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## Dynamics of Temperature and Concentration on Oxidation Reaction Using Reverse Flow Reactor With Periodic Feed Gas Like Square Wave Function: a Numerical Approach

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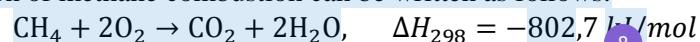
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**Abstract.** Dynamics of oxidation reaction using reverse flow reactor (RFR) are given by a set of convection - diffusion equations that containing the non-linear term corresponding to the reaction rate and provided with certain initial and boundary conditions. In this paper, we investigate the dynamic profiles of temperature and feed concentration on oxidation process using numerical simulation approach. Here we assume the process satisfies 1-D pseudo-homogeneous model and the feed gas form is square wave function. Several different operation parameters have simulated to see the influence towards temperature and feed concentration profile. The results show that period function, small switching time, medium gas velocity and small specific reactor wall surface will make the reactor operated longer..

### 1. Introduction

Climate change induced by global warming is a major issue in the world today. Earlier studies declare that warmth of the earth one of them is result of greenhouse gases (GHG) produced by human activities. Each GHG have a differences effect to global warming. Methane is classified as a GHG, and large volumes of methane in the atmosphere are believed to be a main contributor to climate warming today. Contribution of methane emissions to the greenhouse effect represents 17% of all GHG emissions. Methane has a global warming potential 21 times that of carbon dioxide [1]. Finding efficient methods of reducing methane emissions is very important.

One of strategy to reduce influence the global warming is by convert CH<sub>4</sub> to CO<sub>2</sub>. The stoichiometric reaction of methane combustion can be written as follows:



Each one molar CH<sub>4</sub> gas oxidized will release heat energy of 802,7 kJ. The removal of methane by combustion thus offers the possibility of a net reduction in GHG potential of 87%. Oxidation of methane concentrations smaller than 1%-v can be conducted over appropriate catalysts, such as Pt or Pd active site [2]. Treatment of low-temperature lean methane emission using a catalytic fixed bed reactor with one-through operation usually requires a preheater to achieve the reaction temperature due to its low adiabatic temperature rise.

The reverse flow operation method applied to the catalytic fixed bed reactor or reverse flow reactor (RFR) is proper method to convert methane to carbon dioxide. RFR has advantages over conventional catalytic fixed bed reactor in terms of the ability to operate auto-thermal.

Dynamics of feed gas inside catalytic reactor during the reaction, kept under review [3-9] to acquire the data needed to design a good and appropriate reactor while the feed gas concentration is constant. This problem is usually described by a set of convection – diffusion equation that containing the nonlinear term corresponding to the reaction rate. Simulation used to learn the behavior of feed gas dynamics along the reactor, especially related to the temperature and concentration during the reaction.

In analytical approach, Nuryaman et.al. [10] studied a singular perturbation problem of methane conversion in steady state under certain assumptions. In another article, Nuryaman and Gunawan [11] reported asymptotic solution of the concentration and temperature variables in a singular perturbation problem in steady state of methane combustion using RFR. Both articles use 1-D pseudo-homogeneous model [3] in constructing the singular perturbation problem.

Dynamic of temperature and concentration at start up condition were reported in [9]. In this paper, we investigate the dynamic profiles of temperature and feed concentration on oxidation process with periodic feed gas like square wave function. The effect of parameter operation in model will be studied.

This paper is organized as follows. In Section 2, data/material and method are described. In Section 3, the results of simulation are presented to interpret the behavior of methane concentration and temperature. The conclusions are written in the last section.

## 2. Data and Methods

In this paper, the dynamic behavior profiles of dependent variables were studied using numerical simulation approach. The mathematical model which used in this numerical simulation refers to the 1-D pseudo-homogeneous model that proposed by Khinast et.al [3]. The governing equations in this model are

Heat balance equation:

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

Mass balance equation:

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

where  $K = (1 - \epsilon)(\rho c_p)_s + \epsilon(\rho c_p)_g$  and  $g(T) = \frac{\eta k_\infty k_c a_v \exp(-E_a/RT)}{k_c a_v + \eta k_\infty \exp(-E_a/RT)}$ . Here  $T = T(z, t)$  and  $C = C(z, t)$  respectively correspond to the temperature (K) and feed concentration (molar) at position  $z$  and time  $t$ .

Boundary conditions of heat and mass balances equations can be written as (for flow from left to right)

$$-\frac{\lambda_{ax}}{u(\rho c_p)_g} \frac{\partial T}{\partial z} = T_{in} - T, \quad -\frac{\epsilon D}{u} \frac{\partial C}{\partial z} = C_{in} - C, \quad \text{at } z = 0 \tag{3}$$

$$\frac{\partial T}{\partial z} = 0, \quad \frac{\partial C}{\partial z} = 0, \quad \text{at } z = L \tag{4}$$

Here  $T_{in}$  and  $C_{in}$  correspond to the temperature and concentration of feed gas which entering into reactor and  $L$  denotes reactor length. For flow from right to left, the boundary conditions change on (3) at  $z = L$  and on (4) at  $z = 0$ .

We assume that the temperature of feed gas is constant and its concentration in the form of periodic functions as  $C_{in}(t) = A + B \text{ squire } \omega t$  with  $A > B$  and  $\omega$  related to high and low frequency on specific time period. For initial conditions, at  $t = 0$ , we assume that the reactor has been preheated so reach certain desired temperature,  $T(z, 0) = T_0$  and feed concentration inside reactor,  $C(z, 0) = 0$ .

On numerical simulation, Equations (1)-(2) discretized using finite difference method that is forward time centered diffusion backward convection. We get the discretized equation is obtained as follows :

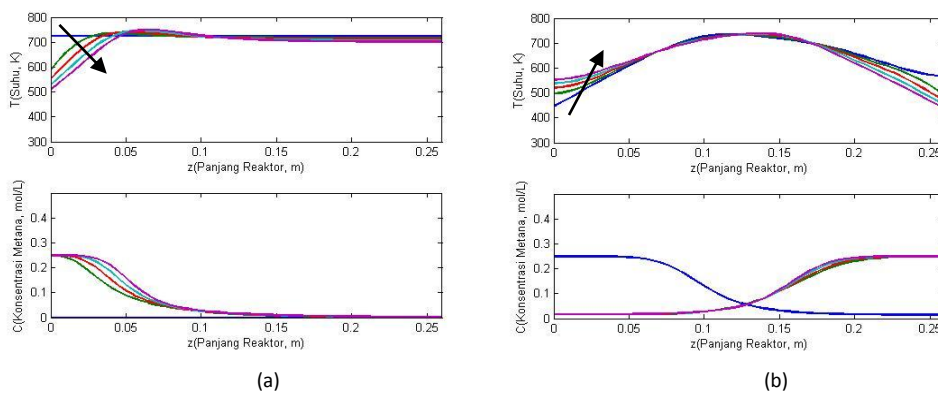
$$T_j^{n+1} = T_j^n + a_1 \frac{\Delta t}{\Delta z} (T_{j+1}^n - 2T_j^n + T_{j-1}^n) - b_1 \frac{\Delta t}{\Delta z} (T_j^n - T_{j-1}^n) - c_1 \Delta t (T_j^n - T_C) + d_1 \Delta t g(T_j^n) C_j^n \tag{5}$$

$$C_j^{n+1} = C_j^n + a_2 \frac{\Delta t}{\Delta z^2} (C_{j+1}^n - 2C_j^n + C_{j-1}^n) - b_2 \frac{\Delta t}{\Delta z} (C_j^n - C_{j-1}^n) - d_2 \Delta t g(T_j^n) C_j^n \tag{6}$$

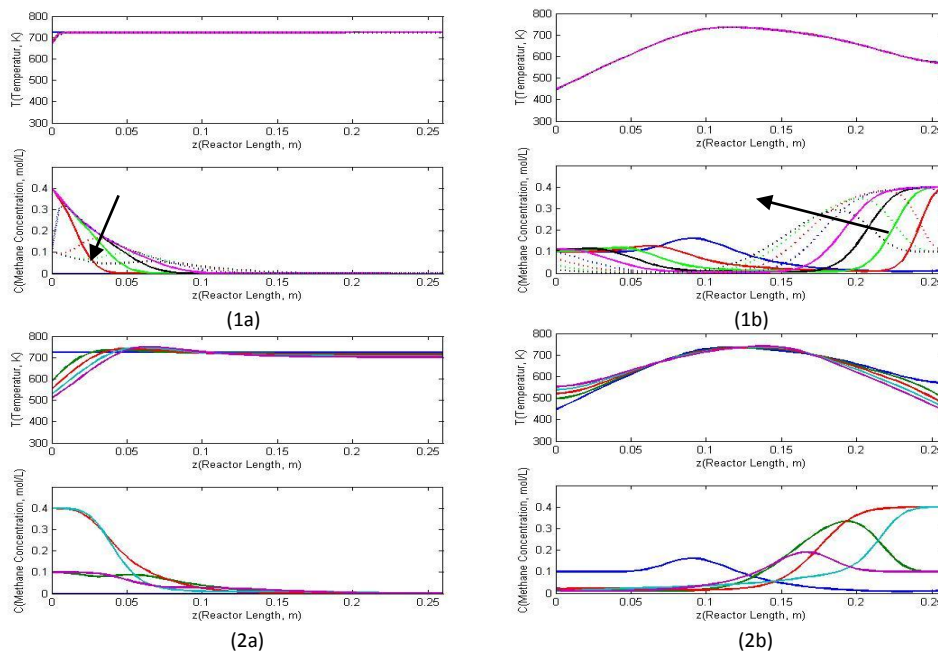
where  $T_j^n = T(z_j, t_n)$ ,  $C_j^n = C(z_j, t_n)$ ,  $\Delta z = L/N_z$  and  $\Delta t = t/N_t$ . Here  $N_z$  and  $N_t$  respectively denote the number of spatial and time coordinate partitions.

### 3. Results and Discussion

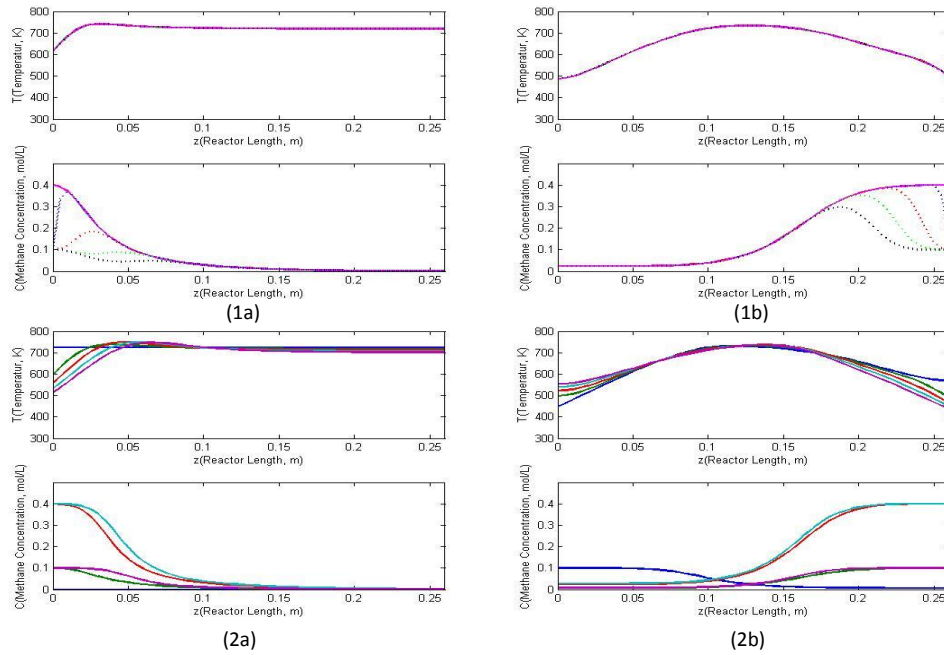
Using finite difference scheme (5)-(6), the boundary conditions (3)-(4) and the initial conditions  $T(z, 0) = T_0$  and  $C(z, 0) = 0$ , then numerical simulation are performed. Parameters values correspond physical properties of RFR that we use in numerical simulation are adopted from [3]. Temperature and concentration profiles obtained as follow:



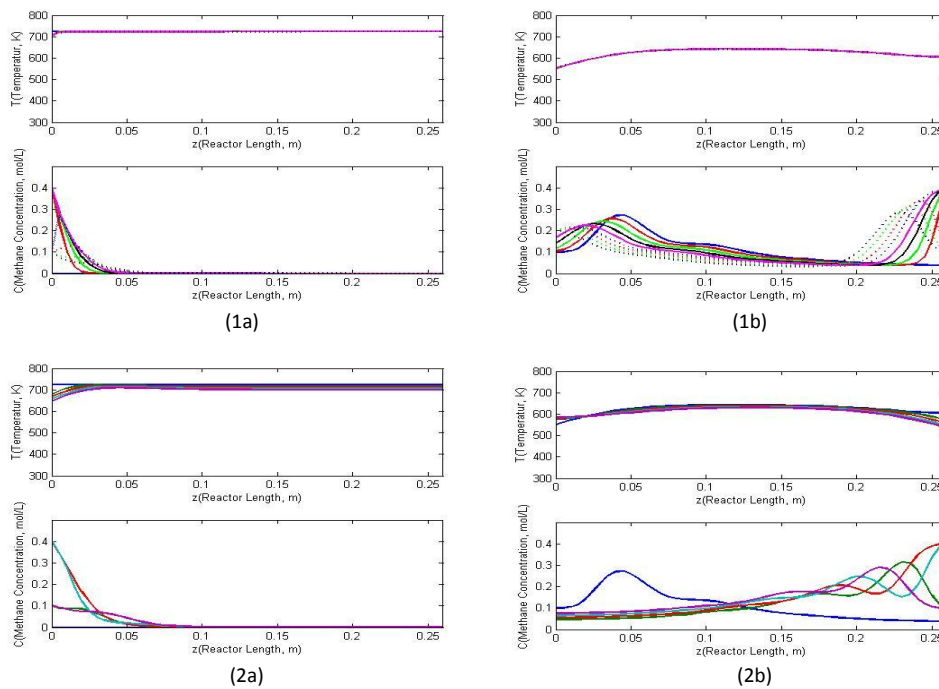
**Figure 1.** Dynamics of temperature and concentration respectively (in the direction of arrow) (a) flow from left to right and (b) after six times reversed, with  $A = 0.25$ ,  $B = 0.15$ ,  $\omega = 0$  (constant concentration).



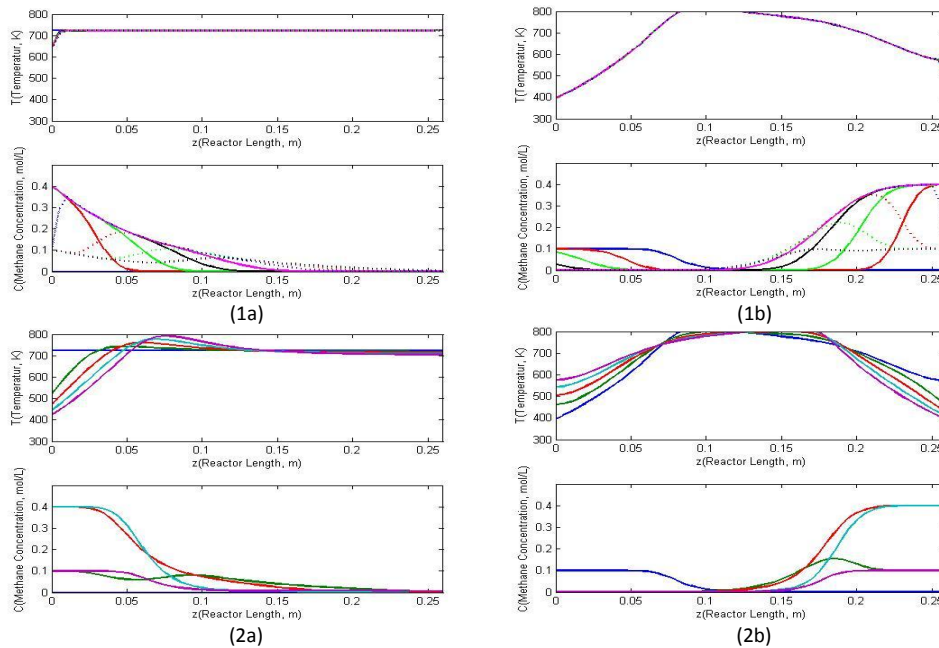
**Figure 2.** Dynamics of temperature and concentration respectively (in the direction of arrow) (1a) and (1b) small  $t$  interval, (2a) - (2b) after six times reversed, with  $A = 0.25$ ,  $B = 0.15$ ,  $\omega = 5\pi$ .



**Figure 3.** Dynamics of temperature and concentration respectively (in the direction of arrow) (1a) - (1b) small  $t$  interval, (2a) - (2b) after six times reversed, with  $A = 0.25, B = 0.15, \omega = \pi/5$ .



**Figure 4.** Dynamics of temperature and concentration respectively (in the direction of arrow) (1a) and (1b) small  $t$  interval, (2a) - (2b) after six times reversed, with  $u = 0.1$  m/s.



**Figure 5.** Dynamics of temperature and concentration respectively (in the direction of arrow) (1a) and (1b) small  $t$  interval, (2a) - (2b) after six times reversed, with  $u = 0.5 \text{ m/s}$ .

In Figure 1, we investigate the dynamics of temperature and concentration in the RFR for some time  $t$  while temperature and concentration of feed gas are constant. While in Figure 1 and Figure 2, we elaborate the dynamics of temperature and concentration in the RFR for constant temperature feed gas and periodic concentration feed gas. Here, periodic concentration refers to  $C_{in}(t)$ . We investigate effect of  $\omega$  (period) value to dynamics of temperature and concentration in RFR. Furthermore, in Figure 4 and Figure 5, we investigate effect of superficial gas velocity to dynamics of temperature and concentration in RFR.

Generally, between constant and periodic like square wave function of feed gas, qualitatively same on temperature profile. Temperature profile in the left end of reactor where feed concentration entering reactor, over time it getting down. This profile caused by dispersion factor. On to the right end of reactor position, the temperature getting up then down. This profile occurs due to the contribution of heat reaction and cooling. When the feed concentration runs out, then the contribution of heat reaction decreases. In other side the cooling continuous, so the temperature getting down. Moreover, with periodic feed concentration like square wave function will have fluctuation because low and high concentration of feed gas that enter the reactor.

While concentration profile for the case of constant feed gas, over time the concentration inside reactor increases, especially near the end of reactor where the concentration entering reactor. It happens because not all of the feed gas to react immediately. But getting to the right, the concentration is getting closer to zero or run out because of reacting. As for the case of periodic feed gas, in general the concentration profile is similar to constant feed gas. The difference lies in the existence of oscillations between high and low concentrations.

Variations in the value of  $\omega$  will effect on the visibility of waveform on the concentration profile along the reactor. When  $\omega$  is large, the waveform is still visible, heading to the right the period wave is getting smaller. When  $\omega$  is small, the waveform becomes invisible because of diffusion.

Variations in the value of  $u$  will effect to the duration of reactor can operate. The smaller  $u$ , the temperature profil will drop quickly. This is because the feed gas movement in the reactor is slow, so that only little feed gas reacts. This will cause the reactor to go out quickly. Whereas with the greater  $u$ , the temperature profile will rise quickly. This is because the feed gas movement in the reactor is fast, so the feed gas reacts a lot. So that the reactor will able to operate longer, but if  $u$  are too large it can cause the reactor to overheat.

#### 4. Conclusions

The study of oxidation reactions using RFR with periodic feed gas like square wave function has been performed. The temperature profile with square wave function will have fluctuation because low and high concentration of feed gas that enter the reactor. The lower and faster superficial gas velocity is very influence to temperature profile which consequence the duration of reactor can operate.

#### 5 Acknowledgments

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