Runaway in micro-channel reactors.

Sunjeev Venkateswaran, Costas Kravaris, Benjamin A. Wilhite*

Department of Chemical Engineering, Texas A&M University,

**Corresponding author: benjaminwilhite@exchange.tamu.edu*

Highlights

- Runaway criteria in micro-channel reactors.
- Asymptotic behavior for extreme values of conduction parameters.
- Influence of conduction and packing losses on critical values.

1. Introduction

Many of the reactions in micro-channel reactors such as combustion are highly exothermic and bring with them the possibility of runaway. Micro-channel reactors are different from conventional tubular reactors due to their larger wall/reactor volume ratios. Consequently, the effect of wall conduction on runaway cannot be neglected. In this work the influence of wall conduction and heat losses through the wall on critical parameters for runaway is studied. The applicability of quick explicit criteria derived for tubular reactors for micro-channel reactors is investigated.

2. Methods

Since our aim is to gauge the effect of conduction on critical runaway parameters, a 1D model is used with an axial wall conduction term in the energy balance for the wall. Radial conduction and diffusion is neglected. The walls are insulated and the coolant temperature is constant. The surface area-volume ratio for both the reactor and the wall is assumed to be equal. Only nth order elementary kinetics is considered. The steady state equations are:

Mass Balance

$$\frac{du}{ds} = -k_0.\,exp^{\left[\frac{\theta}{1+\frac{\theta}{\gamma}}\right]}.\,u^n \quad (1)$$

Energy Balance- Gas Phase

$$\frac{d\theta}{ds} = B.\,Da.\,exp^{\left[\frac{\theta}{1+\frac{\theta}{\gamma}}\right]}.\,u^n - St_1.\,(\theta-\theta_w) \quad (2)$$

Energy Balance- Solid Wall

$$\frac{d^2\theta_w}{ds^2} = -\left[\frac{St_1}{CP}(\theta-\theta_w) + \frac{St_2}{CP}.\,(\theta_c-\theta_w)\right] \quad (3)$$

Boundary Conditions

$$u_A(0) = u_{Ai}, \theta(0) = \theta_i, \frac{d\theta_w}{dz}(0) = Bi.\,(\theta_w - 1), \frac{d\theta_w}{dz}(1) = Bi.\,(1-\theta_w) \quad (4)$$

Where Da-Damkolher Number, B- Dimensionless Adiabatic temperature, St- Stanton Number, CP- conduction parameter, Bi-Biot number. For convenience, St_1 is assumed to be equal to St_2.
Order of magnitude analysis is employed to reduce the model equations to two distinct tubular reactors for low and high values of the conduction parameters (CP) respectively. Influence of wall conduction and heat losses is studied by using parametric sensitivity analysis on the whole model[1, 2]. The critical values obtained from

parametric sensitivity analysis is compared to the values obtained from the explicit criteria by Wu, Morbidelli and Varma[3], and Van Welsenare and Froment[4] for low and high values of CP.

3. Results and discussion

The effect of conduction on the critical stanton number for different Biot numbers (a measure for heat loss) is shown in fig(1).

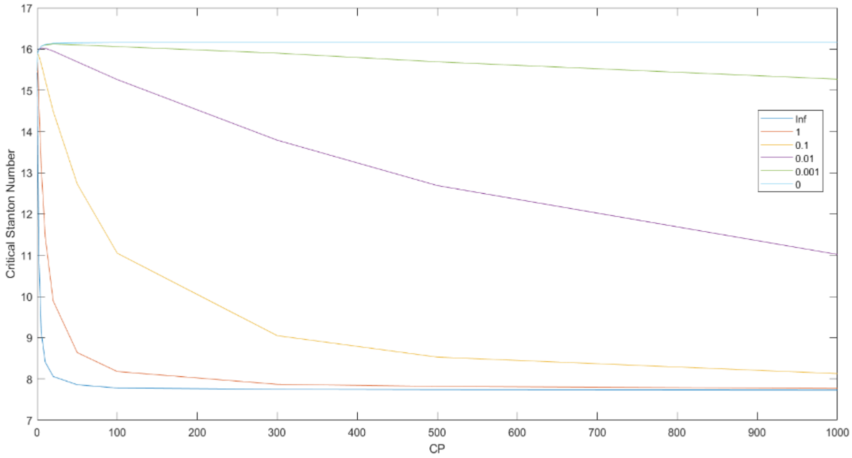

Figure 1 - Effect of CP and heat losses on critical Stanton number. Legend- Different Biot numbers. Parameters: B=40, Da=0.1, γ=20.

<u>Behavior at Low CP-</u> Irrespective of the magnitude heat losses, as the CP is decreased, the critical Stanton number approaches critical value of the tubular reactor approximation derived from order of magnitude estimates. **<u>Behavior at high CP-</u>** The critical stanton number approaches an asymptotic value equal to the critical stanton number of another distinct tubular reactor approximation derived from order of magnitude analysis. Since the micro-channel reactor for low CP approximately mimics a tubular reactor, the explicit criteria by Wu et al and Van Welsenare and Froment work well (Van Welsenare and Froment's criteria is more conservative for low B, but this is because the criterion is inherently conservative).

For intermediate values of CP, it is observed that both packing losses and heat conduction work together. Increasing CP, while keeping the ends insulated restrict the role of conduction because of which the critical Stanton number remains almost constant for practical values of CP. However, as we increase the Biot number the role of conduction is augmented and the approach to the asymptotic value is faster.

4. Conclusions

The behavior of micro-channel reactors mimics two distinct tubular reactors for high and low values of CP. This allows us to use quick explicit criteria for the calculation of critical parameters for runaway for these extreme values. Finally, it is observed that the effect of CP on runaway is enhanced if Bi (packing losses) is high.

References

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Keywords
Runaway; Sensitivity; Wall conduction