Modelling of Unconventionally Catalytic Heated Reactors

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Highlights
- Revised Thiele modulus model for Joule heating and microwave heating
- New temperature-concentration relation for any reaction type
- Applicability to other nonconventional reactors

1. Introduction

Reactors with nonconventional heating schemes, such as those using Joule heating or microwaves, are emerging to replace conventional steam and furnace based heated reactors. Joule heating of catalyst involves applying an electric current [1, 2], whereas microwave heating involves the conversion of electromagnetic radiation into heat, resulting in rapid and selective heating [3-5]. These heating mechanisms can increase heating efficiency and decarbonize the chemical process industry. However, understanding the impact parameters have on achieving optimal operating conditions is key to taking these reactors to industrial scale. Analysis of the efficiency of isothermal catalytic reactions for a single pellet was first done by Thiele in 1939 [6] and others have expanded on the work by accounting for non-isothermal effects due to the heat of the reaction [7].

Here we extend the classical reaction engineering work for endothermic reactions to include unconventionally heated systems. We formulate the models and derive approximations for quick analytical estimations. We also perform simulations to validate the approximations and obtain concentration-temperature profiles. We will present extensions from simple reactions to real endothermic reactions, like methane reforming and propane dehydrogenation. In the classical non-isothermal pellet problem, endothermic reactions effectively remove heat and reduce the temperature and the reaction rate, deviating from isothermal reaction efficiency. We can determine the effective power needed to achieve the equivalent isothermal efficiency.

2. Methods

For constant volumetric heating, the steady state heat and mass equations are given by Eq. 1 and Eq. 2. With these, a new relationship between temperature and concentration can be derived (Eq. 3) which is an advancement on the derivation done by Prater [8], and holds for any reaction type with a form that changes based on the green function that describes the geometry. The parameters are: thermal conductivity: k, temperature: T, heat of reaction: $-\Delta H_{rx}$, reaction rate: r_{pore}, internal heating: Q, mass diffusivity: $\mathcal{D}$, concentration: C, surface: subscript 's', and Green's function: $G(\boldsymbol{r}, \boldsymbol{r}')$.

$$k\nabla^2 T = \Delta H_{rx} r_{pore} + Q \tag{1}$$

$$\mathcal{D}\nabla^2 C = r_{pore} \tag{2}$$

$$T - T_s = \frac{-\Delta H_{rx}\mathcal{D}}{k}(C_s - C) + \frac{Q}{k}\int G(\boldsymbol{r}, \boldsymbol{r}')d\boldsymbol{r}' \tag{3}$$

3. Results and discussion

These three equations are used to derive the three dimensionless numbers that govern the Thiele efficiency, Eq. 4, 5, and 6.

$$\alpha = \frac{QL^2}{kT_s}, \quad \beta = -\frac{C_s\mathcal{D}\Delta H_{rx}}{kT_s}, \quad \gamma = \frac{E_a}{RT_s} \tag{4,5,6}$$

The terms β and γ (Eq. 4 and 5) have been derived previously for the non-isothermal Thiele modulus and refer to the maximum temperature variation due to the reaction and the reaction rate temperature sensitivity, respectively. The new term, α, is a dimensionless power that measures the net heating rate of a catalyst. Fig. 1 shows an example of the power needed to achieve equivalent isothermal efficiency for a pore undergoing a first order endothermic reaction. We show that one can derive simple models to predict the input power needed to operate a reactor with equivalent isothermal efficiency. The generality of how this model is derived also allows us to easily replace Q with a more fundamental heating description of heating, such as voltage for Joule heating, or dielectric properties for microwave heating.
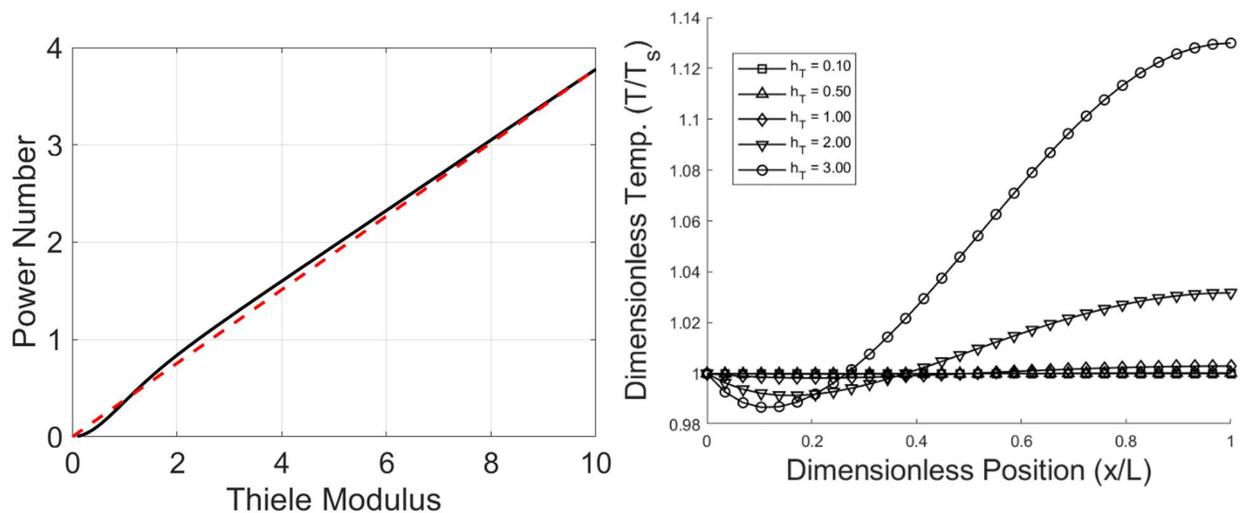
Figure 1. *(left) Power vs, Thiele modulus in a pore (black line) with a linear (red) line of a first order, endothermic reaction with $\beta = -0.5$ and $\gamma = 10$. (Right) Temperature profile under the same conditions*

4. Conclusions

We derive the fundamental models for a single pore to design large scale electrified heated reactors. This multi-scale modelling is key to understanding these next generation reactors. We demonstrate the performance of real reactions and expand the analysis to various catalyst geometries using Eq. 4.

References
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