reaction/diffusion parameters γ, β and ϕ.

2. REACTION AND DIFFUSION IN CATALYST PELLETS

Many industrial reactors involve heterogeneous reaction kinetics of packed catalytic pellets in fixed-bed reactors, as illustrated in equation (1). A single catalyst pellet of radius *R* can be treated as a porous medium through which reactants diffuse while reactions occur simultaneously.

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$$A \xrightarrow[\nabla H]{catalyst} B \tag{1}$$

The species and energy balances for diffusive transport inside the pellet can be written as follows [21]:

$$D_{\varepsilon z}\nabla^2 C_A + r_A = 0 \tag{2}$$

$$K_{\varepsilon z}\nabla^2 T + r_A \Delta H = 0 \tag{3}$$

Equation (2) is represent species balance and equation (3) is represent the heat balance. Where Arrhenius reactions rate is $r_A = -k_{ref}\exp\left[\frac{-E}{R_g T_{ref}}\left(\frac{T_{ref}}{T_s}-1\right)\right]C_{A,s}$ (4)

The boundary conditions are

$$C_A\big|_{r=R} = C_{A,s} \tag{5}$$

$$T\big|_{r=R} = T_s \tag{6}$$

$$\nabla C_A\big|_{r=0} = \nabla T\big|_{r=0} = 0 \tag{7}$$

At the surface, concentration and temperature can be given by a Dirichlet boundary condition such as that in equations (5) and (6). Because of symmetry, the mass and energy flux at the center of the catalyst pellet is zero, as shown in equation (7). The system described by equations (2)-(7) represents the nonlinear PDE system for coupled heat and mass transfer in a spherical non-isothermal catalyst pellet. After inserting the temperature profile into the species balance, equations (2)-(7) can be written in terms of the dimensionless concentration y ($y = C_A/C_A$,s), the dimensionless pellet radius x ($x = r/R$), and dimensionless constants γ, β and ϕ. Using this dimensionless variable dimensionless non-isothermal species and heat transport are as follows [22]:

$$\frac{d^2 y}{dx^2} + \frac{2}{x}\frac{dy}{dx} - \phi^2 y \exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right] = 0 \tag{8}$$

The parameters ϕ, γ and β are in equation (8) represent the dimensionless activation energy, the dimensionless heat of reaction, and the Thiele modulus as evaluated at the surface of the spherical catalyst pellet, respectively. These parameters are expressed in terms of the pellet transport and reaction properties, as well as the pellet surface concentration ($C_{A,S}$) and (T_S) as follows:

$$\phi = R\left\{\frac{k_{ref}}{D}\exp\left[\frac{-E}{RgT_{ref}}\left(\frac{T_{ref}}{T_s}-1\right)\right]\right\}^2 \tag{9}$$

$$\gamma = \frac{E}{R_g T_s} \tag{10}$$

$$\beta = \frac{-\Delta H D_{\varepsilon z}}{K_{\varepsilon z}}\left(\frac{C_{A,S}}{T_S}\right) \tag{11}$$

where C_A is the concentration of reactant A inside the catalyst pellet, $C_{A,s}$ is the concentration of reactant A at the surface of catalyst pellet, $D_{\varepsilon z}$ is the effective diffusivity inside the catalyst pellet, is the activation energy, Δ is the heat of reaction, k_{ref} is the reference reaction constant, $K_{\varepsilon z}$ is the effective thermal conductivity inside the catalyst pellet, r_A is the arrhenius reaction rate, R_g is the universal gas constant, T is the temperature inside the catalyst pellet, T_{ref} is the reference temperature and T_s is the temperature at the surface of catalyst pellet. The boundary conditions in dimensionless forms are

$$y\big|_{x=1} = 1 \tag{12}$$

$$\frac{dy}{dx}\Big|_{x=0} = 0 \tag{13}$$

The overall reaction rate in a catalytic pellet is often expressed by the effectiveness factor (η), which measures the total reaction rate as a scalar multiple of a homogeneous first-order reaction at the surface concentration. The effectiveness factor for spherical pellet is [23]:

$$\eta = \frac{3}{\phi^2}\frac{dy}{dx}\Big|_{x=1} \tag{14}$$

3. ANALYTICAL SOLUTION OF THE CONCENTRATION USING MODIFIED ADOMIAN DECOMPOSITION METHOD (MADM)

In the recent years, much attention is devoted to the application of the Adomian decomposition method to the solution of various scientific models [25]. An efficient modification of the standard Adomian decomposition method for solving singular initial value problem in the second order partial differential equation. The MADM yields, without linearization, perturbation, transformation or discretisation, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms. The decomposition method is simple and easy to use and produces reliable results with few iterations used. The results show that the rate of convergence of modified Adomian decomposition method is higher than standard Adomian decomposition method [26-30]. Using this method (see Appendix A), we can obtain the analytical expression of concentration (see Appendix B), of the substrate as follows:

$$y(x) = 1 - \frac{\phi^2}{6} + \frac{7}{360}\phi^4(1-\gamma\beta) + \phi^2\left(\frac{1}{6} - \frac{\phi^2(1-\gamma\beta)}{36}\right)x^2 + \frac{\phi^4(1-\gamma\beta)}{120}x^4 \tag{15}$$

Using Eq. (10), we can obtain the effectiveness factor

$$\eta = 1 - \frac{\phi^2(1-\gamma\beta)}{15} \tag{16}$$

The Equations (14) and (15) represent the new and simple analytical expression of concentration of substrate and effectiveness factor of vectaut A.

4. NUMERICAL SIMULATION

The non linear diffusion equation (8) for the boundary conditions (equations (12) and (13)) is also solved numerically. We have used the function pdex1 in MATLAB software to solve numerically the initial-boundary value problems for the nonlinear differential equations. This numerical solution is compared with our analytical results in Figures (1) and (2). Upon comparison, it gives a satisfactory agreement for all values of the dimensionless parameters, γ, β and ϕ. The MATLAB program is also given in Appendix *C.*

5. DISCUSSION

The nonlinear PDE system for coupled heat and mass transfer in a spherical non-isothermal catalyst pellet is solved analytically. The concentration of substrate depends on the following there factors, γ (dimensionless activation energy), β (dimensionless heat of reaction) and ϕ (Thiele odulus). Figure 1(a)-(*b*) shows the dimensionless concentration y versus dimensionless pellet radius x. The concentrations were computed for various values of the dimensionless parameter γ, β and ϕ. From figures 1(a)-(b), it is evident that the value of concentration $y \approx 1$ when $x = 1$ and $\phi \le 0.5$ for all values of γ *and* β. The concentration y decreases when ϕ increases.

The normalized numerical simulation of three dimensional substrate concentrations y versus dimensionless pellet raious x is shown in Figures 2 (a) - (c)**.** For fixed value of β (= 0.1) the value of concentration $y(x)$ is slowly decreasing when ϕ is increasing. Then the concentration of $y(x)$=1 when $x = 1$ and for all values of ϕ, γ and β. In these figure, it should be noted that the value of the concentration of substrate decreases for all values of γ. From this Figures, it is apparent that the value of the concentration of substrate increases when β increases.

The variation in effectiveness factor for various values of γ, β and ϕ using Equation (12) is shown in Figures 3- 5. From Figure 3, it is evident that the effectiveness factor increases with the increasing value of the dimensionless parameter β. From Figure 4, it is evident that the effectiveness factor increases with the increasing value of the dimensionless parameter γ. From Figure 5, it is evident that the effectiveness factor increases with the increasing value of the dimensionless parameter $\gamma\,\beta$. The effectiveness factor is equal to one when for ϕ <0.2 and all values parameters β and γ.

6. CONCLUSIONS

The analytical expression of concentration and effectiveness factor of the reactant A inside the catalyst pellets are derived. The approximate analytical expression for the steady state concentration of substrate for all values of parameters ϕ, γ and β in a packed bed reactor was obtained using the modified Adomian decomposition method. A satisfactory agreement with the numerical result is noted. Moreover, we have also presented a closed form expression for the effectiveness factor. These analytical results are useful to analyze the reactivity behaviour of porous catalyst particles subject to both internal mass concentration gradients as well as temperature gradients, in endothermic or exothermic reactions.

Appendix A

Consider the nonlinear differential equation in the form

$$y'' + \frac{2n}{x}y' + \frac{n(n-1)}{x^2}y + F(x,y) = g(x)\,;\, n \geq 0 \tag{A.1}$$

with initial condition

$$y(0) = A,\, y'(0) = B \tag{A.2}$$

where $F(x,y)$ is a real function, $g(x)$ is the given function and A and B are constants. We propose the new differential operator, as below

$$L = x^{-n}\frac{d^2}{dx^2}x^n y \tag{A.3}$$

So, the problem (A.1) can be written as,

$$Ly = g(x) - F(x,y). \tag{A.4}$$

The inverse operator L^{-1} is therefore considered a two-fold integral operator, as below.

$$L^{-1}(.) = x^{-n}\int_0^x\int_0^x x^n\,(.)\,dx\,dx \tag{A.5}$$

Applying L^{-1} of (A.5) to the first three terms $y'' + \frac{2n}{x}y' + \frac{n(n-1)}{x^2}y$ of Equation (A.1) we find

$$\begin{aligned} L^{-1}\left(y'' + \frac{2n}{x}y' + \frac{n(n-1)}{x^2}y\right) &= x^{-n}\int_0^x\int_0^x x^n\left(y'' + \frac{2n}{x}y' + \frac{n(n-1)}{x^2}y\right)dx\,dx \\ &= x^{-n}\int_0^x (x^n y' + nx^{n-1}y)\,dx \\ &= y - y(0) \end{aligned}$$

By operating L^{-1} on (A.4), we have

$$y(x) = A + L^{-1}g(x) - L^{-1}F(x,y) \tag{A.6}$$

The Adomian decomposition method introduce the solution $y(x)$ and the nonlinear function $F(x, y)$ by infinity series

$$y(x) = \sum_{n=0}^{\infty} y_n(x), \tag{A.7}$$

$$F(x, y) = \sum_{n=0}^{\infty} A_n \tag{A.8}$$

where the components $y_n(x)$ of the solution $y(x)$ will be determined recurrently and the Adomian polynomials A_n of $F(x, y)$ are evaluated [22, 23, 25] using the formula

$$A_n(x) = \frac{1}{n!}\frac{d^n}{d\lambda^n} N\left(\sum_{n=0}^{\infty}(\lambda^n y_n)\right)|_{\lambda=0} \tag{A.9}$$

By substituting (A.7) and (A.8) into (A.6),

$$\sum_{n=0}^{\infty} y_n(x) = A + L^{-1}g(x) - L^{-1}\sum_{n=0}^{\infty} A_n \tag{A.10}$$

Through using Adomian decomposition method, the components $y_n(x)$ can be determined as

$$\begin{aligned} y_0(x) &= A + L^{-1}g(x) \\ y_{n+1}(x) &= -L^{-1}(A_n),\ n \geq 0 \end{aligned} \tag{A.11}$$

Which gives

$$\begin{aligned} y_0(x) &= A + L^{-1}g(x) \\ y_1(x) &= -L^{-1}(A_0) \\ y_2(x) &= -L^{-1}(A_1) \\ y_3(x) &= -L^{-1}(A_2) \\ &\cdots \end{aligned} \tag{A.12}$$

From (A.9) and (A.12), we can determine the components $y_n(x)$, and hence the series solution of $y(x)$ in (A.7) can be immediately obtained.

Appendix B

In this appendix, we derive the general solution of nonlinear equation (8) by using Adomian decomposition method. We write the Equation (8) in the operator form,

$$L(y) = \phi^2 y \exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right] \tag{B.1}$$

where $L = x^{-1}\dfrac{d^2}{d\rho^2}x$. Applying the inverse operator $L^{-1}(.) = x^{-1}\displaystyle\int_0^x\int_0^x x\ (.)\,dx\,dx$ on both sides of Equation (B.1) yields

$$y(x) = A\,x + B + \phi^2\ L^{-1}\left(y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]\right) \tag{B.2}$$

where A and *B* are the constants of integration. We let,

$$y(x) = \sum_{n=0}^{\infty} y_n(x) \tag{B.3}$$

$$N[y(x)] = \sum_{n=0}^{\infty} A_n \tag{B.4}$$

$$\text{where } N[y(x)] = \left(y\exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]\right) \tag{B.5}$$

In view of Equations (B. 3), (B. 4) and (B. 5), Eq. (B. 2) gives

$$\sum_{n=0}^{\infty} y_n(x) = A\,x + B + \gamma\, L^{-1}\sum_{n=0}^{\infty} A_n \tag{B.6}$$

We identify the zeroth component as

$$y_0(x) = A\,x + B \tag{B.7}$$

$$y_0 = 1 \tag{B.8}$$

and the remaining components as the recurrence relation

$$y_{n+1}(x) = \phi^2\, L^{-1} A_n, \quad n \geq 0 \tag{B.9}$$

where A_n are the Adomian polynomials of $y_1, y_2, ..., y_n$. We can find the first few A_n as follows:

$$A_0 = N(y_0) = 1 \tag{B.10}$$

$$A_1 = \frac{d}{d\lambda}\left[N(y_0 + \lambda y_1)\right] = \frac{\phi^2}{6}(1-\gamma\beta)(x^2-1) \tag{B.11}$$

The remaining polynomials can be generated easily, and so,

$$y_1 = \frac{\phi^2}{6}(1-\gamma\beta)(x^2-1) \tag{B.12}$$

$$y_2 = \frac{7\,\phi^4(1-\gamma\beta)}{360} + \phi^4(1-\gamma\beta)\left(\frac{x^4}{120} - \frac{x^2}{36}\right) \tag{B.13}$$

Adding (B. 8), (B. 12) and (B. 13) we get Equation (11) in the text.

Appendix C

The Matlab program to find the numerical solution of Equation 8 is as follows.

```
function pdex1
m = 2;
x = linspace(0,1);
t = linspace(0,100);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
u = sol(:,:,1);
surf(x,t,u)
title('Numerical solution computed with 20 mesh points.')
xlabel('Distance x')
ylabel('Time t')
figure
plot(x,u(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u(x,2)')
% --------------------------------------------------------------
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1;
f = DuDx;
Q=1;
B=1.5;
r=1;
s =-(Q^2)*u*exp(r*B*(1-u)/(1+B*(1-u)));
% --------------------------------------------------------------
function u0 = pdex1ic(x)
u0 = 1;
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = 0;
```



```
ql = 1;
pr = ur-1;
qr = 0;
```

Appendix D

Nomenclature

C_A	concentration of reactant A inside the catalyst pellet (cm)
$C_{A,s}$	concentration of reactant A at the surface of catalyst pellet (cm)
D_ε	effective diffusivity inside the catalyst pellet (cm^2/s)
E	activation energy (kJ mol^{-1}.)
g	gradient of $F^T F$
ΔH	heat of reaction (kJ mol^{-1}.)
k_{ref}	reference reaction constant (mmol L^{-1})
k_{ref}	reference reaction constant (mmol L^{-1})
K_ε	effective thermal conductivity inside the catalyst pellet (mmol L^{-1})
r_A	Arrhenius reaction rate (mmol L^{-1})
R_g	universal gas constant (J/K)
T	temperature inside the catalyst pellet (kelvin)
T_{ref}	reference temperature (kelvin)
T_s	temperature at the surface of catalyst pellet (kelvin)
x	dimensionless radius of the spherical catalyst pellet
y	dimensionless concentration along radial direction of catalyst pellet
β	dimensionless heat of reaction
γ	dimensionless activation energy
η	effectiveness factor
ϕ	Thiele modulus

Figures:

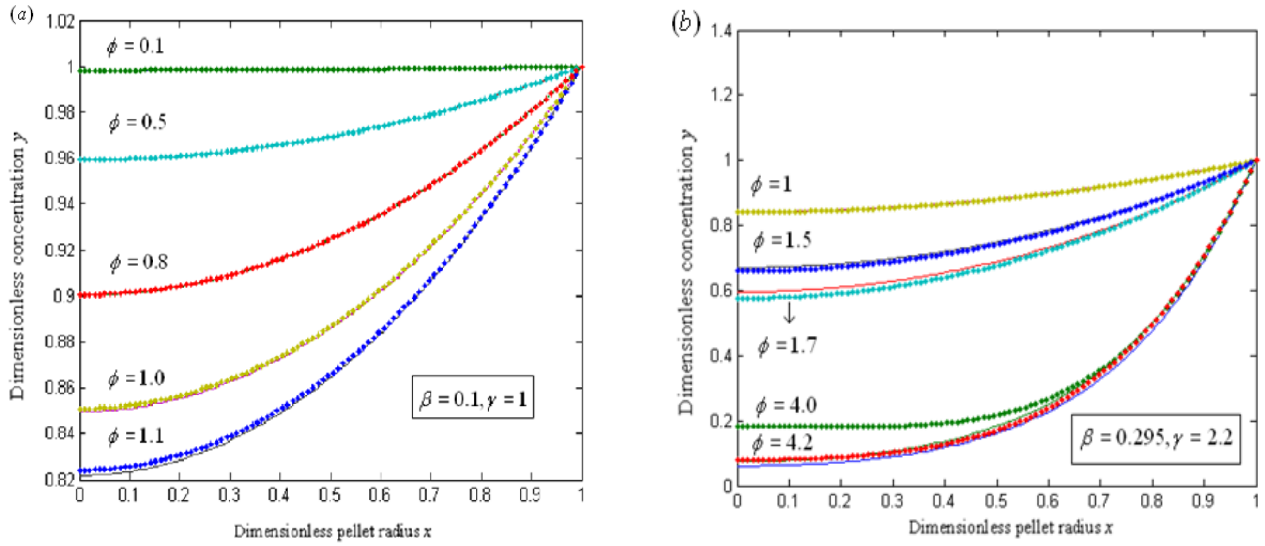

Figure 1: Plot of dimensionless concentration y versus dimensionless pellet radius x. The concentrations were computed for various values of the dimensionless parameter ϕ when (a) $\beta = 0.1, \gamma = 1$ (b) $\beta = 0.295, \gamma = 2.2$. The curves are plotted using equation (15). (—) denotes the analytical results and (• • •) denotes the numerical simulations.

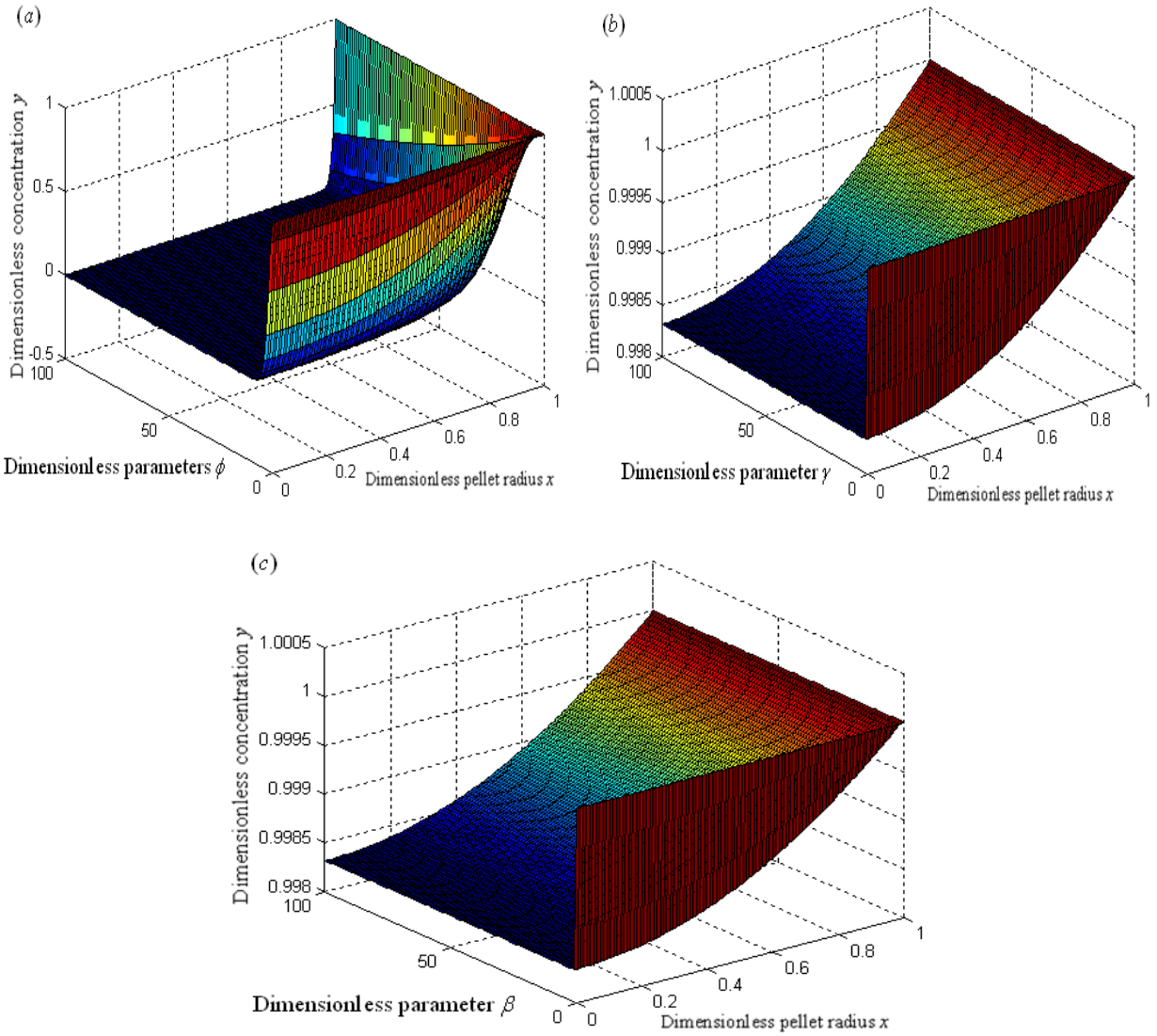

Figure 2: The normalized dimensionless concentration y versus dimensionless pellet radius x. calculated using equation. (15) .The plot was constructed for the values of $(a)\ \beta = 0.1, \gamma = 0.1,\ (b)\ \phi = 0.1, \beta = 0.1$ and $(c)\ \phi = 0.1, \gamma = 0.1$.

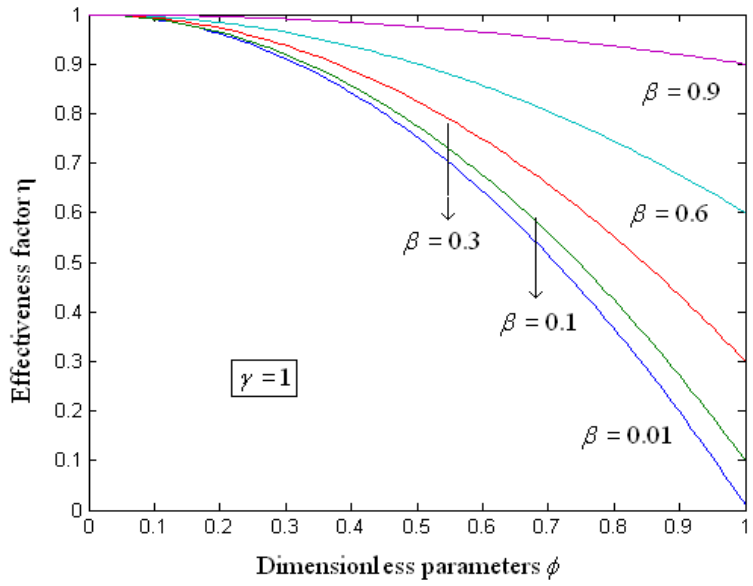

Figure 3: Plot of the effectiveness factor η versus dimensionless parameter β. The effectiveness factor η were computed using equation (16) when $\gamma = 1$.

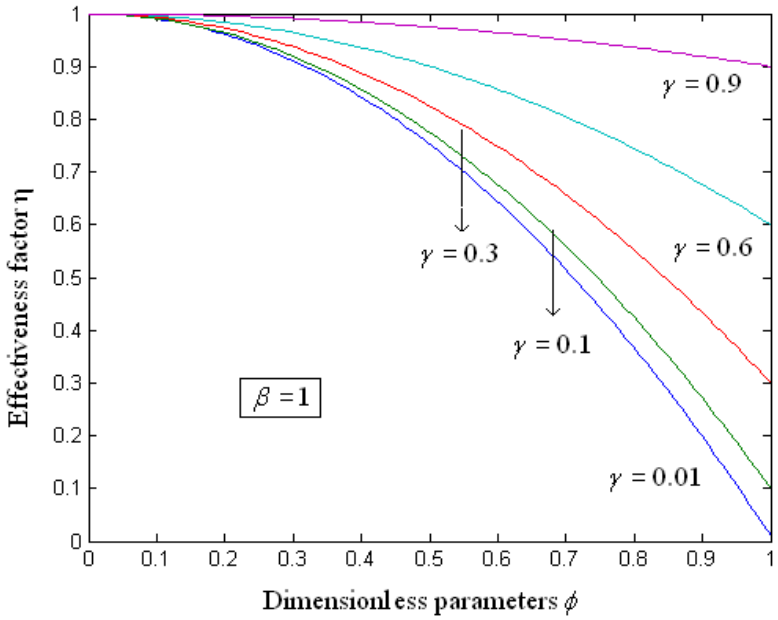

Figure 4: Plot of the effectiveness factor η versus dimensionless parameter γ. The effectiveness factor η were computed using equation (16) when $\beta = 1$.

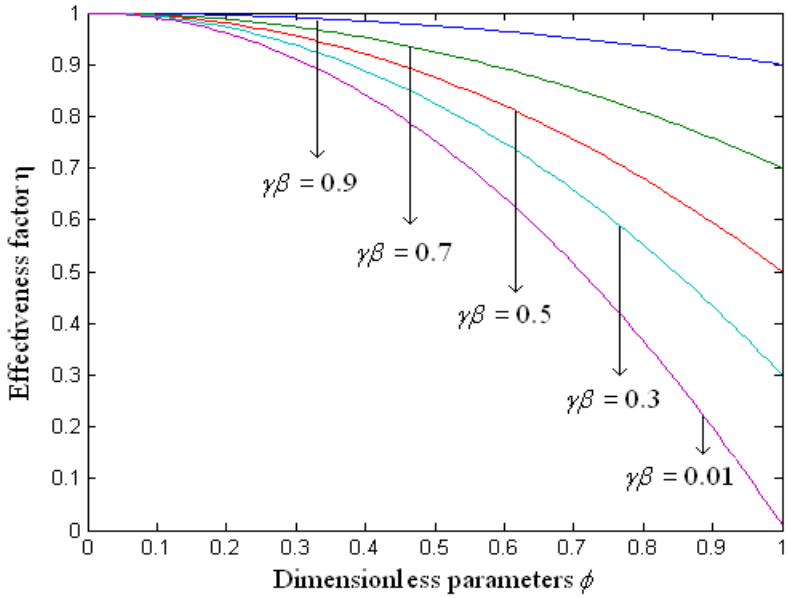

Figure 5: Plot of the effectiveness factor η versus dimensionless parameter $\gamma\beta$. The effectiveness factor η were computed using equation (16).

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