A Computationally Efficient 2D Pseudo-Homogeneous Reactor Model for Evaluating Operational Strategies in Exothermic Packed-bed Reactors

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Highlights

- Two-dimensional model reproduces experimental hotspot location and temperature profile
- Captures temperature gradients without requiring full CFD simulation
- Model enables assessment of catalyst replacement frequency

1. Introduction

In this work, a heterogeneous reactor model is presented for a highly exothermic reaction involving rapid kinetics:

$$A + B \rightleftharpoons C$$

The reaction is carried out in a commercial multi-tubular fixed-bed reactor with the catalyst packed inside the tubes.[1] Heat from the highly exothermic reaction is removed by a coolant circulating on the shell side.[2,3] Catalyst deactivation is an important aspect in the process, and the ability to assess the need for catalyst replacement on the occasion of a reactor shutdown would be a significant asset.

2. Methods

A pseudo-homogeneous reactor model is implemented, accounting for radial heat and mass gradients. Pure transport by convection is assumed in the axial direction, and axial heat and mass dispersion are neglected.

$$u_s \frac{\partial c_k}{\partial z} = D_{er}\left(\frac{\partial^2 c_k}{\partial r^2} + \frac{1}{r}\frac{\partial c_k}{\partial r}\right) + a(r,z)\,\rho_{cat}\,R_k$$

$$u_s \rho_f c_{p,f} \frac{\partial T}{\partial z} = \lambda_{er}\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) + a(r,z)\rho_{cat}\,R_k(-\Delta H_r)$$

BCs: inlet conditions at z = 0, symmetry condition at r = 0, and wall conditions at r = R_t

Catalyst deactivation is taken into account via an activity factor. A kinetic model has been constructed with the parameters determined from internal experimental data. The intrinsic kinetics are expressed as a Langmuir–Hinshelwood–Hougen–Watson (LHHW) rate written in terms of partial pressures P_A, P_B, P_C. The rate expression balances forward and reverse driving forces and includes adsorption terms for A and B in the denominator.

$$R_C = \frac{k\left(P_A P_B - {P_C}/{K_{eq}}\right)}{1 + K_A P_A + K_B P_B}$$

3. Results and discussion

At reactor start-up, the temperature rises rapidly near the inlet due to heat release from the exothermic reaction in the active region. The model captures the main features of the experimental temperature profile, including the position and maximum hotspot temperature. As shown in the contour plot in Figure 1, radial temperature gradients arise from heat removal at the reactor wall through the coolant, which leads to lower temperatures near the wall compared with the reactor centerline. Approximately 1% of the extended reactor operating period can be simulated within about 20 seconds.

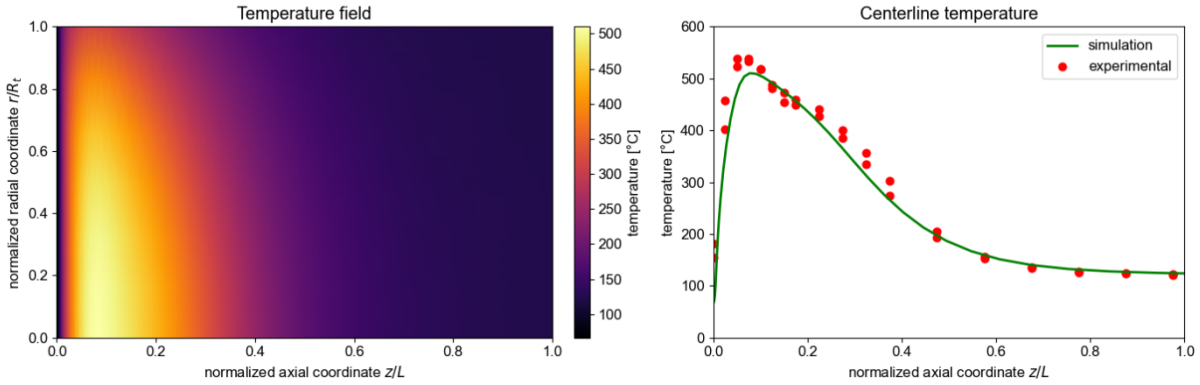

Figure 1. Simulated reactor temperature field as a function of axial and radial position at start-up, together with the corresponding centerline temperature profile, compared with experimental measurements.

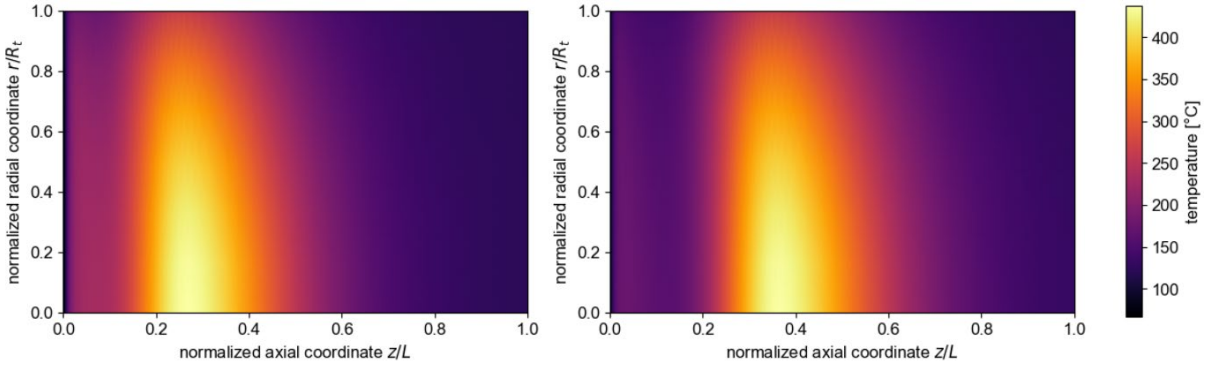

Figure 2. Simulated 2D reactor temperature after 50% (left) and 75% (right) of the total reactor operating period.

Figure 2 shows that after approximately 50% of the reactor operating period, the hotspot has shifted downstream compared with the start of operation. The active reaction zone is no longer located near the reactor inlet and instead moves further into the catalyst bed. After approximately 75% of the reactor operating period, the active region shifts even further downstream as catalyst deactivation progresses.

Deactivation depends on local conditions such as temperature and concentration. As the upstream catalyst gradually loses activity, the reactants survive further into the bed and are no longer fully consumed near the reactor entrance. Consequently, the reactive zone progressively moves deeper into the reactor as a function of time on stream. Analysis of catalyst deactivation behavior can support more efficient reactor operation by reducing the frequency of catalyst replacements and thereby maximizing reactor runtime.

4. Conclusions

The two-dimensional pseudo-homogeneous reactor model reproduces the experimental temperature profile while remaining computationally efficient. It provides reliable reactor predictions without requiring full CFD simulations. The model can therefore be used to predict reactant breakthrough, to support decisions on catalyst replacement frequency, and to develop operational strategies to reduce catalyst deactivation.

References

[1] A. Romero-Limones, J. Poissonnier, C.O. Castillo-Araiza, J.W. Thybaut, Chem. Eng. J. 475 (2023) 146167.
[2] H. Bakhtiary-Davijany, F. Hayer, X.K. Phan, R. Myrstad, H.J. Venvik, P. Pfeifer, A. Holmen, Chem. Eng. J. 167 (2011) 496–503.
[3] H.L. Huynh, W.M. Tucho, Q. Shen, Z. Yu, Chem. Eng. J. 428 (2022) 131106.

Keywords
Reactor model; Exothermic reaction; Fixed-bed reactor