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Applied Mechanics and Materials Vols. 541-542 (2014) pp 108-112
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doi:10.4028/www.scientific.net/AMM.541-542.108

Autothermal Reforming of Ethanol for Hydrogen Production: Modeling and Simulation

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Keywords: Autothermal reforming, Ethanol, Hydrogen production, Modeling, Simulation.

Abstract. Autothermal reforming (ATR), which is the combination of endothermic steam reforming and exothermic partial oxidation, is an attractive process to produce hydrogen using for transportation fuel cell because of its moderate size. ATR is considered to be thermally self-sustaining that the external heat source is not required. In order to keep the adiabatic temperature of ATR reactor, the process control strategy needs in understanding the dynamic characteristics of the ATR system. Thus, the modeling and simulation of ATR process for hydrogen production fueled by ethanol is carried out in this work. The open loop responses of the feed and ATR temperatures are simulated by the dynamic models of ATR system. The simulation results showed the predominantly influence of the electrical power of preheater on the feed and ATR temperatures while the air flowrate has an inverse effect on the feed temperature and a direct effect on the ATR temperature. As a result, the match of control loop is very sensible for an effective control strategy in the development of control system design for maintaining the adiabatic temperature of ATR reactor for sustaining the effectiveness of hydrogen production.

Introduction

Hydrogen is very attractive clean energy carrier for future automobile fuel used in a fuel cell to generate electricity with high efficiency. To support sustainable hydrogen economy, it is vital to produce hydrogen cleanly and renewably. Among the various feedstocks, ethanol is one of the most attractive options because it can be produced renewably by fermentation of biomass or agricultural waste products. Moreover, it is non-toxicity and easy to store and transportation. There are three major thermochemical reforming techniques used to produce hydrogen from ethanol, namely steam reforming (SR), partial oxidation (POX) and autothermal reforming (ATR). The endothermic reaction of SR process is the oldest and most widely applied, but it has a difficulty of slow start-up that makes it more suitable for a stationary system rather than for a mobile system [1]. Though SR leads to a high efficiency of hydrogen production at the outlet stream, the endothermic reaction requires a large amount of heat to be provided by an external source such as burner. POX can reduce the use of burner, but the high temperature causes the formation of hot spots in the catalyst [2], while the low hydrogen production is presented. ATR combines the thermal effects of the exothermic POX and endothermic SR reactions by feeding the fuel, water, and air together into the reactor [3] that makes it practical for moderate size fuel processor [4-5]. A benefit of lower energy requirement of ATR compared to SR, that it is because of a presence of oxygen in the exothermic reaction, appears to have attracted much interest.

There are many works concerning the hydrogen production via ATR mostly focused on developing catalytic reaction and optimizing of operating conditions. The experimental, modeling and dynamics tasks are mainly aimed towards determining the suitable amount of reactants at steady state operations that obtain maximum hydrogen production and maintain safe operating conditions for the reformer [5-8] and most favorable values are also determined. Analysis of the effects of operating conditions

such as amount of water and air in the system and reaction temperature on the product distribution via ATR is investigated in [4, 9-10]. A process control of autothermal reformer is very important as Chen and Sun [11] presented that the control objective of ATR is to produce adequate hydrogen efficiently to support the fuel cell load while maintaining the operation temperature of the reactors within the safe range in order to avoid carbon formation. Hu et al. [12] reported the control system options available to an ATR of gasoline for on-board fuel process using in fuel cell application. It has been recognized that the dynamic models is very important for process control design and there are several works on the modeling and simulation of ATR of methane [6, 10], JP5 fuel [8] and gasoline [12] but, however, there is not enough published paper describing modeling and simulation of ATR of ethanol. In our previous work [13], the steady state modeling of ATR of ethanol for hydrogen production was investigated and the estimated functions of adiabatic temperature as function of steam-to-carbon ratio and air-to-carbon ratio were proposed.

In the present work, the modeling and simulation for ATR from ethanol for hydrogen production has been performed. The mathematical models of energy balances of the ATR system are proposed. The simulation results of the open-loop response of the feed temperature, which is the temperature before entering the ATR reactor, and of the temperature of ATR reactor are presented. An idea of control system design strategy is also discussed in this paper.

System Description of Autothermal Reforming System

A process flow diagram of ATR process for hydrogen production from ethanol is shown in Fig. 1. The ethanol fuel, water and air are mixed and fed together into a preheater before entering the ATR reactor. The ATR is used for converting ethanol to hydrogen-rich gas used as the fuel in fuel cell systems. In the ATR, ethanol is reacted with both steam and oxygen in the air to obtain the wet gas, mainly consisting of hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4), unreacted nitrogen (N_2) and water (H_2O) which are then separated in a flash separator.

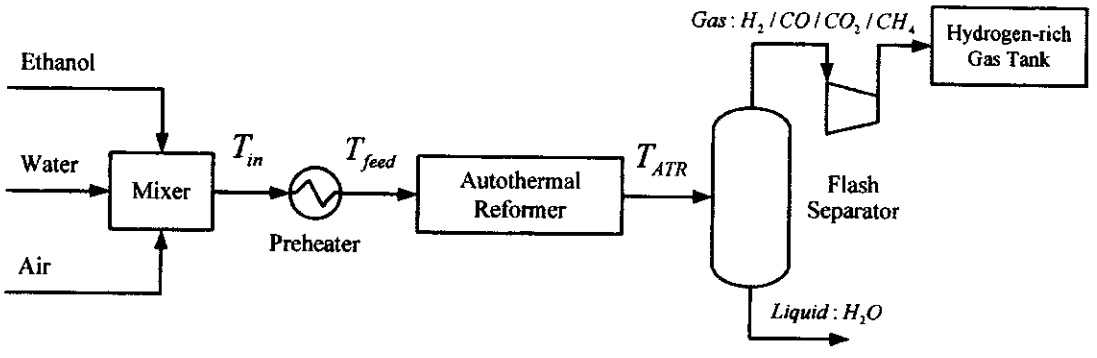

Fig. 1 Process flow diagram for ATR system.

Models of Autothermal Reforming System

Because of the complex mathematical models taking place in the ATR system, the assumptions and simplifications made are:

1. As no reaction kinetic is available, the minimization of Gibbs free energy method is used to simplify the calculation of mass balance dynamics of gas production in the ATR [14].
2. The ATR of ethanol is assumed to be completed.
3. The pressure in the reactor is considered to be constant.
4. All the gases are assumed to be ideal.
5. The influence of radiation is neglected.
6. The well insulated reactor and preheater is assumed.
7. The reactor is considered as an adiabatic device.

The need of the adiabatic temperature control of ATR reactor is a main idea. The unsteady-state energy balances around the preheater and the ATR reactor can be written as

$$\rho_{HT}V_{HT}\overline{C}_{p,HT}\frac{dT_{feed}(t)}{dt}=\Sigma(\dot{N}_i(t)\overline{C}_{p,i})(T_{in}(t)-T_{feed}(t))+x(t)P \quad (1)$$

$$\rho_{ATR}V_{ATR}\overline{C}_{p,ATR}\frac{dT_{ATR}(t)}{dt}=\Sigma(\dot{N}_i(t)\overline{C}_{p,i})(T_{feed}(t)-T_{ref})-\Sigma(x_j\overline{C}_{p,j})\dot{N}_f(t)(T_{ATR}(t)-T_{ref})$$
$$+\Sigma(\dot{N}_i(t)\Delta H_i^f)-\Sigma(x_j\Delta H_i^f)\dot{N}_f(t) \quad (2)$$

where ρ is the density, V the volume, $\overline{C}_p$ the average heat capacity, $\dot{N}_i$ the molar flowrate of species i at inlet stream, $\dot{N}_f$ the molar flowrate of ATR outlet stream, x_j the mole fraction of species j at outlet stream, T_{ref} the reference temperature of 298 K, H_i^f the enthalpy of formation of species i, P the maximum electrical load of heating coil of preheater, x the heating power fraction, and the HT and ATR subscripts represent the preheater and the ATR reactor, respectively.

Simulation Results

It is very crucial to realize dynamic responses of the ATR system in order to design an effective control strategy. Nominal parameters and operating points of this ATR system are given in Table 1. From the dynamic models described earlier, the open loop responses of the temperature of ATR system were investigated at which the operation near the nominal conditions is of our primary research interest for this work.

Table 1 Nominal parameters for the ATR system

Parameters	Value	Parameters	Value
Ethanol molar flowrate	0.1 mol/s	T_{ref}	298 K
Water molar flowrate	0.4 mol/s	T_{in}	298 K
Air molar flowrate	0.35 mol/s	T_{feed}	473 K
ATR Outlet stream flowrate	1.1593 mol/s	T_{ATR}	912 K
Mole fraction of $H_2/CO_2/CO/CH_4/H_2O/N_2$	0.31/0.147/0.05/0.007/0.28/0.24	Max. Load of preheater	50 kW
		Heating power fraction	0.546

Fig. 2 illustrates the dynamic response of the feed temperature (T_{feed}) at preheater outlet stream during transitions of input parameters, namely air flowrate ($\dot{N}_{Air}$), ethanol flowrate ($\dot{N}_{C_2H_6O}$), water flowrate ($\dot{N}_{H_2O}$) and heating power fraction (x). The step inputs were +0.035, +0.0435, +0.11 mol/s of $\dot{N}_{Air}$, $\dot{N}_{C_2H_6O}$ and $\dot{N}_{H_2O}$, respectively, and +10% of the nominal value of x. The changes of step inputs of $\dot{N}_{Air}$, $\dot{N}_{C_2H_6O}$ and $\dot{N}_{H_2O}$ decreased the T_{feed} of 3.3, 14, and 34 K, respectively. The change of step input of x increased the T_{feed} of 32 K. The open loop responses of the ATR temperature (T_{ATR}) during the changes of $\dot{N}_{Air}$, $\dot{N}_{C_2H_6O}$, $\dot{N}_{H_2O}$ and x are shown in Fig. 3. The input step changes of $\dot{N}_{Air}$, $\dot{N}_{C_2H_6O}$ and x increased the T_{ATR} of 11, 2.1, and 26 K, respectively whereas the transition of $\dot{N}_{H_2O}$ decreased the T_{ATR} of 12.5 K.

In the control system design, the match of controlled variables and manipulated variables can be considered from the positive influence with the largest gain of control loop. As shown in Fig. 2, it can be found that the controlled variable is the T_{feed} and the possible manipulated variable is x because it showed the highest positive effect on the T_{feed}.

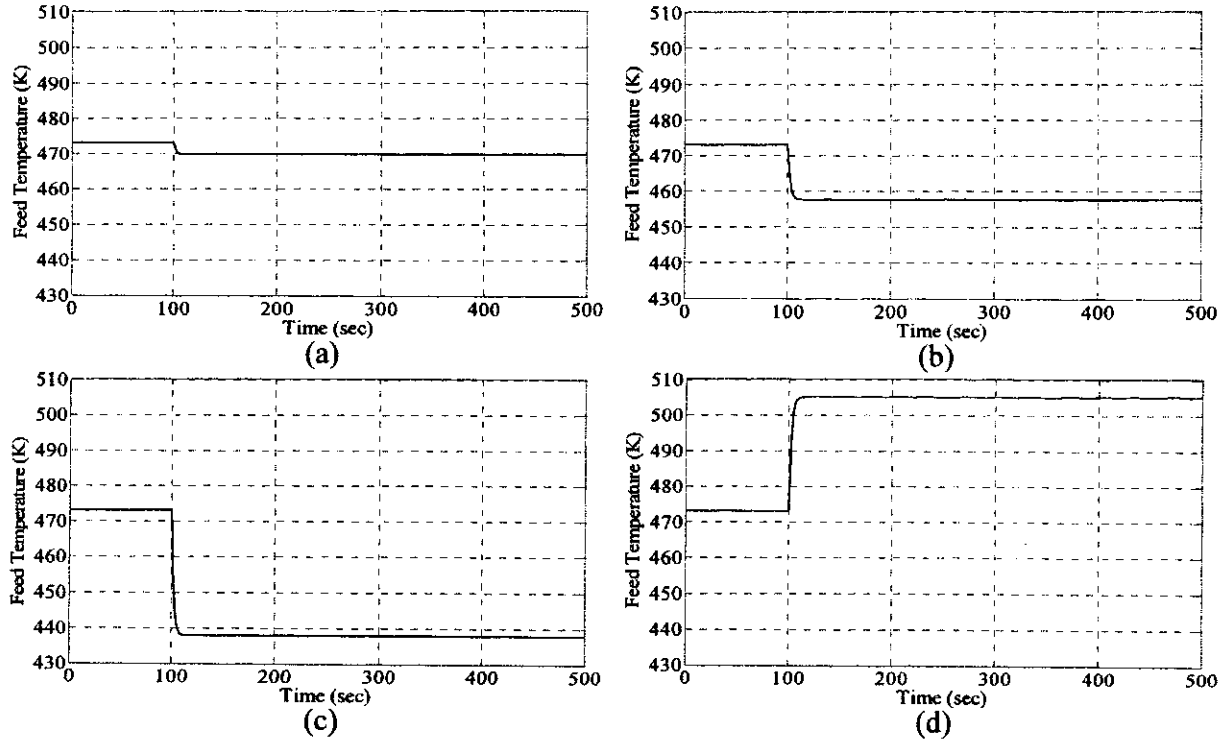

Fig. 2 Open loop responses of the feed temperature (T_{feed}) to input step changes: (a) $\dot{N}_{Air}$, (b) $\dot{N}_{C_2H_6O}$, (c) $\dot{N}_{H_2O}$ and (d) x.

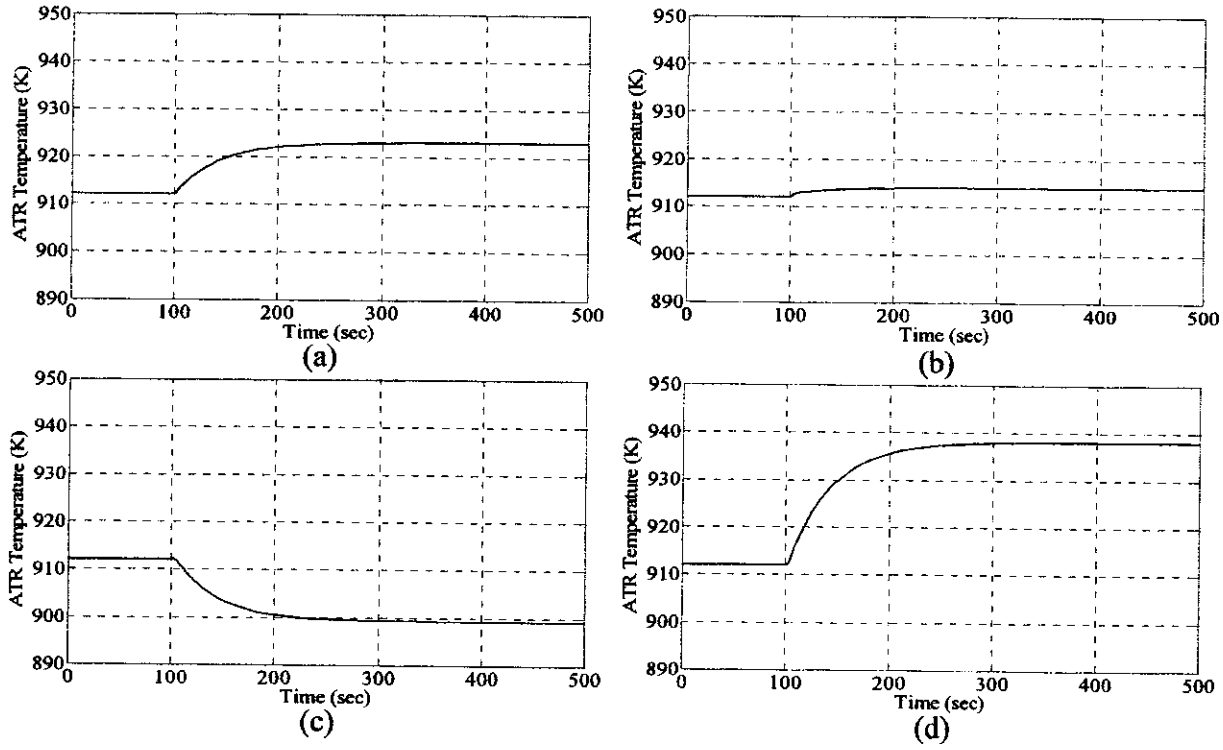

Fig. 3 Open loop responses of the ATR temperature (T_{ATR}) to input step changes: (a) $\dot{N}_{Air}$, (b) $\dot{N}_{C_2H_6O}$, (c) $\dot{N}_{H_2O}$ and (d) x.

On the other hand, if the controlled variable of T_{ATR} is considered, the feasible manipulated variables can be both of the x and $\dot{N}_{Air}$ in which the input step change of x showed the larger gain than

that of $\dot{N}_{Air}$. It seems that the x should be chosen as the manipulated variable of this T_{ATR} control loop but, however, the T_{feed} has an important influence considered as a major disturbance of ATR reactor. Consequently, the $\dot{N}_{Air}$ is probably optioned as the manipulated variable for T_{ATR} control loop instead of the x, which is the possible manipulated variable of T_{feed} control loop.

Conclusion

Due to the difficulty for maintaining the adiabatic operating temperature in the ATR reactor to keep the efficiency of hydrogen yield, the dynamic response is necessary for the effective control system design strategy. Therefore, the modeling and simulation of ATR system for hydrogen production has been performed in this work. As the dynamic models of energy balances for the ATR process were described, the open loop responses of the feed temperature and the ATR temperature can be useful for making the decision to design the control system strategy. It can be concluded that, the ATR temperature should be controlled by adjusting the air flowrate. However, since the feed temperature being the major disturbance has a main effect on the ATR temperature, the feed temperature can be designed as another controlled variable of which the fraction of heating power should be the manipulated variable.

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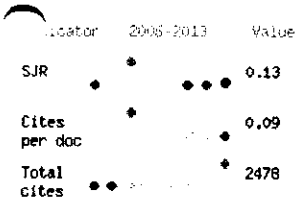

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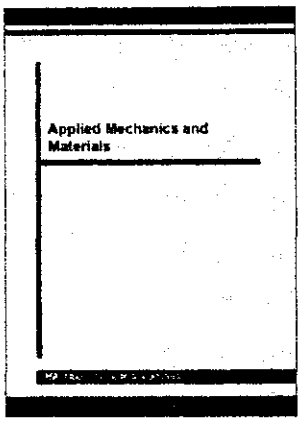

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