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Dimensionless description of non-isothermal fixed-bed catalytic reactors

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ABSTRACT

This paper presents a dimensionless reaction–diffusion–energy model for a non-isothermal fixed-bed reactor. The model integrates chemical kinetics, mass transfer, heat transfer, and wall heat exchange within a unified framework. It is formulated in terms of dimensionless parameters, including the Damköhler, Péclet, Lewis, and Biot numbers, enabling the analysis of coupled transport and reaction processes within a consistent parametric space. To evaluate the stability of operating regimes, an integral energy-efficiency index η_e is introduced, quantifying the balance between heat generation and heat removal. Numerical results show that increasing the Damköhler number enhances conversion but also intensifies temperature gradients. Higher temperature sensitivity leads to stronger thermal feedback and the formation of pronounced temperature maxima. An optimal operating region ($Da \approx 2$) is identified, where η_e reaches a maximum (0.74–0.76), indicating that maximum conversion does not coincide with maximum energy efficiency. Model validation against data from an industrial phosphine oxidation reactor shows deviations within 5–7%, confirming its predictive capability. The proposed approach can be used for reactor design, optimization, and thermal regime analysis, providing a computationally efficient alternative to more complex models while preserving physical fidelity.

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1. INTRODUCTION

Catalytic reactors with a fixed bed catalyst are widely used in chemical and petrochemical processes due to their high selectivity and operational reliability. The productivity of such reactors is determined by the combined interaction of chemical kinetics, mass transfer, and heat transfer inside the porous catalytic layer. In exothermic conditions, this interaction becomes strongly nonlinear. When local heat is released, reaction rates accelerate and temperature gradients increase, which can lead to the formation of hot spots. This effect

limits the stability of the process, imposing strict requirements on thermal regulation and reactor design [1]–[5]. Existing one-dimensional models can describe conversion and temperature profiles, whereas computational fluid dynamics (CFD) models provide detailed local information at high computational cost. However, none of these approaches is usually used to obtain a compact dimensionless criterion that directly relates reaction intensity, heat dissipation, and thermal stability. This gap is important for the preliminary design of the reactor, where a quick assessment of safe and energy-compatible modes of operation is required.

In this study, a one-dimensional non-isothermal reaction-diffusion-energy model is proposed in dimensionless form. The model combines kinetic reactions, mass transfer, heat transfer and heat transfer through the walls into a single system of equations. To evaluate the operation of the reactor, which goes beyond the scope of conversion only, the integral indicator of energy efficiency η_e, is introduced. This indicator characterizes the balance between the heat released by the reaction and the heat removed through the walls of the reactor.

The model was validated using data from an industrial phosphine oxidation reactor, which allows us to estimate its prognostic ability in realistic operating conditions [6]. The main results of this study: i) development of dimensionless reaction-diffusion-energy model for non-isothermal fixed-bed reactors; ii) introduction of the integral indicator of energy efficiency η_e to estimate the thermal stability of work modes; iii) analysis of the relationship between energy efficiency and dimensionless parameters Da, Pe, Le, and Bi; and iv) validation model based on industrial reactor.

The purpose of the study is the numerical analysis of the proposed model and the determination of operating modes that provide a balance between energy conversion, thermal stability, and energy efficiency.

2. RELATED WORKS

Fixed-bed reactors have long been used as reference systems for studying the interaction between reaction kinetics and transport processes in heterogeneous catalysis. Early analytical and numerical studies described the fundamental mechanisms of nonisothermal behavior, including temperature maxima and multiple steady states. Later models incorporated axial dispersion and effective thermal conductivity, improving the agreement between calculated and observed reactor behavior [7], [8].

Computational fluid dynamics (CFD) has extended the analysis of coupled flow, heat, and mass transfer by incorporating reactor geometry and catalyst structure. Multidimensional, particle-resolved models provide detailed local information and high prediction accuracy. Their main limitation is computational cost, which limits their use in routine engineering calculations and large-scale parametric studies [9], [10]. Therefore, one-dimensional models remain relevant for reactor design. They offer a practical balance between physical adequacy and computational efficiency. In these models, dimensionless parameters, including the Damköhler, Peclet, Lewis, and Biot numbers, describe the relative roles of kinetics, diffusion, convection, and heat transfer [11].

Despite these developments, existing approaches rarely relate transport phenomena to the overall reactor energy efficiency in a dimensionless form. This limits their use in problems where heat management and thermal stability are design constraints [12], [13]. Table 1 summarizes the evolution of fixed-bed reactor modeling approaches and shows the status of this work. The proposed model extends traditional one-dimensional formulations by adding an energy-based performance metric while maintaining computational efficiency [14]. The studies reviewed demonstrate that reaction-diffusion modeling is well-developed for describing kinetic and transport phenomena, while energy-based estimation remains less formalized. This study addresses this limitation by combining a dimensionless one-dimensional formulation with an integral exponent for heat generation and removal. The next section presents the model formulation and assumptions [15].

Table 1. Evolution of fixed-bed reactor modeling approaches and the status of this work

Study	Dimensionality	Core focus/coupling	Method	Energy efficiency	Validation/limitation
Froment *et al*. (1990) [5]	1D	Reaction–diffusion and stability	FD	—	Analytical; no energetic link
Luss and Amundson (1967) [2]	1D	Non-isothermal kinetics and hot spots	FD/analytical	—	Theoretical; small scale
Stegehake *et al*. (2019) [7]	1D–2D	Heat–mass transport; validation	FEM/CFD-assisted	—	Benchmark; high computational cost
Jurtz *et al*. (2019) [11]	3D	Particle-resolved flow and heat transfer	CFD	—	Experimental; geometry-specific
Dixon and Partopour (2020) [16]	1D–3D	Reactor design; hybrid coupling	Hybrid CFD	Partial	Industrial; weak energy link
Present work (2025)	1D	Unified reaction–diffusion–energy model	Crank–Nicolson + Newton–Raphson	Yes (η_e)	Industrial validation (±6%)

3. METHOD

The model describes coupled reaction kinetics, mass transfer, and heat transfer in a non-isothermal fixed-bed reactor. It is formulated in dimensionless variables using the Damköhler (Da), Péclet (Pe), Lewis (Le), temperature sensitivity (β), and Biot (Bi) numbers [17], [18]. The problem is treated as a boundary value problem for a nonlinear system of differential equations. The numerical solution is obtained using a finite-difference scheme, and the nonlinear algebraic system is solved iteratively. The implementation was carried out in Python using the NumPy and SciPy libraries [19], [20]. The overall research procedure is summarized in Figure 1. The workflow includes parameter selection, nondimensionalization of the governing equations, numerical solution of the boundary value problem, parametric analysis, validation against industrial data, and interpretation of the results using the energy-efficiency indicator η_e.

3.1. Physical model and assumptions

A tubular reactor with a fixed bed of porous catalyst is considered. A gas mixture flows through the catalyst bed in the axial direction, and the reaction occurs on the catalyst surface, releasing heat. The one-dimensional approximation is justified by the reactor geometry, with L/D much greater than 10, for which axial gradients dominate radial variations [20]. The pseudo-homogeneous model assumes local thermal equilibrium between the gas and solid phases. This approximation is acceptable for small catalyst particles and efficient heat transfer within the bed, when the thermal equilibration time is shorter than the reaction time [5]. The model includes convective and diffusive transport, thermal conduction, reaction heat release, and heat exchange with the reactor wall. Radiative effects and radial gradients are neglected, and thermophysical properties are treated as constant, which is consistent with standard engineering assumptions for this class of systems [5]. These assumptions limit the model to regimes with moderate radial non-uniformity and negligible radiative effects. A schematic representation of the coupled processes is shown in Figure 2 [21].

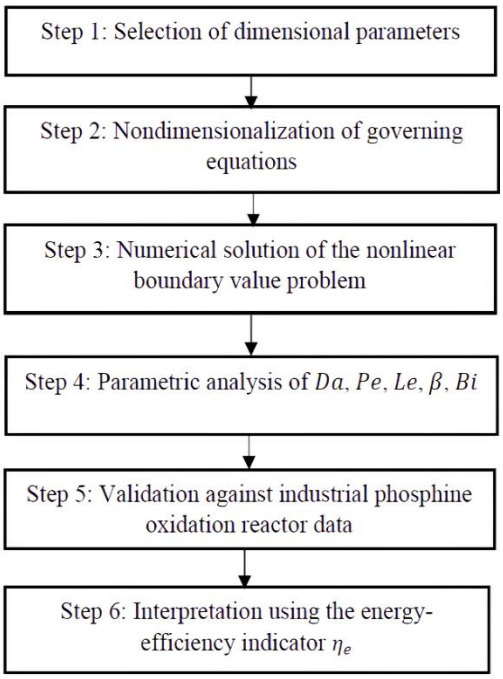


Figure 1. Structured workflow of the proposed study

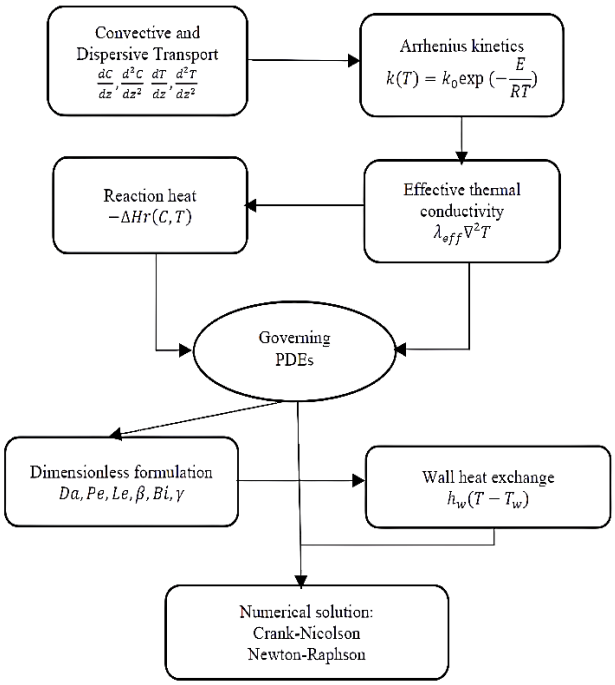


Figure 2. Schematic representation of the one-dimensional non-isothermal reaction–diffusion–energy model

3.2. Governing equations

The model considers steady-state concentration and temperature distributions along the reactor axis for an irreversible first-order reaction. In dimensionless form, the governing equations are (1) and (2):

$$\frac{1}{Pe}\frac{d^2C}{dz^2} - \frac{dC}{dz} - Da\, f(C,T) = 0 \quad (1)$$

$$\frac{1}{PeLe}\frac{d^2T}{dz^2} - \frac{dT}{dz} + \gamma\, Da\, f(C,T) - Bi\,(T - T_w) = 0 \quad (2)$$

The reaction rate is expressed as (3):

$$f(C,T) = C * \exp\left(\beta \frac{T-1}{T}\right) \quad (3)$$

where $\beta = E/RT_0$ is the dimensionless temperature sensitivity, which controls the strength of thermal feedback. Higher values of β lead to stronger thermal coupling and more pronounced temperature maxima. The boundary conditions are defined as (4):

$$z = 0: C = 1, T = 1, z = 1: dC/dz = 0, dT/dz = 0 \quad (4)$$

This formulation represents a convective system and avoids non-physical reflections at the outlet.

3.3. Dimensionless parameters and energy efficiency index

The main dimensionless parameters of the model are summarized in Table 2.

Table 2. Dimensionless parameters governing transport, kinetics, and heat exchange in the model

Symbol	Definition	Physical meaning
Da	kL/u	Ratio of reaction rate to convective transport
Pe	uL/D	Ratio of convective to diffusive transport
Le	α/D	Ratio of thermal to mass diffusivity
β	$E/(RT_0)$	Temperature sensitivity of reaction rate
Bi	$hwL/\lambda eff$	External heat transfer intensity
γ	$(-\Delta HC0)/\rho cpT0$	Dimensionless heat generation (adiabatic temperature rise)

The integral energy-efficiency indicator is defined as (5):

$$\eta_e = \frac{\int_0^L h_w(T-T_w)dz}{\int_0^L (-\Delta H) r(C,T) dz} \quad (5)$$

This indicator represents the ratio of heat removed through the reactor wall to the total heat generated by the reaction. Values of η_e close to unity correspond to a thermally balanced regime. Lower values indicate imbalance caused either by insufficient heat generation at low Da or by heat localization near the hot spot at high Da. Unlike conversion, which measures reactant consumption, and unlike maximum temperature, which reflects only a local thermal extreme, η_e provides an integral measure of the heat balance along the reactor bed. It compares the total heat removed through the reactor wall with the heat generated by the reaction. Therefore, η_e can distinguish between regimes with similar conversion but different thermal safety and heat-removal consistency.

The selected parameter ranges correspond to typical fixed-bed reactor conditions and cover transitions between kinetically controlled and transport-limited regimes. The range $Da = 0.5 - 5.0$ describes the transition from kinetic control to regimes with pronounced thermal and diffusion effects. The range $Pe = 20 - 100$ represents diffusion-influenced and convection-dominated transport, while $Le = 1 - 5$ reflects the relative importance of thermal and mass diffusivity.

3.4. Parameter selection, numerical scheme, and model validation

Model parameters were selected based on literature data and established correlations for porous catalytic systems [5]. The parameter values and ranges used in the simulations are summarized in Table 3. The governing equations were solved using an implicit Crank–Nicolson finite-difference scheme combined with the Newton–Raphson method. The spatial domain was discretized by a uniform grid with N nodes and step size $\Delta z = 1/(N - 1)$. Diffusion terms were approximated by second-order central differences, while convective terms were discretized using a first-order upwind scheme.

Convergence was assessed using the $L\infty$ norm, defined as the maximum absolute residual of the governing equations over all grid points. The iteration was stopped when the residual became lower than 10^{-6} for both temperature and concentration. Grid independence was checked by varying N from 50 to 200; the relative deviation in peak temperature with respect to the finest grid did not exceed 1.2%. Linear temperature and concentration profiles were used as the initial approximation. No spurious oscillations were observed during grid refinement.

Table 3. Model parameters and ranges used in simulations

Parameter	Symbol	Range/value	Unit	Source/note
Gas velocity	U	0.5–1.5	m s^{-1}	Typical operation
Effective diffusivity	$Deff$	1×10^{-8}–5×10^{-7}	m^2 s^{-1}	Porous media
Thermal conductivity	λeff	0.2–1.0	W m^{-1} K^{-1}	Froment *et al.* (1990) [5]
Volumetric heat capacity	$(\rho\, c_p)eff$	1000–2000	J kg^{-1} K^{-1}	$Ni/\gamma - Al_2O_3$ catalyst
Inlet concentration	C_0	0.5–1.0	mol m^{-3}	Feed data
Inlet temperature	T_0	300–350	K	Operating range
Wall heat-transfer coeff.	hw	100–300	W m^{-2} K^{-1}	Equipment data
Reaction enthalpy	$-\Delta H$	60–120	kJ mol^{-1}	Exothermic systems
Pre-exponential factor	k_0	10^5–10^8	s^{-1}	Literature range
Activation energy	E	60–90	kJ mol^{-1}	Typical kinetics
Reactor length	L	1–3	m	Pilot scale
Bed diameter	D	0.01–0.1	m	Geometry
Biot number	Bi	0.1–1.0	—	Defined as $Bi = hw\,L\,/\,\lambda eff$

Model validation was performed using data from an industrial phosphine oxidation reactor reported in [6]. The validation case corresponds to a tubular fixed-bed reactor operating under gas-phase flow conditions. The reactor contains a packed bed of porous catalyst and the reacting gas mixture passes through the bed in the axial direction. The process is exothermic; therefore, heat release within the catalyst bed and wall heat exchange determine the temperature field. The validation conditions included a temperature range of 300–350 K and a contact time of 0.3–0.4 s. Model accuracy was assessed using relative errors for temperature profiles, outlet conversion, and integral reactor characteristics such as residence time and bed height. Deviations did not exceed 5–7%. Uncertainty arises from three sources: model assumptions, parameter estimation, and measurement errors in industrial data. The largest deviations occur near the hot spot region, where local temperature gradients may be underestimated. Within the considered operating range, the model reproduces the main features of reactor behavior [22].

4. RESULTS AND DISCUSSION

Numerical simulations were performed for parameter ranges corresponding to typical operating conditions of non-isothermal fixed-bed reactors. The reference case was defined as $u = 1.0\,m\,s^{-1}$, $Deff = 2\times10^{-7}\,m^2\,s^{-1}$, $\lambda eff = 0.5\,W\,m^{-1}\,K^{-1}$, $Bi = 0.5$, $Da = 1$, $Pe = 50$, $Le = 2$, and $\beta = 15$.

Under these conditions, the steady-state profiles shown in Figure 3 indicate a conversion of 94–96%. The maximum dimensionless temperature reaches $T_{max} \approx 1.13 - 1.16\,T_0$ and is located at $z \approx 0.35 - 0.45$. The concentration decreases monotonically along the reactor bed, while the temperature profile has a single maximum in the reaction zone.

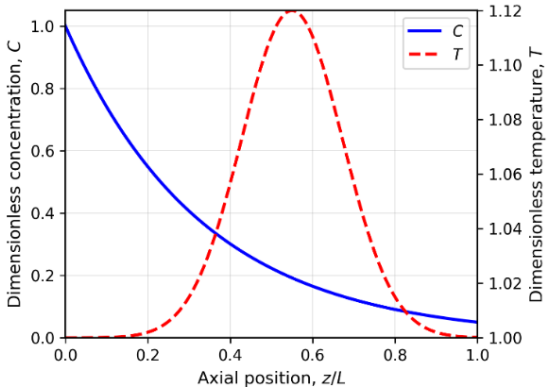
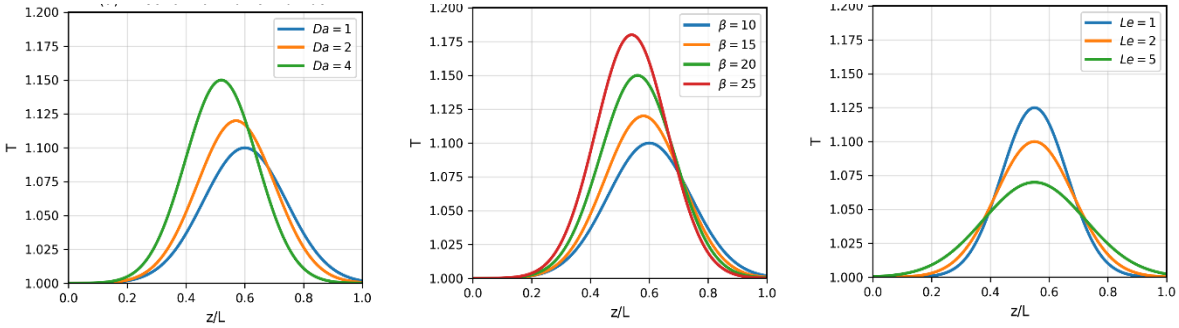


Figure 3. Axial profiles of dimensionless temperature and concentration

4.1. Numerical results

The influence of the main dimensionless parameters on the axial temperature profiles was analyzed for $Da = 0.5 - 5.0$, $\beta = 10 - 20$, and $Le = 1 - 5$, with the results summarized in Figure 4. Increasing Da from 0.5 to 2 increases conversion from approximately 75% to 97% and raises T_{max} by 8–12%, as shown in

Figure 4(a). At $Da > 3Da$, the additional conversion gain remains below 2%, whereas T_{max} continues to increase and the hot spot shifts toward the reactor inlet. The effect of temperature sensitivity is presented in Figure 4(b). Increasing β from 10 to 20 produces a nonlinear rise in the maximum temperature because of stronger thermal feedback. At $\beta > 18$, T_{max} reaches approximately 1.20–1.25 T_0, indicating an increased risk of thermal instability. Figure 4(c) demonstrates that increasing Le from 1 to 5 reduces T_{max} by approximately 5–10% and smooths the axial temperature profile because of more effective heat redistribution relative to mass transport.



(a) (b) (c)

Figure 4. Effects of dimensionless parameters on axial temperature profiles: (a) Damköhler number (Da); (b) temperature sensitivity (β); and (c) Lewis number (Le)

The energy-efficiency indicator η_e also shows a non-monotonic dependence on the governing parameters, as presented in Figure 5. In the range $Da = 0.5 - 2.5$, η_e increases from 0.66 to 0.74–0.76 and reaches its maximum near $Da \approx 2$ and $Pe \approx 40 - 60$. At $Da > 3$, η_e decreases to 0.68–0.70, although conversion remains above 97%. At $Pe < 20$, stronger axial diffusion lowers T_{max} but reduces η_e by 5–8%. At Le>3, the dependence of η_e on Da becomes weaker.

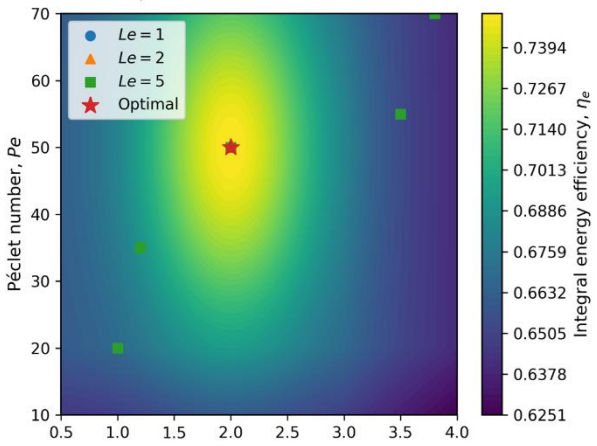
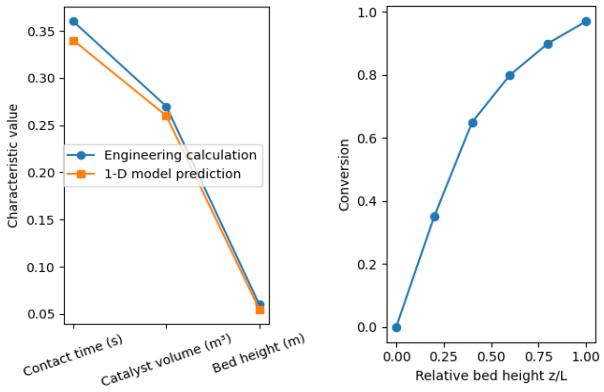


Figure 5. Dependence of η_e on Da and Pe for different Le

Model validation was performed using industrial phosphine oxidation reactor data, and the overall validation results are presented in Figure 6. Figure 6(a) compares the engineering calculations with the predictions of the one-dimensional model for the principal reactor parameters. The deviations between the two approaches remain within 5–6%, as summarized in Table 4, while the relative error in the predicted temperature profiles does not exceed 5–7%. Figure 6(b) shows the axial conversion profile along the reactor bed. The model predicts a progressive increase in conversion and an outlet value of approximately 97–98%, demonstrating satisfactory agreement with the reference industrial reactor performance.



(a) (b)

Figure 6. Model validation under representative operating conditions: (a) engineering calculations versus 1D model predictions and (b) axial conversion profile

Table 4. Comparison of engineering data and model predictions

Parameter	Engineering	Model	Deviation
Contact time (s)	0.360	0.340	5.6%
Catalyst volume (m³)	0.267	0.255	4.5%
Bed height (m)	0.060	0.057	5.0%
PH_3 conversion (%)	Design target	97–98	Within tolerance

4.2. Physical discussion

The numerical results show that the Damköhler number mainly controls reaction intensity. At low Da, the reaction rate is insufficient to produce high conversion and a strong thermal response. As Da increases, the reaction zone becomes more active, conversion rises, and local heat release increases. When Da exceeds 3, conversion is already close to its limiting value, but additional reaction intensification mainly increases the temperature maximum. This explains why high Da produces a stronger hot spot without a proportional gain in conversion.

The temperature sensitivity parameter β determines the strength of thermal feedback. Larger β values make the reaction rate more sensitive to local temperature changes. As a result, heat release becomes concentrated in a narrower region of the bed, and the temperature maximum increases sharply. Values of $\beta > 18$ indicate a regime close to thermal instability, especially when heat removal is insufficient.

The Lewis number affects the balance between thermal and mass diffusion. Higher Le values improve heat redistribution relative to mass transport, which reduces the temperature maximum and smooths the profile. This explains the stabilizing effect observed in Figure 4(c). The Péclet number affects axial redistribution: low Pe enhances axial diffusion, which lowers the peak temperature but spreads heat along the bed and reduces η_e. The predicted temperature rise of 10–25% above T_0 is consistent with published experimental and numerical data for exothermic catalytic reactions, including CO oxidation on supported catalysts [23]–[25]. Unlike detailed CFD models, the present formulation does not resolve local flow and particle-scale effects, but it captures the main integral behavior of the reactor with lower computational cost.

4.3. Engineering interpretation

The results indicate that maximum conversion and maximum energy efficiency do not occur under the same conditions. The most favorable operating range is $Da \approx 1.5 - 2.5$, where conversion is high and η_e reaches its maximum without excessive temperature growth. At larger Da, conversion remains high, but heat localization reduces thermal consistency and increases the risk of hot spot formation.

For reactors operating at high β, heat removal becomes a critical design factor. Stronger wall heat exchange or higher effective thermal conductivity is required to prevent localized overheating. Increasing Le has a stabilizing effect and can be used as a design direction through catalyst-bed properties, reactor internals, or heat-transfer enhancement.

The proposed model is suitable for preliminary reactor analysis. It can be used to define safe operating ranges, compare thermal regimes, estimate overheating risk, and select conditions in which reaction intensity and heat removal remain balanced. It is not intended to replace CFD calculations for detailed geometry-dependent analysis, but it can reduce the number of cases requiring high-fidelity simulation.

4.4. Limitations and future work

The accuracy of the model is limited by its one-dimensional, pseudo-homogeneous, and steady-state assumptions. The pseudo-homogeneous approximation neglects pore diffusion and interphase heat transfer, which may lead to underestimation of local temperatures at high reaction rates. The one-dimensional formulation does not capture radial gradients; this becomes important under intense heat release or non-uniform flow. The steady-state formulation also excludes startup, shutdown, and dynamic instability [26].

The largest errors are expected near the hot spot, where local temperature gradients are strongest. At high Da and β, pore diffusion and local heat-transfer resistance may become significant. For complex reactor geometries, non-uniform packing, or strong radial heat losses, CFD or multidimensional models are required.

Future work should focus on direct comparison with CFD simulations, extension of the model to transient conditions, inclusion of pore diffusion and interphase heat transfer, and testing with more complex reaction kinetics.

5. CONCLUSION

This study developed a dimensionless reaction–diffusion–energy model for a non-isothermal fixed-bed reactor. The model combines reaction kinetics, mass transfer, heat transfer, and wall heat exchange and introduces the integral energy-efficiency indicator η_e to evaluate the relation between heat generation and heat removal. The simulations show that Da increases conversion but also strengthens temperature gradients; β controls the intensity of thermal feedback; and Le reduces peak temperatures through enhanced heat redistribution. The most favorable operating range is $Da \approx 1.5 - 2.5$, where high conversion is achieved without excessive thermal gradients and η_e reaches its maximum.

Validation against industrial phosphine oxidation data shows deviations of 5–7%, which is acceptable for preliminary engineering analysis. The proposed formulation can therefore be used to evaluate operating regimes before applying more detailed CFD-based models. The model remains limited by its one-dimensional, pseudo-homogeneous, and steady-state assumptions. Further development should include transient behavior, pore-scale diffusion effects, interphase heat transfer, and systematic comparison with CFD simulations.

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AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

CONFLICT OF INTEREST STATEMENT

The authors state that there are no conflicts of interest related to this work.

DATA AVAILABILITY

The authors confirm that the data supporting the findings of this study are available within the article.

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