

Formula 1

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Formula 2

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Formula 3

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Detailed Explanation

Internal diffusion limitations arise when the rate of molecular transport (via Knudsen diffusion, molecular diffusion, or surface diffusion) inside catalyst pores becomes slower than the surface reaction rate, leading to concentration gradients and non-uniform active site utilization. The effectiveness factor (η) — defined as the ratio of the observed (overall) reaction rate to the rate that would occur if the entire catalyst interior were exposed to bulk-phase concentrations — serves as the central quantitative metric. Experimental determination typically involves varying catalyst particle size while holding external conditions (temperature, pressure, flow rate, concentration) constant and measuring the resulting change in observed rate; a strong dependence on particle size signals significant internal diffusion resistance. Additional methods include comparing Arrhenius activation energies (diffusion-limited reactions exhibit lower apparent E_a than intrinsic kinetics) and analyzing Thiele modulus (ϕ) behavior across operating conditions. Practically, this protocol informs catalyst selection, pellet sizing, washcoat thickness optimization in monoliths, and reactor scale-up decisions — ensuring kinetic data reflect true surface chemistry rather than transport artifacts.

Key Components

#	Component
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1	Catalyst particle size series (e.g., 10–100 mesh sieved fractions)
2	Isothermal fixed-bed or differential reactor with precise flow/pressure control
3	Analytical instrumentation (GC, HPLC, or online MS) for product distribution and conversion quantification

Applications

#	Application
1	Diagnosing pore diffusion limitations in supported metal catalysts (e.g., Pt/Al ₂ O ₃ for hydrogenation)
2	Validating kinetic models prior to reactor simulation (e.g., in ASPEN Plus or COMSOL)
3	Optimizing extrudate or microsphere geometry for industrial hydroprocessing catalysts

Related Concepts

#	Concept
1	Effectiveness factor
2	Thiele modulus
3	Weisz-Prater criterion

Tags

catalysis, reaction engineering, mass transfer, kinetics, diffusion limitation