Modeling of cellulose assisted combustion synthesis technique for catalyst preparation for hydrogen production from ethanol reforming

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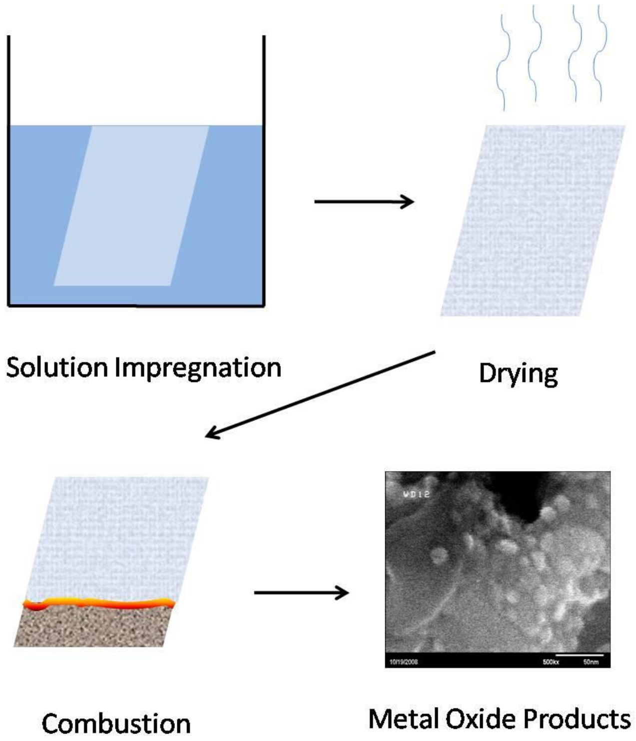
XXIV International Conference on Chemical Reactors CHEMREACTOR-24
September 12 - 17, 2021

Cellulose Assisted Combustion Synthesis

- Reaction media is impregnated in a thin cellulose paper
- Eliminates the preheating stage
- Relatively low combustion temperature (~600 ˚C)
- Fast Cooling rate due to thin layer
- High product yield



- Helps in achieving steady state propagation in weakly exothermic system.
- Continuous catalysts synthesis in stable conditions.

Appl. Catal. A: Gen. **372** (2010), pp. 175-183
Ind. Eng. Chem. Res. **58** (2019), pp. 7681-7689

Catalyst Synthesis: reaction mixture

Metal Nitrate

Fuel: Glycine, Urea, Hydrazine…

Oxygen

$$Me^{v}(NO_3)_v \quad + \quad {}^{5}/_{9}\, v\, \varphi\, NH_2CH_2COOH \quad + \quad {}^{5}/_{4}\, v(\varphi-1)O_2$$

φ = 1 : stoichiometric

φ > 1 : fuel rich

φ < 1 : fuel lean

$$MeO_{v/2} \quad + \quad {}^{10}/_{9}\, v\, \varphi\, CO_2 + {}^{25}/_{18}\, v\, \varphi\, H_2O + \{{}^{(5\varphi+9)}/_{18}\}\, vN_2$$

Metal Oxide

Gas Phase products

Model Description

Reactants:

$$\rho_1 c_{p1}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_1 \frac{\partial T}{\partial x}\right) + (-\Delta H_r) r(C_A, T) - \left(\frac{4U}{d}\right)_1 (T - T_0) - n_g r(C_A, T) c_p^g (T - T_0)$$

Products:

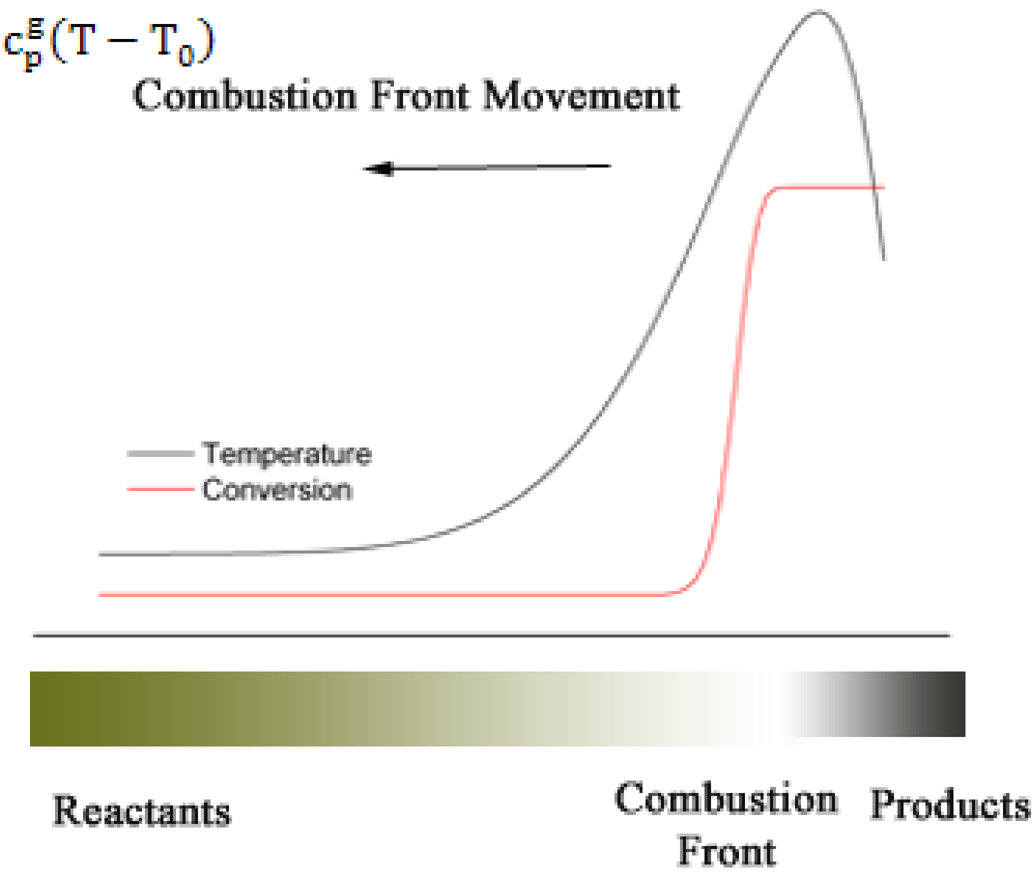
$$\rho_2 c_{p2}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_{p2} \frac{\partial T}{\partial x}\right) - \left(\frac{4U}{d}\right)_2 (T - T_0)$$

Where $\frac{\partial C_A}{\partial t} = -r(C_A, T)$ and $r(C_A, T) = k_0 C_A \exp\left(-\frac{E}{RT}\right)$

IC^s: For $t \leq 0, T = T_0, C_A = C_{A0};\ 0 < x < l$

BC^s: $-\lambda_2 \frac{\partial T}{\partial x} = q; 0 < t < t_q,\ x = 0$ and $\lambda_2 \frac{\partial T}{\partial x} = U(T - T_0);\ t > t_q, x = 0$

$-\lambda_1 \frac{\partial T}{\partial x} = U(T - T_0); t > 0, x = l$



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Ind. Eng. Chem. Res. 2010, 49, 21, 11001–11008

Model Description - Dimensionless parameters

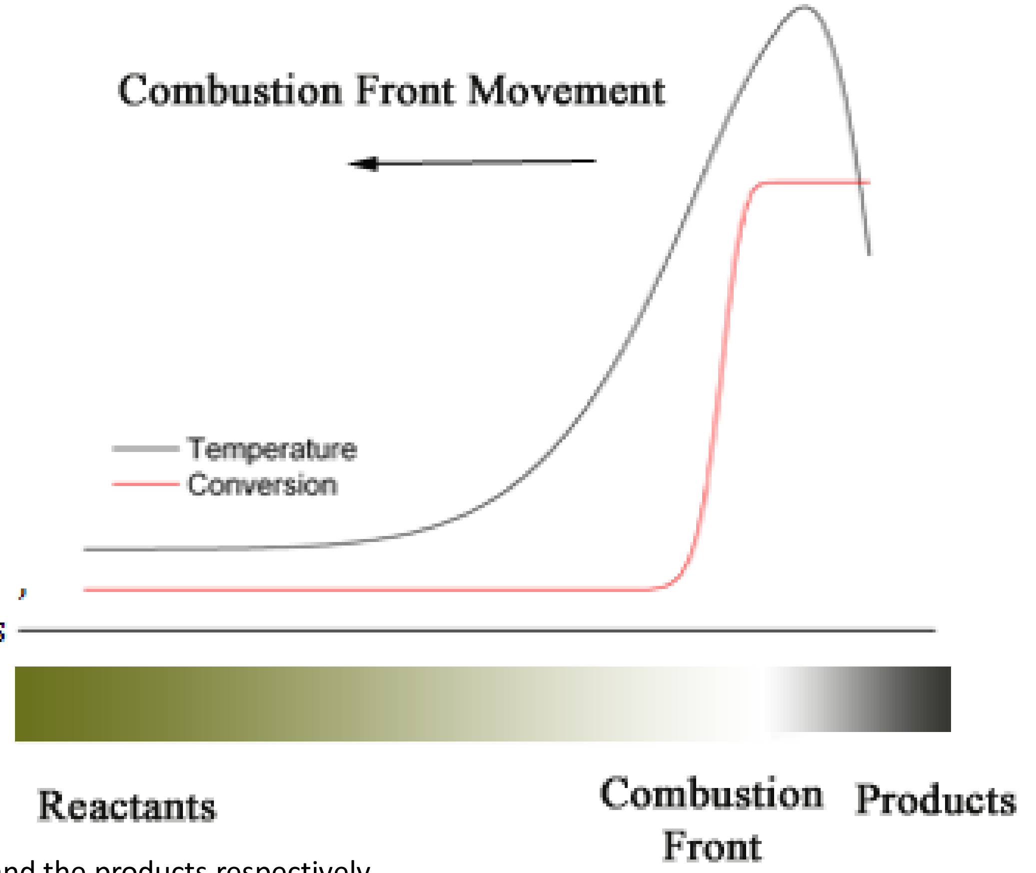
$$\theta = \frac{T}{T^*}, \quad \eta = 1 - \frac{C_A}{C_{A0}}, \quad \tau = \frac{t}{t^*}, \quad \xi = \frac{x}{x^*}, \quad t^* = \frac{\exp(\gamma)}{k_0}, \quad x^* = \left(\frac{\lambda_1 t^*}{\rho_1 c_{p1}}\right)^{\frac{1}{2}},$$

$$L = \frac{l}{x^*}, \quad \beta = \frac{(-\Delta H) C_{A0}}{c_{p1}\rho_1 T^*}, \quad \gamma = \frac{E}{RT^*},$$

$$\psi = \frac{q x^*}{\lambda_1 T^*}, \quad \alpha = \frac{\left(\frac{4U}{d}\right)_1 t^*}{c_{p1}\rho_1}, \quad Bi = \frac{U x^*}{\lambda_1},$$

$$a_p = \begin{cases} 1 & \text{for reactants} \\ \dfrac{\left(\frac{\lambda_2}{\rho_2 c_{p2}}\right)}{\left(\frac{\lambda_1}{\rho_1 c_{p1}}\right)} & \text{for products} \end{cases}, \qquad \delta = \begin{cases} 1 & \text{for reactants} \\ \dfrac{\left(\frac{\left(\frac{U}{d}\right)_2}{\rho_2 c_{p2}}\right)}{\left(\frac{\left(\frac{U}{d}\right)_1}{\rho_1 c_{p1}}\right)} & \text{for products} \end{cases},$$

$$N_f = \frac{n_g c_p^g}{-\Delta H}, \quad \mu = \frac{\left(\frac{\left(\frac{U}{d}\right)_2 dx^*}{\lambda_2}\right)}{\left(\frac{\left(\frac{U}{d}\right)_1 dx^*}{\lambda_1}\right)}$$



where the subscripts 1 and 2 represent the reactants and the products respectively.

Model Results

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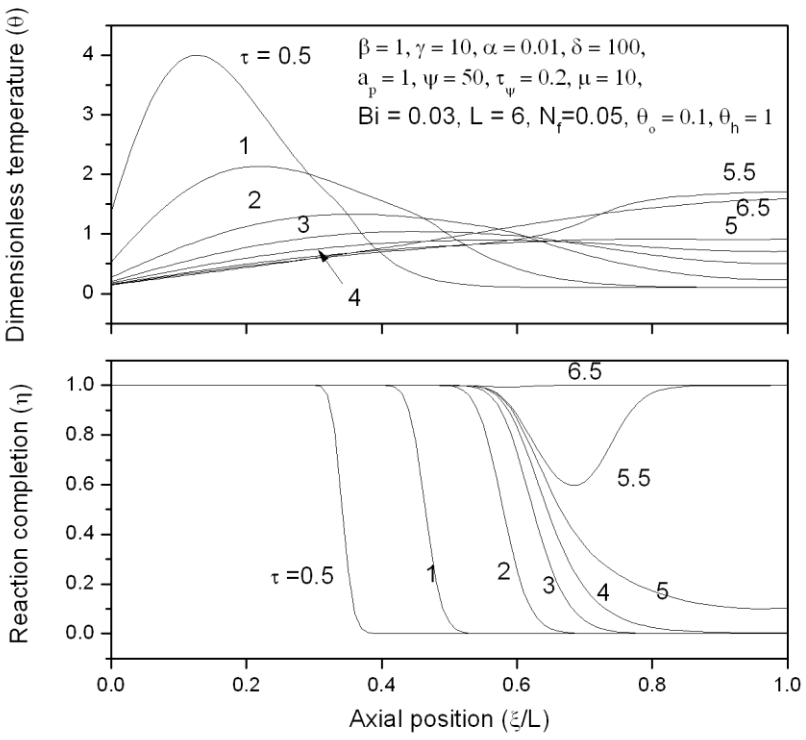
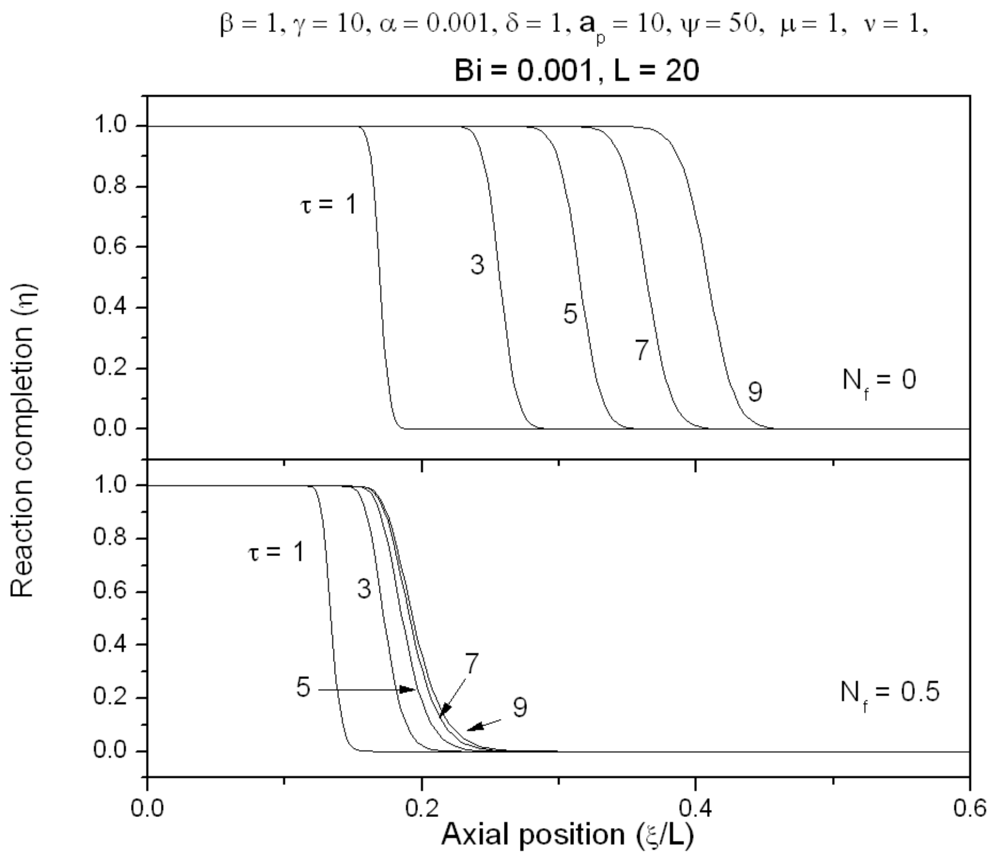
Temperature profile and combustion front with time



Effect of gas phase products:



Model Results

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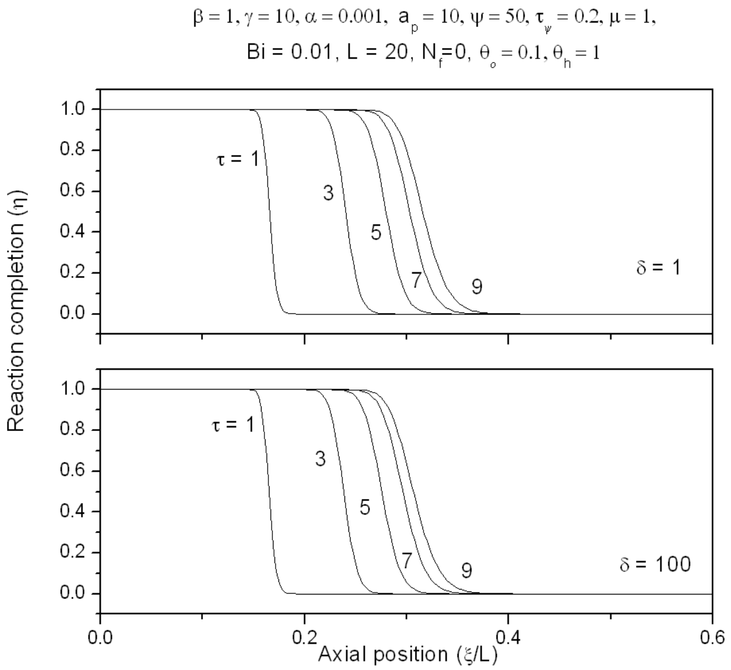
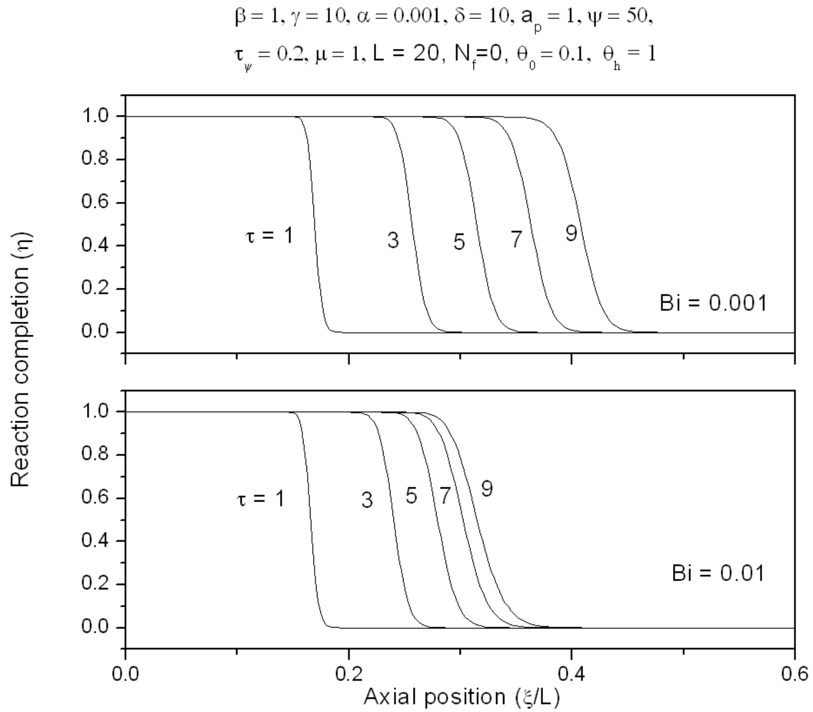
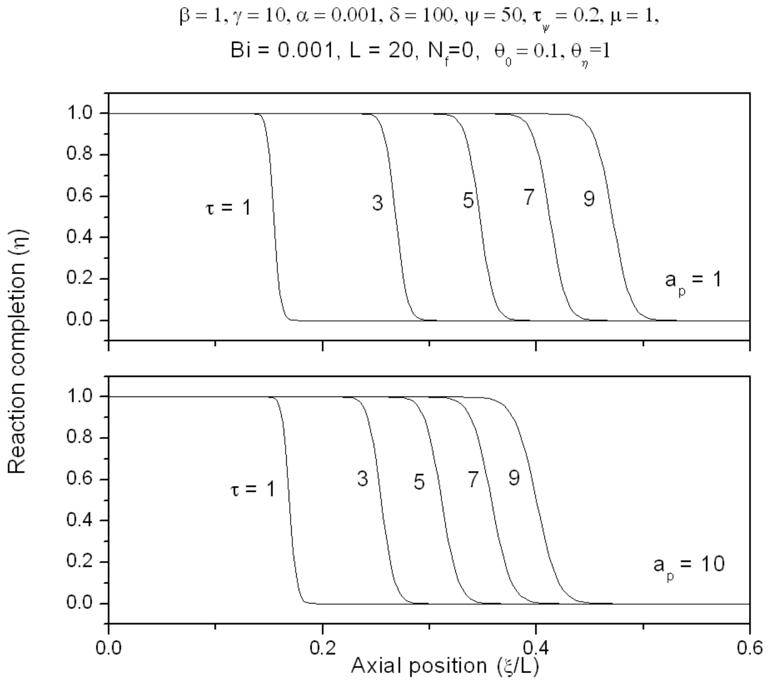
Effect of convective heat transfer: Due to change is surface area



Effect of change in Biot number:



Effect of change in thermal diffusivity:



Summary Points

In a typical self propagating process, the product gases evolved reduce the combustion temperature and slow down the front velocity.

The pores generated by these gases increase the total surface area and in turn further increases heat loss to the environment.

High thermal diffusivity of the product decreases the combustion front velocity and increases the width of combustion peak.

Heat loss from the product boundary increase the sharpness of the combustion peak.