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A SINGULAR PERTURBATION PROBLEM IN STEADY STATE OF METHANE COMBUSTION USING REVERSE FLOW REACTOR

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Abstract

In this paper, we study a solution of a set of convective-diffusion equations arising from methane combustion in reverse flow reactor. Here, temperature and concentration of methane are dependent variables. By scaling process, a nonlinear reaction rate term can be approximated as a linear term, resulting in linear convective-diffusion equations. We consider the steady state regime for small ratio of the diffusion and convective terms. This leads to a singular perturbation problem. Using variable transformation, the problem can be converted into a regular perturbation-like problem. Asymptotic solution shows that, up to and including the second order of approximation, the solution is in agreement with numerical solutions of the boundary value problem.

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1. Introduction

A reverse flow reactor (RFR) is a packed-bed reactor in which the flow direction is periodically reversed to trap a hot zone within the reactor. The common features of combustion process in an RFR were described by convective-diffusion equations with the corresponding boundary and initial conditions [7]. Many previous studies [1-6] mostly determined the features of the RFR dynamic with numerical approach. For example, Gupta and Bhatia [1] proposed a Newton's technique to directly solve for the cyclic profiles. Salinger and Eigenberger (see [4] and [5]) studied periodic state profile by direct calculation. Garg et al. [9] used the direct computation approach that proposed Gupta and Bhatia [1] to observe the periodic state at which the temperature and concentration profiles at the beginning and end of a flow reversal period are mirror images. In steady state profile, simulation of Gosiewski and Warmuzinsky [6] showed that the heat recovery by hot gas withdrawal from the reactor guaranteed more favorable symmetry of the half-cycle-temperature profile.

In this paper, we study the behavior profile of temperature and concentration in methane combustion by analytical approach. As common convective-diffusion equation, some methods can be applied to this problem, for examples Green's function method (see [12]), classical integral transform techniques [13], generalized and extended classical integral transform method [14, 3]. Nuryaman et al. [2] presented an asymptotic solution of a singular perturbation problem for steady state conversion of methane oxidation in reverse flow reactor. They considered a one-dimensional pseudo-homogeneous model with a certain reaction rate in which the whole process of the reactor was still workable and in one direction only from the left to the right end. These assumptions lead to an equation in terms of the conversion variable only. In this paper, we extend the problem by considering a complete equation as a system of convective-diffusion equations. Here, temperature and concentration of methane are dependent variables. We construct a singular perturbation problem with rescaling variable and solve it simultaneously.

This paper is organized as follows: In Section 2, mathematical models for steady state concentration and temperature of methane are described. In Section 3, the asymptotic analysis is presented to find the approximate solution of steady state concentration and temperature, by using asymptotic expansion technique. In Section 4, the numerical simulation is presented to confirm the asymptotic solution. The conclusions are written in the last section.

2. Problem Formulation

Consider a mathematical model of single phase cooled reverse flow reactor model described by 1-D pseudo-homogeneous model [7]:

$$\epsilon \frac{\partial C}{\partial t} = \epsilon D \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} - g(T)C,$$

$$((1-\epsilon)(\rho c_p)_s + \epsilon(\rho c_p)_g)\frac{\partial T}{\partial t} = \lambda_{ax} \frac{\partial^2 T}{\partial x^2} - u(\rho c_p)_g \frac{\partial T}{\partial x} - U_w a_w (T - T_c) + (-\Delta H) g(T) C \tag{1}$$

with

$$g(T) = \frac{\eta k_\infty k_c a_v \exp(-E_a/RT)}{k_c a_v + \eta k_\infty \exp(-E_a/RT)}.$$

Boundary conditions in direction from the left to the right end are written as

$$\frac{\epsilon D}{u}\frac{\partial C}{\partial x} = c_0 - C, \quad -\frac{\lambda_{ax}}{u(\rho c_p)_g}\frac{\partial T}{\partial x} = T_0 - T, \text{ at } x = 0, \tag{2}$$

$$-\frac{\partial C}{\partial x} = \frac{\partial T}{\partial x} = 0, \text{ at } x = L. \tag{3}$$

In order to facilitate the analysis, we introduce the following nondimensional variables and parameters, $T = T_0 + \frac{RT_0^2}{E_a}\theta$, $x = Lz$, $t = t_f \tau$, $C = c_0 \chi$. During our discussion, we assume that the cooler temperature takes places as same as the feed gas temperature, thus $T_c = T_0$. Therefore, the dimensionless governing equations are

$$k_1 \frac{\partial \chi}{\partial \tau} = \frac{1}{Le} \frac{\partial^2 \chi}{\partial z^2} - \frac{\partial \chi}{\partial z} - k_2 g(\theta)\chi, \tag{4}$$

$$k_3 \frac{\partial \theta}{\partial \tau} = \frac{1}{Pe} \frac{\partial^2 \theta}{\partial z^2} - \frac{\partial \theta}{\partial z} - k_4 \theta + k_5 g(\theta)\chi \tag{5}$$

with

$$g(\theta) = \frac{\exp\left(\frac{\theta}{\mu\theta + 1}\right)}{\hat{\varepsilon} + \exp\left(\frac{\theta}{\mu\theta + 1}\right)}, \tag{6}$$

where $\hat{\varepsilon} = k_c a_v / (\eta k_\infty \exp(-E_a / RT_0))$. The boundary conditions are now

$$\frac{1}{Le} \frac{\partial \chi}{\partial z} = \chi - 1, \quad \frac{1}{Pe} \frac{\partial \theta}{\partial z} = \theta, \text{ at } z = 0, \tag{7}$$

$$\frac{\partial \chi}{\partial z} = \frac{\partial \theta}{\partial z} = 0, \text{ at } z = 1. \tag{8}$$

In the present, we consider that $\hat{\varepsilon}$ is very small $(\hat{\varepsilon} \ll 1)$ such that the function $g(\theta)$ can be approximated by $g(\theta) \approx 1$. Furthermore, we assume that the effect of diffusive term in temperature and concentration equations is very much smaller than the convective term, so $\frac{1}{Le} = \frac{1}{Pe} = O(\varepsilon)$, where $\varepsilon \ll 1$. For the steady state, equations (4)-(5) now become

$$\varepsilon\chi'' - \chi' - k_2\chi = 0, \quad \varepsilon\chi'(0) = \chi(0) - 1, \quad \chi'(1) = 0, \tag{9}$$

$$\varepsilon\theta'' - \theta' - k_4\theta + k_5\chi = 0, \quad \varepsilon\theta'(0) = \theta(0), \quad \theta'(1) = 0, \tag{10}$$

where $u'' = \frac{d^2 u}{dz^2}$ and $u' = \frac{du}{dz}$.

In the next section, we present an asymptotic expansion method for the system (9)-(10) (see [10] and [11]).

3. Asymptotic Solution

For $\varepsilon = 0$, equations (9)-(10) become a first order differential equation with two boundary conditions for each. Thus, (9)-(10) lead to singular perturbation problems. To solve this problem, we introduce a new variable $r = \frac{z}{\varepsilon}$. Using the chain rule, in the new variable r, equations (9)-(10) become

$$\ddot{\chi} - \dot{\chi} - \varepsilon k_2 \chi = 0, \quad \dot{\chi}(0) = \chi(0) - 1, \quad \dot{\chi}(1/\varepsilon) = 0, \tag{11}$$

$$\ddot{\theta} - \dot{\theta} - \varepsilon(k_4 \theta - k_5 \chi) = 0, \quad \dot{\theta}(0) = \theta(0), \quad \dot{\theta}(1/\varepsilon) = 0, \tag{12}$$

where $\ddot{\chi} = \frac{d^2\chi}{dr^2}$ and $\dot{\chi} = \frac{d\chi}{dr}$. Let us assume that the solutions of system (11)-(12) can be expanded in power of ε as follows:

$$\chi(r) \sim u_0(r) + \varepsilon u_1(r) + \cdots, \tag{13}$$

$$\theta(r) \sim v_0(r) + \varepsilon v_1(r) + \cdots. \tag{14}$$

Substituting (13)-(14) into (11)-(12), we obtain

$$(\ddot{u}_0 + \varepsilon \ddot{u}_1 + \cdots) - (\dot{u}_0 + \varepsilon \dot{u}_1 + \cdots) - \varepsilon k_2 (u_0 + \varepsilon u_1 + \cdots) = 0, \tag{15}$$

$$(\ddot{v}_0 + \varepsilon \ddot{v}_1 + \cdots) - (\dot{v}_0 + \varepsilon \dot{v}_1 + \cdots) - \varepsilon(k_4 (v_0 + \varepsilon v_1 + \cdots) - k_5 (u_0 + \varepsilon u_1 + \cdots)) = 0. \tag{16}$$

The $O(1)$ equations of (15)-(16) are

$$\ddot{u}_0 - \dot{u}_0 = 0, \quad \dot{u}_0(0) = u_0(0) - 1, \quad \dot{u}_0(1/\varepsilon) = 0, \tag{17}$$

$$\ddot{v}_0 - \dot{v}_0 = 0, \quad \dot{v}_0(0) = v_0(0), \quad \dot{v}_0\left(\frac{1}{\varepsilon}\right) = 0. \tag{18}$$

The solutions of these boundary value problems are

$$u_0(r) = 1, \tag{19}$$

$$v_0(r) = 0. \tag{20}$$

Next, the $O(\varepsilon)$ equations of (15) and (16) are

$$\ddot{u}_1 - \dot{u}_1 - k_2 = 0, \quad \dot{u}_1(0) = u_1(0), \quad \dot{u}_1(1/\varepsilon) = 0, \tag{21}$$

$$\ddot{v}_1 - \dot{v}_1 + k_5 u_0 = 0, \quad \dot{v}_1(0) = v_1(0), \quad \dot{v}_1(1/\varepsilon) = 0. \tag{22}$$

The solution of (21) is

$$u_1(r) = -k_2(r + 1 - e^{r-1/\varepsilon}). \tag{23}$$

By substituting equation (19) into equation (22), we get the solution of (22) given by

$$v_1(r) = k_5(r + 1 - e^{r-1/\varepsilon}). \tag{24}$$

The $O(\varepsilon^2)$ equation of (15) is given by

$$\ddot{u}_2 - \dot{u}_2 + k_2^2(r + 1 - e^{r-1/\varepsilon}) = 0, \quad \dot{u}_2(0) = u_2(0), \quad \dot{u}_2(1/\varepsilon) = 0. \tag{25}$$

The solution of (25) is

$$u_2(r) = k_2^2\left(\frac{1}{2}r^2 + (2 + e^{-1/\varepsilon})(r + 1) + (1/\varepsilon + 2 + e^{-1/\varepsilon})e^{r-1/\varepsilon}\right). \tag{26}$$

From (23) and (24), the $O(\varepsilon^2)$ equation of (16) is

$$\ddot{v}_2 - \dot{v}_2 - A(r + 1 - e^{r-1/\varepsilon}) = 0, \quad \dot{v}_2(0) = v_2(0), \quad \dot{v}_2(1/\varepsilon) = 0, \tag{27}$$

where $A = k_5(k_2 + k4)$. The solution of this boundary value problem is given by

$$v_2(r) = -A\left(\frac{1}{2}r^2 + (2 - e^{-1/\varepsilon})(r + 1) + (1/\varepsilon + 2 - e^{-1/\varepsilon})e^{r-1/\varepsilon}\right). \tag{28}$$

Therefore, the solutions of system (15)-(16) up to and including the first order are

$$\chi(r) = 1 - \varepsilon k_2(r + 1 - e^{r-1/\varepsilon}), \tag{29}$$

$$\theta(r) = \varepsilon k_5(r + 1 - e^{r-1/\varepsilon}), \tag{30}$$

or in variable z,

$$\chi(z) = 1 - \varepsilon k_2\left(\frac{z}{\varepsilon} + 1 - e^{(z-1)/\varepsilon}\right), \tag{31}$$

$$\theta(z) = \varepsilon k_5\left(\frac{z}{\varepsilon} + 1 - e^{(z-1)/\varepsilon}\right). \tag{32}$$

If we extend the solutions of system (15)-(16) up to and including the second order, then the solutions are

$$\begin{aligned}\chi(z) &= 1 - \varepsilon k_2\left(\frac{z}{\varepsilon} + 1 - e^{(z-1)/\varepsilon}\right)\\ &\quad + \varepsilon^2 k_2^2\left(\frac{z^2}{2\varepsilon^2} + B_1\left(\frac{z}{\varepsilon} + 1\right) + B_2 e^{(z-1)/\varepsilon}\right),\end{aligned} \tag{33}$$

$$\begin{aligned}\theta(z) &= \varepsilon k_5\left(\frac{z}{\varepsilon} + 1 - e^{(z-1)/\varepsilon}\right)\\ &\quad - \varepsilon^2 A\left(\frac{z^2}{2\varepsilon^2} + C_1\left(\frac{z}{\varepsilon} + 1\right) + C_2 e^{(z-1)/\varepsilon}\right),\end{aligned} \tag{34}$$

where $B_1 = (2 + e^{-1/\varepsilon})$, $B_2 = \left(\frac{1}{\varepsilon} + 2 + e^{-1/\varepsilon}\right)$, $C_1 = (2 - e^{-1/\varepsilon})$ and $C_2 = (1/\varepsilon + 2 - e^{-1/\varepsilon})$.

4. Numerical Simulation

In comparison, we compare our asymptotic solution with numerical solution of system (15)-(16) as a boundary value problem. If we substitute $\psi_1(z) = \chi(z)$, $\psi_2(z) = \chi'(z)$, $\psi_3(z) = \beta(z)$ and $\psi_4(z) = \theta'(z)$, then we get a system of first order ordinary differential equations as follows:

$$\psi_1' = \psi_2,$$

$$\psi_2' = \frac{1}{\varepsilon}(\psi_2 + k_2\psi_1),$$

$$\psi_3' = \psi_4,$$

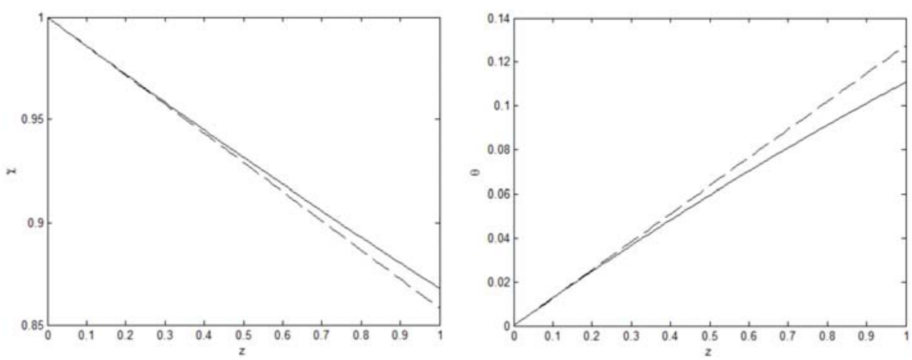
$$\psi_4' = \frac{1}{\varepsilon}(\psi_4 + k_4\psi_3 - k_5\psi_1) \tag{35}$$

with the boundary conditions

$$\varepsilon\psi_2(0) = \psi_1(0) - 1, \quad \psi_2(1) = 0, \quad \varepsilon\psi_4(0) = \psi_3(0) \quad \text{and} \quad \psi_4(1) = 0. \tag{36}$$

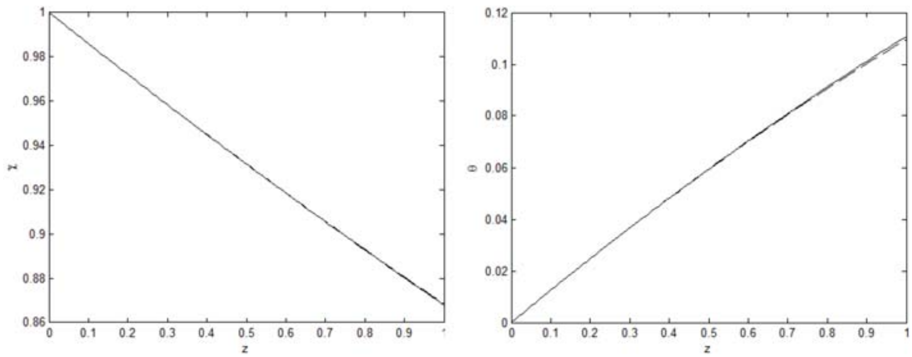
We solve the boundary problem (35)-(36) using the boundary value problem toolbox in Matlab.

In illustration, plots of the asymptotic solution up to and including first order and the numerical solution of (15)-(16), for $\varepsilon = 10^{-6}$, $k_2 = 0.156$; $k_4 = 0.13925$, $k_5 = 0.1275$ are shown in Figure 1. While, Figure 2 shows plots of the asymptotic solution up to and including second order and the numerical solution of (15)-(16). The results show that the asymptotic solution up to and including the second order is quite in agreement with the numerical solutions. In addition, we also confirm our asymptotic solution of methane concentration and the analytical solution of (9) proposed by Guerrero et al. [3], as shown in Figure 3. The result shows that the asymptotic solution up to and including the second order coincides with the analytical solution.



(a) (b)

Figure 1. Plot of methane concentration (a) and methane temperature (b) as a function of z where the dashed line represents the asymptotic solution up to and including first order and the solid line represents the numerical solution.



(a) (b)

Figure 2. Plot of methane concentration (a) and methane temperature (b) as a function of *z* where the dashed line represents the asymptotic solution up to and including second order and the solid line represents the numerical solution.

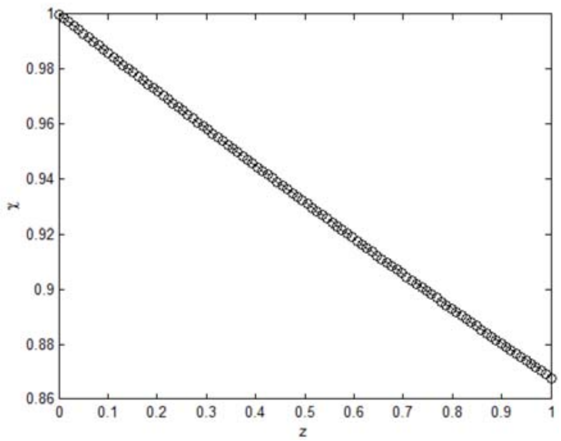


Figure 3. Plot of methane concentration as a function of *z* where the dashed line represents the asymptotic solution up to and including the second order and the circle symbol represents the analytical solution that proposed in [3].

5. Conclusion

In this paper, we have constructed singular perturbation problems for the steady state concentration and temperature of feed gas in the methane combustion process using a reverse flow reactor. The small parameter in our problem took place in front of the diffusive terms. Using the variable transformation and asymptotic expansion method, we solved the equations up to and including the second order approximation. The present asymptotic solutions were quite in agreement with the numerical solutions.

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