

RESEARCH ARTICLE

Screening of Isothermal Plug-Flow Reactor Length for Cumene Synthesis Using Aspen HYSYS

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Correspondence: Rudy Agustriyanto (rudy.agustriyanto@staff.ubaya.ac.id)**Received:** 8 May 2026 | **Revised:** 3 October 2026 | **Accepted:** 6 October 2026**Keywords:** Aspen HYSYS | cumene synthesis | kinetic-model uncertainty | plug-flow reactor | reactor-length screening

ABSTRACT

An auditable Aspen HYSYS workflow was developed to screen isothermal plug-flow reactor length for cumene synthesis at a benzene-to-propene molar ratio of 1.2 and to test the robustness of the resulting length decision. An apparent-rate model was compared with a reversible Langmuir–Hinshelwood–Hougen–Watson (LHHW) formulation, whereas Peng–Robinson and Soave–Redlich–Kwong were assessed as property-method alternatives. The apparent-rate formulation supported a shorter candidate relative to its reference case, whereas the Han–LHHW model-form test yielded no passing length within the investigated range. Reactor-length inference was, therefore, strongly kinetic-model dependent, and the thermal and hydraulic results remain preliminary screening quantities rather than validated design predictions.

1 | Introduction

Cumene (isopropylbenzene) is the principal intermediate used in the large-scale manufacture of phenol and acetone [1–5]. It is commonly produced by alkylating benzene with propene. Modern processes employ solid-acid and zeolite catalysts because their acidity and pore structure can improve activity and selectivity relative to older Friedel–Crafts catalyst systems [4, 6–9]. A persistent selectivity challenge is the further alkylation of cumene to diisopropylbenzene (DIPB), which consumes desired product and increases the load on downstream separation and recycle operations [8–10].

Cumene reactor performance depends on reaction kinetics, catalyst characteristics, temperature, pressure, residence time, and the benzene-to-propene ratio. Increasing benzene relative to propene generally suppresses secondary alkylation, but it also increases material circulation and separation requirements [8,

10–13]. Reactor geometry is, therefore, coupled to selectivity, thermal management, and process economics. This coupling is especially important for exothermic alkylation, for which the heat-release profile and available heat-transfer area constrain safe isothermal operation.

Previous simulation studies have mainly addressed complete cumene processes, separation intensification, plantwide control, and energy integration. Luyben [10] developed a widely used process design and control basis for vapor-phase cumene production. Norouzi et al. [8] examined economic design and optimization of a zeolite-based plant, whereas Flegiel et al. [14] applied multiobjective optimization to capital cost, utility demand, and material losses. Zhai et al. [6] and Jamshidi et al. [15] investigated intensified separation configurations, including dividing-wall and reactive dividing-wall columns. Junqueira et al. [4] compared economic and environmental performance across alternative process designs, and Samad et al. [5] identified energy-recovery

Abbreviations: DIPB, diisopropylbenzene; EOS, equation of state; HTC, heat-transfer coefficient; LHHW, Langmuir–Hinshelwood–Hougen–Watson; PFR, plug-flow reactor; PR, Peng–Robinson; SRK, Soave–Redlich–Kwong; TAC, total annual cost; VLE, vapor–liquid equilibrium.

opportunities through thermodynamic analysis. Sutjahjo et al. [16] further demonstrated the importance of reactor-effluent heat recovery. These contributions provide process-wide insight but do not directly establish a minimum effective plug-flow reactor (PFR) length from coupled axial conversion, by-product, and isothermal-duty profiles.

Reactor-focused studies also differ substantially in catalyst system and operating window. Reported benzene-to-propene ratios range from approximately 3 to 10, and temperatures range from 70°C to 260°C [11–13]. Consequently, literature conversion values cannot be transferred directly to a model operating at a benzene-to-propene ratio of 1.2. Moreover, the use of apparent kinetic expressions introduces model-form uncertainty, particularly for secondary alkylation when the local cumene concentration is not explicitly represented.

The present work addresses a narrower and reproducible screening question: under explicitly stated kinetic, thermodynamic, thermal, and hydraulic assumptions, how does the inferred PFR-length decision change with model form and numerical resolution relative to a 10 m reference? The novelty is the auditable decision workflow rather than a new cumene reaction route. It combines axial-grid verification, kinetic-model-form comparison, property-method sensitivity, local and global heat-removal checks, explicit hydraulic-boundary-condition assessment, and a reactor-only relative cost indicator in a single screening sequence. This scope is intentionally different from reactive or dividing-wall distillation studies, which intensify reaction and separation but require column equilibrium, catalyst-location, and operability decisions [6, 15], and from detailed nonisothermal multitubular design, which requires a rated coolant circuit and validated transport coefficients. The workflow is intended to reject unsupported length savings early and to identify which higher fidelity models are required before detailed design.

2 | Methodology

2.1 | Computational Tool and Workflow

The calculations were performed in Aspen HYSYS V15 in steady state. The workflow comprises (i) an apparent-kinetics reference matrix; (ii) a reversible Han–Langmuir–Hinshelwood–Hougen–Watson (LHHW) kinetic-model comparison; (iii) a common-grid length screen at $\Delta z = 0.0125$ m; (iv) an apparent-rate property-method sensitivity using the Peng–Robinson (PR) and Soave–Redlich–Kwong (SRK) equations of state; (v) global and local isothermal heat-removal screening; and (vi) prescribed model-specific pressure-drop boundary conditions. The same feed and nominal geometry were used unless a sensitivity case was explicitly labeled. The complete reactor-length screening workflow and the associated supporting assessments are summarized in Figure 1.

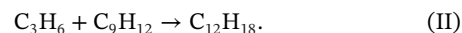
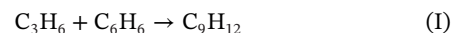
The modeled components were benzene, propene, propane, cumene, and 1,3-DIPB (the HYSYS component used as the lumped DIPB surrogate). Propane represented an inert impurity. PR was used as the base property method, whereas SRK was evaluated as a sensitivity case using the apparent-rate model. This comparison assesses property-method sensitivity and does

not constitute experimental thermodynamic or reactor-model validation.

2.2 | Reaction Network and Kinetic Models

2.2.1 | Apparent Reference Model

The modeled reaction network consisted of primary cumene formation and secondary alkylation to DIPB:



The primary pathway was represented by the apparent first-order expression:

$$-r_1 = k_1 C_{\text{C}_3\text{H}_6} \quad (1)$$

$$k_1 = 6510 \exp\left(-\frac{52\,564}{RT}\right). \quad (2)$$

The secondary pathway was represented in the submitted model by

$$-r_2 = k'_2 C_{\text{C}_3\text{H}_6}, \quad (3)$$

$$k'_2 = 450 \exp\left(-\frac{55\,000}{RT}\right). \quad (4)$$

The reaction structure and numerical parameter set were adopted from the cumene process-modeling basis reported by Norouzi et al. [8]. Here, r_i denotes the liquid-phase volumetric rate, $C_{\text{C}_3\text{H}_6}$ is the propene concentration, T is the absolute temperature, and R is the universal gas constant. The numerical values were entered using the time and energy-unit basis of the HYSYS reaction set and the resulting rates were reported in $\text{kmol m}^{-3} \text{s}^{-1}$.

These expressions are retained only as the submitted-model reference and as a controlled uncertainty screen. Because the secondary expression omits local cumene concentration and adsorption competition, its DIPB prediction is not used as independent evidence of catalyst selectivity. Final length conclusions must be checked against the literature LHHW model below.

2.2.2 | Reversible Literature LHHW Model

Han et al. [17] derived an intrinsic Langmuir–Hinshelwood model for benzene alkylation over H-beta zeolite ($\text{Si/Al} = 35$) after eliminating external and internal diffusion in stirred-autoclave experiments. Their reaction network is reversible: $B + P \rightleftharpoons I$ and $I + P \rightleftharpoons D$, where B , P , I , and D denote benzene, propene,

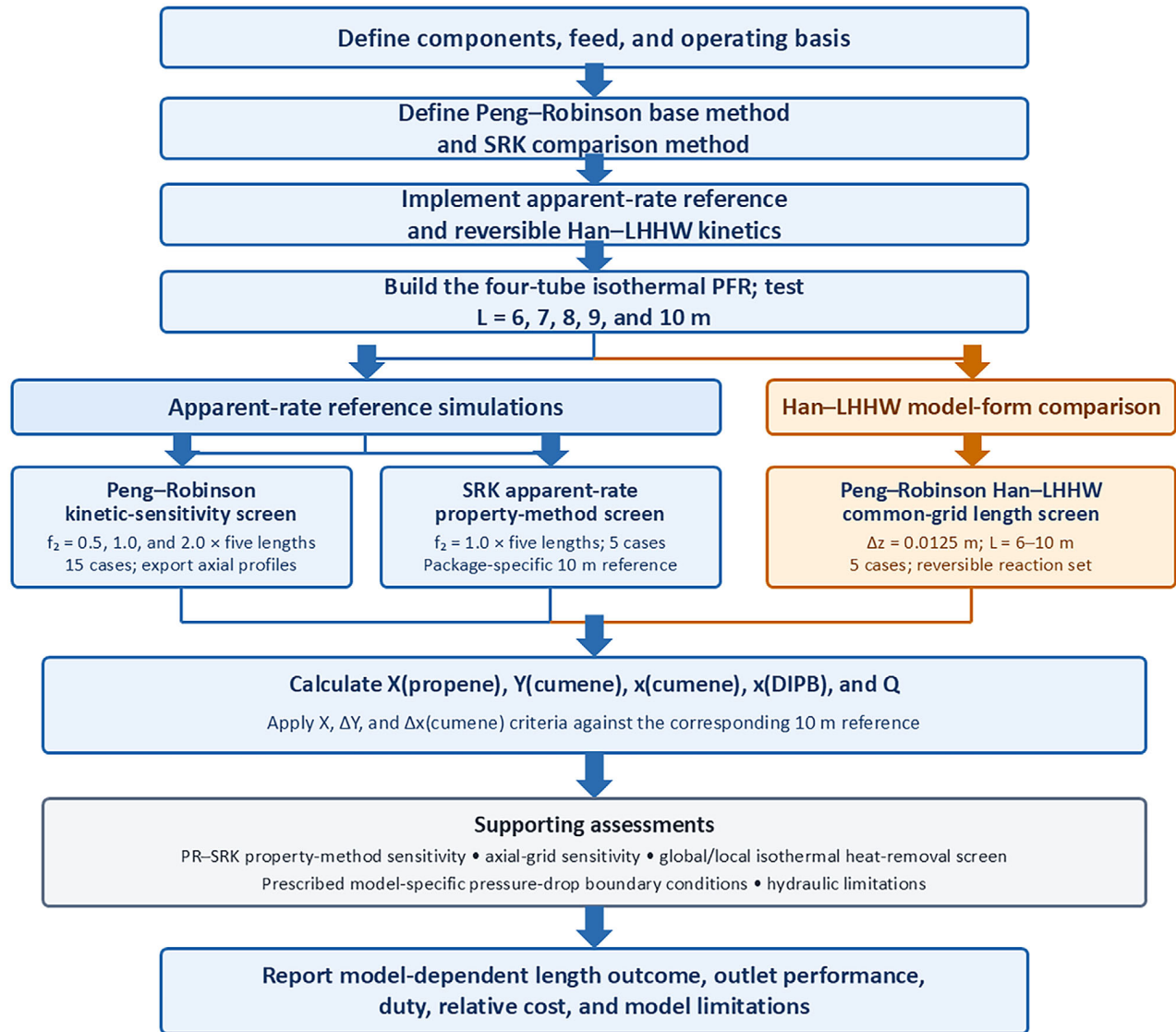


FIGURE 1 | Reactor-length simulation workflow for the Peng–Robinson and SRK apparent-rate cases and the Peng–Robinson Han–LHHW common-grid model-form comparison, including supporting numerical and feasibility assessments. DIPB, diisopropylbenzene; LHHW, Langmuir–Hinshelwood–Hougen–Watson; PFR, plug-flow reactor; SRK, Soave–Redlich–Kwong.

cumene, and DIPB. The two rates share a competitive-adsorption denominator:

$$w_1 = \frac{k_1 C_B C_P - k_{-1} C_I}{D_{\text{ads}}^2} \quad (5)$$

$$w_2 = \frac{k_2 C_I C_P - k_{-2} C_D}{D_{\text{ads}}^2} \quad (6)$$

$$D_{\text{ads}} = 1 + K_P C_P + K_B C_B + K_I C_I + K_D C_D. \quad (7)$$

The temperature functions are reproduced in Table 1A in the original $\exp(b/T)$ form. For HYSYS fields written as $A \exp(-E/RT)$, the corresponding E values are positive for the four

kinetic constants and negative for the adsorption constants. The HYSYS implementation uses liquid-phase molar concentrations in kmol m^{-3} and a volumetric reaction-rate basis of $\text{kmol m}^{-3} \text{s}^{-1}$. Because Han et al. did not explicitly report the dimensional basis of the fitted kinetic constants, the absolute numerical rate scale remains unverified. Accordingly, the Han–LHHW calculations are used here only as a model-form sensitivity test and not as quantitative validation of reactor performance.

Han et al. fitted the model at 353–433 K and 0.255–0.725 MPa using catalyst particles smaller than 0.1 mm. The present nominal condition, 443.15 K and 3.54 MPa, is outside both fitted ranges; the LHHW calculation is, therefore, an extrapolative model-form test, not experimental validation at the reactor condition. HYSYS 1,3-DIPB is treated as the lumped D species, and that surrogate assumption is retained in all comparisons.

TABLE 1A | Han–Langmuir–Hinshelwood–Hougen–Watson (LHHW) parameter functions [17] and equivalent HYSYS exponent entries.

Parameter	A in $A \exp(b/T)$	b (K)	Equivalent E (kJ kmol ⁻¹)
k_1	2.90×10^7	-3.91×10^3	3.2510×10^4
k_{-1}	2.91×10^6	-7.65×10^3	6.3606×10^4
k_2	3.80×10^7	-4.31×10^3	3.5835×10^4
k_{-2}	4.50×10^6	-7.85×10^3	6.5269×10^4
K_p	0.768	$+3.18 \times 10^3$	-2.6440×10^4
K_B	0.019	$+2.33 \times 10^3$	-1.9373×10^4
K_I	0.426	$+2.34 \times 10^3$	-1.9456×10^4
K_D	0.108	$+2.62 \times 10^3$	-2.1784×10^4

TABLE 1B | Model basis for the reactor-length screening.

Item	Model input
Benzene feed	120 kmol h ⁻¹
Propene feed	100 kmol h ⁻¹
Propane impurity	5 kmol h ⁻¹
Benzene-to-propene molar ratio	1.2
Reactor inlet temperature	170°C
Reactor inlet pressure	3.54 MPa
Thermodynamic model	Peng–Robinson (base); SRK (sensitivity)
Reactor representation	Legacy ideal PFR; revised heterogeneous-catalytic packed-bed cases
Tube internal diameter	0.500 m
Tube wall thickness	0.005 m
Tube external diameter (calculated)	0.510 m
Base-case length	10 m
Candidate lengths evaluated	6, 7, 8, 9, and 10 m
Pressure-drop specification (user input)	34.47 kPa in the legacy cases; in the revised Han–LHHW screening, a user-specified constant pressure-drop gradient of 3.447 kPa m ⁻¹ was applied, corresponding to total ΔP values of 20.68, 24.13, 27.58, 31.02, and 34.47 kPa for $L = 6, 7, 8, 9$, and 10 m, respectively.
Tube-packing void fraction in reported cases	1.000 legacy; 0.400 revised packing screen
Parallel-tube flow distribution	Equal split assumed; no distribution model
Catalyst particle diameter	1.0 mm base; 0.1 and 3.0 mm sensitivity
Particle sphericity	1.0 (screening assumption)
Solid/Bulk density	2500/1500 kg m ⁻³ (screening assumptions)
Han fitted range	353–433 K; 0.255–0.725 MPa
Common axial spacing	0.0125 m (80 segments m ⁻¹)

Abbreviations: LHHW, Langmuir–Hinshelwood–Hougen–Watson; PFR, plug-flow reactor; SRK, Soave–Redlich–Kwong.

2.3 | Feed Operating Conditions and Reactor Configuration

Table 1B distinguishes the submitted ideal-PFR reference from the revised heterogeneous-catalytic packed-bed cases. Four

equal-flow horizontal tubes are retained. The reference calculations use a void fraction of 1.000 and an imposed total pressure drop of 34.47 kPa. The Han–LHHW cases use the catalyst/packing screen below: bed void fraction 0.400, particle diameter 1.0 mm, sphericity 1.0, solid density 2500 kg m⁻³, and bulk density

1500 kg m⁻³. The density relation $\varepsilon_b = 1 - \frac{\rho_{\text{bulk}}}{\rho_{\text{solid}}}$ gives 0.400, so the three quantities are internally consistent. These are screening assumptions rather than measured properties of the Han catalyst. Particle-diameter sensitivity at 0.1, 1.0, and 3.0 mm spans the sub-0.1 mm intrinsic-powder scale reported by Han et al. [17] and larger hypothetical pellet sizes used only for sensitivity screening.

2.4 | Length-Selection Criterion and Performance Metrics

The 10 m configuration was used as the reference case. Candidate lengths of 6, 7, 8, 9, and 10 m were compared using the criteria formalized in Section 2.5: propene conversion of at least 99.9%, a relative net-cumene-yield difference no greater than 0.1%, and an absolute cumene-outlet-mole-fraction difference no greater than 0.001. A final reaction-performance selection requires the shortest tested length satisfying all criteria on a numerically verified grid. Decisions from the earlier screening dataset are retained only as initial-grid outcomes. This designation does not imply thermal or hydraulic design validation.

For component i , the molar-flow change was defined as

$$\Delta F_i = F_{i,\text{out}} - F_{i,\text{in}} \quad (8)$$

Propene conversion, net cumene yield, and net cumene selectivity were calculated as

$$X(\text{C}_3\text{H}_6) = \frac{F_{\text{C}_3\text{H}_6,\text{in}} - F_{\text{C}_3\text{H}_6,\text{out}}}{F_{\text{C}_3\text{H}_6,\text{in}}} \quad (9)$$

$$Y(\text{cumene}) = \frac{F_{\text{cumene,out}} - F_{\text{cumene,in}}}{F_{\text{C}_3\text{H}_6,\text{in}}} \quad (10)$$

$$S(\text{cumene}) = \frac{F_{\text{cumene,out}} - F_{\text{cumene,in}}}{F_{\text{C}_3\text{H}_6,\text{in}} - F_{\text{C}_3\text{H}_6,\text{out}}} \quad (11)$$

The metrics in Equations (8)–(11) distinguish molar-flow change, conversion, yield, and selectivity. DIPB formation was reported as the outlet mole fraction. Yield and selectivity are nearly identical at essentially complete propene conversion; both quantities were retained to distinguish their definitions while avoiding interpretation of either as independent experimental validation. Calculated results are generally reported to four significant figures as a presentation convention, without implying additional accuracy in rounded source data. Conversion percentages and their differences in percentage points are reported to four decimal places. Stream-composition values, small differences available only from rounded exports, and numerical-grid coordinates retain the precision supported by their source. Model inputs, including the equivalent HYSYS energy entries in Table 1A, and source-reported kinetic parameters are retained. Derived comparisons are calculated before rounding the reported results.

2.5 | Kinetic Uncertainty and Model-Form Assessment

A secondary-rate sensitivity analysis was completed to quantify the effect of the uncertain apparent secondary kinetics on conversion, cumene yield, DIPB formation, and reactor-length screening. The base secondary pathway was expressed as

$$-r_2 = k'_2 C_{\text{C}_3\text{H}_6}, \quad (12)$$

where k'_2 is the apparent rate coefficient defined in Equation (4). A dimensionless multiplier, f_2 , was applied to this coefficient:

$$k'_{2,\text{sens}} = f_2 k'_2. \quad (13)$$

For Equations (12) and (13), values of $f_2 = 0.5, 1.0$, and 2.0 were examined by setting the pre-exponential coefficient to 225, 450, and 900, respectively, on the unchanged time and energy-unit basis of the HYSYS reaction set. The activation energy, reaction orders, and primary kinetic expression were held fixed. At the imposed temperature, these changes multiply the secondary-rate coefficient by the stated factors. The half-rate and double-rate cases constitute a factor-of-two scenario range around the base case, not an experimentally estimated confidence interval.

For each value of f_2 , reactor lengths of 6, 7, 8, 9, and 10 m were simulated, giving 15 steady-state cases. The feed flow rates, benzene-to-propene molar ratio, reactor temperature, inlet pressure, tube diameter, tube count, thermodynamic model, and isothermal specification were maintained at the values listed in Table 1B.

Propene conversion, net cumene yield, net cumene selectivity, cumene outlet mole fraction, DIPB outlet mole fraction, and isothermal heat-removal duty were recorded for each case. At each value of f_2 , the corresponding 10 m result was used as the reference. A shorter length was considered effective when

$$X(\text{propene}) \geq 99.9\% \quad (14)$$

$$\frac{|Y(\text{cumene}, L) - Y(\text{cumene}, 10 \text{ m})|}{Y(\text{cumene}, 10 \text{ m})} \times 100\% \leq 0.1\% \quad (15)$$

$$|x(\text{cumene}, L) - x(\text{cumene}, 10 \text{ m})| \leq 0.001. \quad (16)$$

For each secondary-rate factor, the shortest tested length satisfying all three criteria was recorded on the numerical basis used for that study. Table 3 reports these completed screening outcomes and their 10 m endpoint values. Because the later refinement changes the base-case pass/fail result, the original outcomes are interpreted as dataset-specific decisions rather than a grid-independent optimum. The sensitivity study itself is complete; the separate refinement study limits how its length decisions can be generalized.

The factor-of-two secondary-rate study quantifies parameter-magnitude sensitivity within the submitted apparent model.

TABLE 2 | Latest base-case comparison at 170°C and 3.54 MPa ($\Delta z = 0.0125$ m); endpoint estimates for screening.

Metric	10 m reference	8 m candidate
Propene conversion, %	99.9895	99.9427
Net cumene yield, mol mol ⁻¹ propene feed	0.929928	0.929548
Net cumene selectivity, mol mol ⁻¹ propene reacted	0.930026	0.930081
Cumene outlet mole fraction	0.7439	0.7433
DIPB outlet mole fraction	0.0280	0.0280
Heat-removal duty, 10 ⁷ kJ h ⁻¹	1.091176	1.090680
Heat-removal duty, MW	3.03104	3.02967
Imposed HYSYS pressure drop, kPa	34.47	34.47
Relative purchased-cost index	1.00	0.8554–0.8747
Number of axial segments	800	640

Abbreviation: DIP0042, diisopropylbenzene.

TABLE 3 | Apparent-kinetics sensitivity results on the original numerical grid: 10 m endpoint performance and the shortest tested length satisfying Equations (14)–(16).

f_2	Shortest passing length, L^* (m)	$X(\text{C}_3\text{H}_6)$ (%)	$Y(\text{cumene})$ (mol mol ⁻¹)	$x(\text{cumene, out})$ (mol mol ⁻¹)	$x(\text{DIPB, out})$ (mol mol ⁻¹)	Duty (MW)
0.5	No passing length (6–10 m)	99.8979	0.954728	0.763159	0.017686	3.029
1.0	10	99.9412	0.918031	0.734079	0.032537	3.029
2.0	10	99.9769	0.857963	0.686242	0.056714	3.028

Note: L^* denotes the shortest passing length reported in the original 6–10 m study, not a grid-independent design optimum. All performance columns refer to 10 m, including $f_2 = 0.5$, for which no passing length was found. Values are reproduced from the completed kinetic-sensitivity dataset. The refined $f_2 = 1.0$ results in Table 2 are not substituted here, so numerical refinement is not confused with changing the kinetic coefficient.

It is complemented, rather than relabeled, by the mechanistically different Han–LHHW calculation. The LHHW series uses 6 m/480, 7 m/560, 8 m/640, 9 m/720, and 10 m/800 segments. For each length, the reported outputs are propene conversion, net cumene yield and selectivity, cumene and DIPB outlet mole fractions, isothermal duty, total prescribed pressure drop, and outlet pressure. The final length decision was based on the same criteria specified in Equations (14)–(16). A reactor length was designated as passing only when all three criteria were satisfied; otherwise, the outcome was reported as no passing length within the investigated 6–10 m interval.

2.6 | Thermodynamic-Package Sensitivity

PR was retained as the base property method. To assess whether the original reactor-length screening was sensitive to the selected cubic equation of state (EOS), the apparent-rate length series at $f_2 = 1.0$ and $L = 6, 7, 8, 9$, and 10 m was repeated using the SRK EOS. Feed composition and flow rates, kinetic parameters, reactor temperature and inlet pressure, tube geometry, imposed pressure-drop specification, axial discretization, and isothermal specification were held unchanged.

For each property method, the corresponding 10 m result was used as the reference, and the criteria in Equations (14)–(16) were applied independently. Propene conversion, net cumene

yield, outlet cumene and DIPB mole fractions, reactor duty, and the shortest passing length were compared. The resulting legacy PR–SRK comparison is presented in Section 3.5.

Because this comparison was performed using the apparent-rate model and its original numerical grid, it was kept separate from the common-grid Han–LHHW results reported in Section 3.4.1. Furthermore, the two equations of state were not benchmarked against experimental benzene–cumene vapor–liquid equilibrium (VLE) data. The comparison is, therefore, interpreted as a property-package sensitivity test rather than experimental thermodynamic validation, and it does not establish that the Han–LHHW length-screening result is independent of the selected property method.

2.7 | Isothermal Heat-Removal Screening and Hydraulic Boundary Condition

The isothermal HYSYS reactor exchanges energy through the stream Q using the Direct Q Value representation. No coolant material stream, coolant circulation geometry, coolant flow rate, or overall heat-transfer coefficient (HTC) was specified. The reported Q is the heat-removal requirement consistent with the imposed 170°C condition and the model energy balance; it does not demonstrate that a physical cooling system can supply that duty. For a separate utility-demand estimate, a hypothetical

cooling-water mass flow was calculated from

$$\dot{m}_{CW} = \frac{Q}{C_{p,CW} \Delta T_{CW}}, \quad (17)$$

using C_p , $CW = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ and an assumed temperature rise of 10–15 K. This estimate is not a simulated coolant flow or an input to the reactor model.

To address the heat-transfer-area question, an illustrative post-processing screen was performed for the PR base-kinetics cases at $L = 8$ and 10 m, without changing their Q -based reactor specification. All four bare tube surfaces were assumed to be cooled over their full cylindrical length; end surfaces were excluded. Water at 30°C inlet and 40°C outlet was selected solely as a cooling scenario. Against the prescribed 170°C reactor, the terminal differences are 140 and 130 K, giving $\Delta T_{lm} = (140-130)/\ln(140/130) = 134.9 \text{ K}$. The globally required area was calculated as

$$A_{req} = \frac{Q}{U_o \Delta T_{lm}}. \quad (18)$$

Illustrative U_o values of 250, 500, and 750 $\text{W m}^{-2} \text{ K}^{-1}$ were adopted on an external-area basis for this screen. This range was based on the organic-solvent/water cooler entry in Dimian and Bildea [18] (Table B.4, p. 477), with 500 $\text{W m}^{-2} \text{ K}^{-1}$ selected as the midpoint. The tabulated values include fouling, so no separate generic fouling allowance was added. This cooler analogy is not a correlation or validated coefficient for the present large-diameter tubes with reacting, partly two-phase flow. These U_o values are not HYSYS inputs or outputs. Available external area was calculated using $N_t = 4$ and $D_o = 0.510 \text{ m}$:

$$A_{avail} = N_t \pi D_o L. \quad (19)$$

The globally required coefficient and the area assigned to axial segment j were calculated from

$$U_{o,req} = \frac{Q}{A_{avail} \Delta T_{lm}} \quad (20a)$$

$$A_j = N_t \pi D_o \Delta z. \quad (20b)$$

The base-case exports contained 20, 80, 160, 320, and 640 segments at $L = 8 \text{ m}$ and 20, 200, 400, and 800 segments at $L = 10 \text{ m}$. Matched spacings of 0.050, 0.025, and 0.0125 m were compared using the 160/200, 320/400, and 640/800 pairs. Total heat-removal duty was obtained by summing the displayed segment duties; differences from the rounded unit-operation total were within reporting precision. Segment-average heat flux and the locally required coefficient were calculated as

$$q''_j = \frac{Q_j}{A_j}, U_{o,req,j} = \frac{Q_j}{A_j (T_r - T_{CW,j})}, \quad (20c)$$

where $T_{CW,j}$ denotes the local cooling-water temperature. Because an axial coolant-temperature profile was not calculated, $T_{CW,j}$ was bounded by the assumed inlet and outlet temperatures of 30°C and 40°C. For Equations (18), (20a), and (20c), duties in kJ h^{-1}

were divided by 3.6 to obtain W. The assumed 30–40°C coolant range therefore gives local temperature-difference bounds of 130–140 K. No design margin was applied. The local maxima are finite-segment averages, not converged pointwise peaks. The HYSYS Inside HTC and Overall HTC fields were unpopulated. Neither Q alone nor this post-processing calculation determines the actual reactor U_o , which would depend on both fluid films, wall resistance, fouling, and cooling configuration.

Axial-discretization sensitivity was assessed separately at each reactor length by halving Δz and comparing total duty, maximum segment-average heat flux, final-profile conversion, and cumene yield. Relative changes use the coarser result as denominator. The latest Δz is 0.0125 m and external area per segment is 0.08011 m^2 . Final reported component-flow rows were used to estimate X , Y , and S ; Stream-2 screenshots independently confirmed outlet mole fractions at four-decimal precision. These tests quantify sensitivity rather than establish grid independence. The global area screen is reported separately from the unresolved local-peak convergence.

Pressure drop was specified as a model boundary condition rather than predicted from a hydraulic correlation. All legacy apparent-rate, kinetic-sensitivity, and PR–SRK property-package cases used an imposed total pressure drop of 34.47 kPa. For the revised Han–LHHW length screen, a user-specified constant pressure-drop gradient of 3.447 kPa m^{-1} was applied, corresponding to total pressure drops of 20.68, 24.13, 27.58, 31.02, and 34.47 kPa for reactor lengths of 6, 7, 8, 9, and 10 m, respectively.

The reactor was assumed to be horizontal, thereby eliminating the hydrostatic elevation contribution. However, the specified pressure drops do not constitute a prediction of packed-bed frictional losses, acceleration effects, or gas–liquid distribution. Because a validated horizontal two-phase packed-bed hydraulic model was not implemented, no pressure-drop advantage, pumping-power reduction, or hydraulic equivalence among the candidate lengths is claimed. Detailed two-phase packed-bed hydraulic design remains outside the scope of this screening study.

2.8 | Relative Equipment-Cost Indicator

A detailed mechanical design and dated cost basis were unavailable; therefore, the economic comparison was restricted to a dimensionless purchased-equipment cost index. For geometrically similar equipment,

$$\frac{I_{C,2}}{I_{C,1}} = \left(\frac{V_2}{V_1} \right)^n, \quad (21)$$

where I_C is the relative purchased-cost index, V is reactor volume, and $n = 0.6 - 0.7$ is a commonly used preliminary scaling exponent [19, 20]. At constant diameter and tube count, reactor volume is proportional to length. Therefore,

$$\frac{I_{C,8m}}{I_{C,10m}} = \left(\frac{8}{10} \right)^{0.6-0.7} = 0.8554 - 0.8747. \quad (22)$$

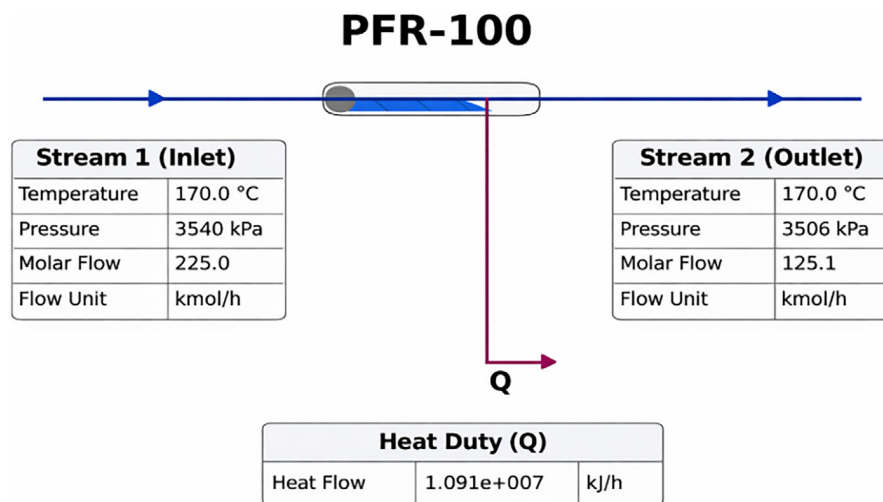


FIGURE 2 | Schematic of the Aspen HYSYS PFR configuration for the 10 m apparent-kinetics reference case with 800 axial segments. PFR, plug-flow reactor.

3 | Results and Discussion

3.1 | Apparent-Kinetics Reference Results

Figure 2 presents a schematic of the Aspen HYSYS PFR configuration for the refined 10 m apparent-kinetics reference case. The displayed numerical values correspond to this reference case and are summarized in Table 2. The inlet molar flow was 225 kmol h^{-1} , comprising benzene, propene, and propane. With 800 axial segments, the total heat-removal duty for the 10 m reactor was $1.091 \times 10^7 \text{ kJ h}^{-1}$ (3.031 MW), and the outlet propene conversion was approximately 99.9895%.

Figure 3 shows the axial propene and cumene profiles from the completed three-factor kinetic study. The profiles document rapid propene consumption and a product plateau whose level depends on f_2 ; quantitative endpoint and length-screening comparisons are discussed in Section 3.4. These reported profiles are distinct from the later base-case refinement. On the original numerical basis, the 8 m conversion of 99.8046% failed the 99.9% criterion; at 640 segments, its estimate is 99.9427%. Thus, the original 8 m rejection is a dataset-specific result, not a final length recommendation. The refined endpoints are reported separately in Tables 2 and 6.

3.2 | Secondary Reaction and Selectivity Limitation

In the latest base-case outlet streams, the DIPB mole fraction is 0.0280 at both 8 and 10 m at the displayed precision (Table 2). The benzene-to-propene ratio of 1.2 provides only a modest benzene excess compared with ratios of 3–10 reported in several experimental studies. Consequently, the high predicted selectivity should not be attributed to benzene excess alone. It also depends strongly on the adopted secondary kinetic expression [11–13].

The outlet DIPB values are useful for comparing candidate lengths within the same model, but their absolute magnitude has not been independently validated. In particular, Equation (3) does

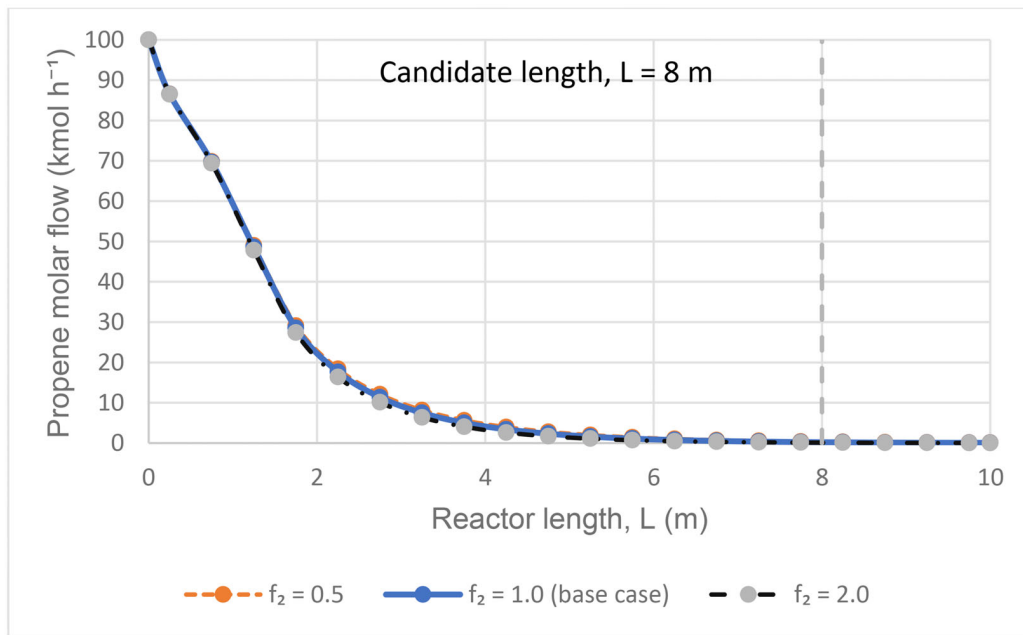
not include the local cumene concentration. A two-reactant or catalyst-specific kinetic expression could, therefore, change the predicted location and magnitude of DIPB formation. This model-form uncertainty remains in addition to the observed dependence on axial discretization.

3.3 | Performance Comparison

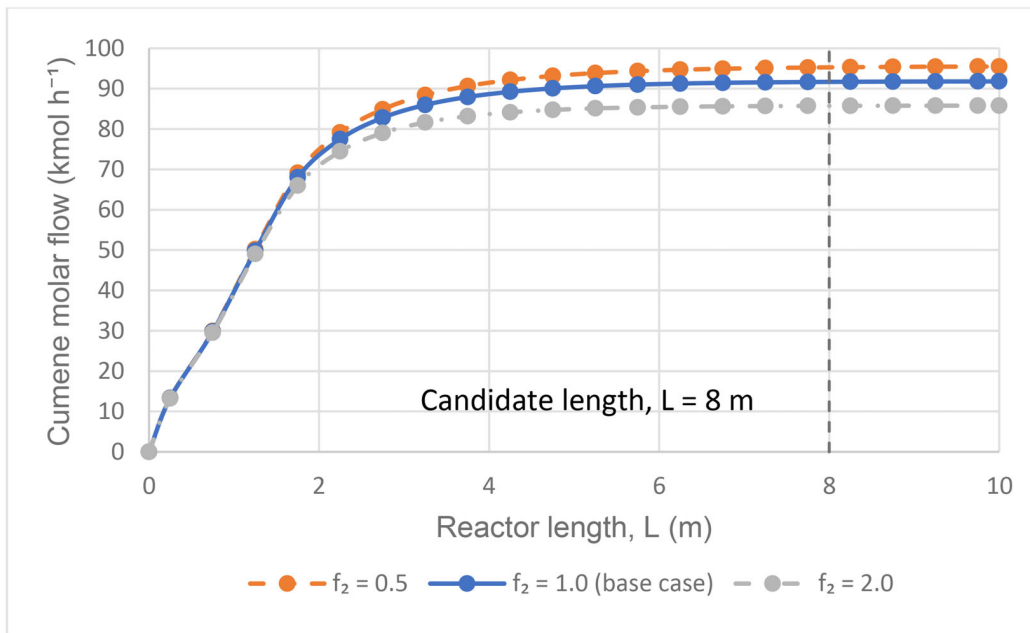
X , Y , and S are calculated from the final reported component molar-flow rows (labeled $z = 9.994$ and 7.994 m), rather than full-precision outlet-flow exports. Cumene and DIPB mole fractions were checked directly on Stream 2 at four-decimal precision. Duties are sums of printed segment values, not unrounded solver exports. The kJ h^{-1} entries in Table 2 are used for the duty difference and utility comparison in Section 3.3; the MW entries are independently rounded.

At the matched spacing of 0.0125 m, the 8 m base case provisionally satisfies all three reaction-performance criteria against 10 m: conversion is 99.9427%, the relative cumene-yield difference is 0.04086%, and the absolute difference in displayed outlet cumene mole fraction is 0.0006. This supersedes the initial-grid rejection of 8 m but does not establish the shortest acceptable length or robustness to kinetics and property method. Those claims require consistent reassessment of the other candidate lengths and sensitivity matrices.

The heat-removal duties are 3.031 MW at 10 m and 3.030 MW at 8 m, a difference of 1.378 kW or 0.04546% calculated from the segment-sum duties in kJ h^{-1} listed in Table 2, before rounding to MW. The separate utility estimate with an assumed water-temperature rise of 10–15 K gives approximately $174.0\text{--}261.0 \text{ m}^3 \text{ h}^{-1}$ at 10 m (water density 1000 kg m^{-3}); the corresponding reduction at 8 m is only about $0.07911\text{--}0.1187 \text{ m}^3 \text{ h}^{-1}$. These values are hypothetical utility requirements, not results from a modeled cooling circuit. Shortening the reactor mainly changes size and the preliminary purchased-cost index, not total heat-removal duty.



(a)



(b)

FIGURE 3 | Axial molar-flow profiles of (a) propene and (b) cumene for the apparent-kinetics sensitivity cases ($f_2 = 0.5, 1.0$, and 2.0). The dashed vertical line indicates the 8 m candidate length.

The identical pressure-drop entries in Table 2 document a shared HYSYS input, not hydraulic equivalence of the two lengths. Consequently, no pressure-drop or pumping-power advantage is assigned to the 8 m candidate. Its provisional comparison is restricted to the reported reaction-performance criteria, heat-removal requirement, and preliminary size-based cost index under that imposed pressure boundary condition.

3.4 | Sensitivity of Reactor-Length Selection to Secondary-Reaction Kinetics

The completed 15-case study quantified the influence of the apparent secondary-rate magnitude on the screening results. Table 3 reports the 10 m endpoints and the shortest passing length recorded for each factor on that study's original numerical basis. At $f_2 = 0.5$, no tested length up to 10 m passed all criteria;

at $f_2 = 1.0$ and 2.0, the recorded length was 10 m. These are conditional screening outcomes, distinguished below from the later refined-grid base-case result.

As f_2 increased from 0.5 to 2.0, the reported 10 m propene conversion increased from 99.8979% to 99.9769%, a change of only 0.0790 percentage points. In contrast, net cumene yield decreased from 0.9547 to 0.8580 mol mol⁻¹ propene feed (10.14% relative), whereas DIPB mole fraction increased from 0.01769 to 0.05671 (3.207-fold). Relative to $f_2 = 1.0$, yield changed by +3.997% and -6.543% in the half-rate and double-rate cases, respectively. The simultaneous increase in conversion and decrease in desired-product yield is consistent with propene being consumed by secondary alkylation. Thus, nearly complete conversion alone does not ensure comparable cumene production or by-product loading.

The reported length-screening margins explain why the kinetic perturbation matters. At $f_2 = 0.5$, the 10 m conversion fell below 99.9% by only 0.0021 percentage points. At $f_2 = 1.0$ and 8 m, the yield difference of 0.0788% and cumene-mole-fraction difference of 0.000223 passed their limits, but conversion of 99.8046% did not. At $f_2 = 2.0$ and 8 m, the corresponding differences were 0.2608% and 0.001412%, both above their limits; the 9 m yield difference of 0.1085% also narrowly failed. These comparisons use the 10 m reference at the same f_2 and the original dataset throughout.

The apparent-model factor study establishes that conversion alone is insufficient, but it does not validate selectivity. The mechanistic model-form comparison below is therefore the decision-relevant kinetic check.

3.4.1 | Han-LHHW Model-Form Comparison

To determine whether the reactor-length decision was robust to the assumed kinetic model form, the two-reaction liquid-phase Han-LHHW model was evaluated using the same feed conditions, PR property method, reactor geometry, and isothermal temperature as the apparent-rate model, while applying the revised prescribed pressure-drop gradient defined in Section 2.7. A common axial spacing of $\Delta z = 0.0125$ m was maintained by increasing the number of segments from 480 at 6 m to 800 at 10 m. Here, X denotes the overall propene conversion, Y is the net molar cumene yield based on propene feed, S is the net molar cumene selectivity based on propene reacted, x_{cumene} and x_{DIPB} are the overall outlet mole fractions, and Q is the magnitude of the isothermal reactor duty.

The Han-LHHW calculation predicted a monotonic increase in propene conversion from 14.8113% at 6 m to 28.3644% at 10 m, accompanied by an increase in the outlet cumene mole fraction from 0.06534 to 0.1250. Net cumene yield based on propene feed increased from 0.1373 to 0.2458 mol mol⁻¹ propene feed, whereas net cumene selectivity decreased from 0.9273 to 0.8666 mol mol⁻¹ propene reacted. The DIPB mole fraction increased from 0.002562 to 0.009621, and the required isothermal duty increased from 0.5147 to 0.9683 MW. These trends indicate increasing overall reaction extent together with increasing secondary alkylation

as residence time increases. The common-grid Han-LHHW reactor-length results are summarized in Table 4.

No reactor length within the investigated 6–10 m interval satisfied the original near-complete-conversion criterion. Consequently, the 10 m case is retained only as the upper-bound comparison case because it provides the highest conversion and outlet cumene mole fraction within the prescribed screening interval; it is not identified as a validated design length.

At 10 m, the Han-LHHW model reduced the predicted propene conversion from 99.9895% for the apparent-rate reference to 28.3644% and reduced the outlet cumene mole fraction from 0.7439 to 0.1250. Net cumene yield based on propene feed decreased from 0.9299 to approximately 0.2458 mol mol⁻¹ propene feed, whereas net cumene selectivity decreased from 0.9300 to 0.8666 mol mol⁻¹ propene reacted. The outlet DIPB mole fraction decreased from 0.0280 to 0.009621. This lower DIPB mole fraction must not be interpreted as improved selectivity because it occurs together with a substantially lower overall reaction extent.

The large difference between the two kinetic formulations demonstrates that the earlier apparent-rate 8 m result is strongly dependent on the assumed kinetic model and cannot be considered kinetically robust without independent calibration data. Furthermore, the present operating condition of 443.15 K and 3.54 MPa lies outside the temperature and pressure ranges used to regress the Han parameters (353–433 K and 0.255–0.725 MPa). Therefore, these calculations constitute a model-form sensitivity test rather than catalyst validation or a quantitatively validated reactor design.

3.5 | Thermodynamic-Package Sensitivity

To isolate property-method sensitivity from kinetic model-form sensitivity, the earlier PR and SRK comparison was retained as a legacy calculation. Both property packages were evaluated using the submitted apparent-rate reaction set, $f_2 = 1.0$, and the original axial discretization. Consequently, these results are not combined with the common-grid Han-LHHW calculations reported in Section 3.4.1.

At 10 m, replacing PR with SRK decreased the calculated propene conversion by only 0.0018 percentage points. The corresponding changes in cumene yield, outlet cumene mole fraction, and outlet DIPB mole fraction were 6×10^{-6} mol mol⁻¹, 1.5×10^{-5} , and 4×10^{-6} , respectively. The most noticeable difference was the reactor duty, which increased from 3.029 to 3.047 MW, equivalent to approximately 0.5943%. Both property methods therefore produced the same 10 m selection on the original numerical grid, with negligible differences in the predicted reaction-performance indicators.

However, this agreement does not constitute experimental validation of either EOS. It also does not demonstrate that the revised Han-LHHW length screen is independent of the thermodynamic method because the common-grid Han-LHHW calculations were completed only with PR. Accordingly, PR is retained as the base property package, whereas the results in Table 5 are interpreted only as a legacy sensitivity test of the apparent-rate

TABLE 4 | Common-grid Han–Langmuir–Hinshelwood–Hougen–Watson (LHHW) reactor-length sensitivity ($\Delta z = 0.0125$ m).

L (m)	Segments	X (%)	Y (mol mol ⁻¹ propene feed)	S (mol mol ⁻¹ propene reacted)	x_{cumene}	x_{DIPB}	Q (MW)
6	480	14.8113	0.13734	0.92729	0.065343	0.002562	0.5147
7	560	17.8096	0.16269	0.91348	0.078521	0.003719	0.6161
8	640	21.0302	0.18904	0.89891	0.092682	0.005212	0.7244
9	720	24.5234	0.21663	0.88338	0.108060	0.007133	0.8411
10	800	28.3644	0.24581	0.86660	0.125006	0.009621	0.9683

TABLE 5 | Legacy apparent-rate thermodynamic-package sensitivity at $f_2 = 1.0$ on the original numerical grid.

EOS	Original-grid selected L (m)	$X(\text{C}_3\text{H}_6)$ (%)	Y_{cumene} (mol mol ⁻¹)	$x_{\text{cumene,out}}$	$x_{\text{DIPB,out}}$	Duty (MW)
PR	10	99.9412	0.918031	0.734079	0.032537	3.029
SRK	10	99.9394	0.918025	0.734064	0.032533	3.047

Abbreviations: EOS, equation of state; PR, Peng–Robinson; SRK, Soave–Redlich–Kwong.

TABLE 6 | Illustrative post-processing heat-removal screen (8 m/640 and 10 m/800 segments); not a cooling-system rating.

Parameter	8 m	10 m
Total heat-removal duty (MW)	3.02967	3.03104
Available external area (m ²)	51.27	64.09
Global required area at assumed $U_o = 250$ W m ⁻² K ⁻¹ (m ²)	89.81	89.85
Global required area at assumed $U_o = 500$ W m ⁻² K ⁻¹ (m ²)	44.90	44.92
Global required area at assumed $U_o = 750$ W m ⁻² K ⁻¹ (m ²)	29.94	29.95
Globally required U_o (W m ⁻² K ⁻¹)	437.9	350.5
Segment length (m)	0.0125	0.0125
External area per segment (m ²)	0.080111	0.080111
Maximum segment duty (kW)	36.008	36.096
Maximum segment-average heat flux (kW m ⁻²)	449.48	450.57
Required U_o at highest-duty segment (W m ⁻² K ⁻¹)	3211–3458	3218–3466

model. A benzene–cumene VLE benchmark and repetition of the Han–LHHW length screen using the selected alternative property method would be required before making a property-package-independent reactor-length claim.

3.6 | Illustrative Heat-Removal Screening and Hydraulic Limitations

All exported axial temperatures are 170.0°C, consistent with the imposed isothermal condition. The inlet contains vapor and liquid, whereas downstream points have zero vapor fraction; a liquid-phase reaction basis therefore does not imply single-liquid-phase flow throughout. The latest profiles first report zero vapor fraction at the row labeled 0.906 m, close to the highest duty segment. Table 6 evaluates hypothetical heat-transfer requirements from the Q -based results, not the performance of a simulated coolant system.

Basis: four fully cooled bare tube surfaces, $D_o = 0.510$ m; imposed reactor temperature 170°C; assumed cooling water 30–40°C and $\Delta T_{\text{lm}} = 134.9$ K. Q comes from the simulation; U_o values and coolant conditions are screening assumptions. Local U_o bounds use temperature difference of 130–140 K. No design margin is included. Peak values are finite-segment averages with unresolved grid sensitivity.

Available total external areas are 51.27 and 64.09 m² at 8 and 10 m. At the assumed $U_o = 250$ W m⁻² K⁻¹, both are below the global requirement of 89.81 and 89.85 m² at 8 and 10 m, respectively. At $U_o = 500$ or 750 W m⁻² K⁻¹, aggregate area exceeds the calculated global requirement. Equivalently, the global coefficient requirements are 437.9 and 350.5 W m⁻² K⁻¹. These conditional comparisons do not establish that those coefficients are achievable or resolve the nonuniform local demand.

TABLE 7 | Axial-discretization sensitivity of the apparent-rate reference calculations.

L (m)	Segments	Δz (m)	Q (MW)	Maximum q'' (kW m ⁻²)	X_{propene} (%)	Y_{cumene} (mol mol ⁻¹ propene feed)
8	20	0.400	3.02555	225.18	—	—
8	80	0.100	3.02893	344.09	—	—
8	160	0.050	3.02939	392.65	99.9340	0.928256
8	320	0.025	3.02957	422.05	99.9399	0.929103
8	640	0.0125	3.02967	449.48	99.9427	0.929548
10	20	0.500	3.02920	204.63	—	—
10	200	0.050	3.03087	392.55	99.9876	0.928669
10	400	0.025	3.03099	421.35	99.9888	0.929502
10	800	0.0125	3.03104	450.57	99.9895	0.929928

Note: Q is the sum of displayed segment duties; q'' is the maximum segment-average flux. X_{propene} and Y_{cumene} were calculated using the final reported outlet component molar-flow row and the corresponding inlet-flow basis. A dash indicates that no component-flow data were paired with that particular duty-profile export. Values from unmatched earlier sensitivity runs were excluded from the present discretization sequence.

In both latest cases, the maximum duty occurs over 0.8875–0.9000 m (center 0.89375 m, printed as 0.894 m). Segment-average heat fluxes are 449.5 and 450.6 kW m⁻² for 8 and 10 m, implying local U_o requirements of 3211–3458 and 3218–3466 W m⁻² K⁻¹ under the assumed coolant bounds. These exceed all three illustrative coefficient scenarios. Thus, the selected scenarios fail the local screen despite adequate aggregate area at the higher U_o values; the extra downstream area at 10 m does not materially relieve the upstream demand.

The Q -based model and the global/local area screening do not validate a four-tube cooling design. A defensible detailed design would require reactor-specific two-phase transport, wall resistance, fouling, coolant distribution, and a coupled reactor-coolant model.

Table 7 reports the axial-discretization history for the apparent-rate reference calculations. Halving Δz from 0.025 to 0.0125 m changed the total duty by only 0.003301% at 8 m and 0.001650% at 10 m, whereas the maximum segment-average heat flux increased by 6.499% and 6.935%, respectively. The corresponding relative changes in cumene yield were 0.04790% and 0.04583%. These relative changes were recalculated from the printed values in Table 7; their reporting precision does not imply unrounded solver accuracy. Thus, the global area estimate is substantially less sensitive to axial discretization than the local peak heat flux. The global screening calculation may, therefore, be reported as a preliminary result, but local grid independence is not claimed. These numerical results apply only to the apparent-rate reference calculations and are not used to select the reactor length following the Han–LHHW model-form comparison.

Pressure drop was imposed as a model boundary condition rather than predicted using a packed-bed hydraulic correlation. For the Han–LHHW length screen, a constant pressure-drop gradient of 3.447 kPa m⁻¹ was applied, corresponding to total pressure drops of 20.68, 24.13, 27.58, 31.02, and 34.47 kPa for reactor lengths of 6, 7, 8, 9, and 10 m, respectively. These values are prescribed inputs

and do not establish hydraulic equivalence or pumping-power savings.

3.7 | Comparison With Published Operating Windows

Table 8 compares the present simulation with selected published operating conditions.

The first four entries report high conversion, but the agreement does not constitute validation because the catalyst, kinetic basis, reactor representation, and benzene excess differ. The present model uses a substantially lower benzene-to-propene ratio than the literature cases. A lower ratio would generally be expected to increase the risk of secondary alkylation, making the DIPB prediction particularly sensitive to the simplified kinetic model. Thus, Table 8 supports only the plausibility of a high-conversion operating window; it does not demonstrate that the reported selectivity or required length is transferable to an industrial catalyst bed.

Process-wide studies provide a second context for interpretation. Junqueira et al. [4], Flegiel et al. [14], and Samad et al. [5] show that meaningful economic and environmental conclusions require separation, recycle, heat integration, and utility systems in addition to the reactor. The present 12.53%–14.46% cost-index reduction applies only to the reactor size parameter. It should not be equated with the same percentage reduction in total installed plant cost. Similarly, the nearly unchanged cooling duty does not preclude energy savings from heat recovery of the reactor effluent, as considered by Sutjahjo et al. [16].

3.8 | Scope and Remaining Uncertainty

The final interpretation is bounded by four documented limitations. First, the Han–LHHW model is extrapolated beyond its fitted temperature and pressure ranges, and Han et al.

TABLE 8 | Comparison of the refined 10 m base case with selected published operating conditions.

Source	Reactor/Catalyst context	Benzene:propene	Temp.	Pressure (MPa)	Propene conversion
Panming et al. [12]	Ni/ γ -Al ₂ O ₃ catalytic reactor	3:1	70°C	1.5	99.9%
Bokade and Kharul [11]	Catalytic membrane reactor	3:1–10:1	200–260°C	3–4	99.3%
Dong et al. [13]	Molecular-sieve catalyst screening	7.4:1	150°C	3	99%
Present study	Ideal four-tube isothermal PFR; apparent kinetics	1.2:1	170°C	3.54	≈99.9895%
Han et al. [17]	Intrinsic H-beta zeolite LHHW kinetics; stirred autoclave	Variable	80–160°C	0.255–0.725	Model fitted to transient data

did not explicitly report the dimensional basis of the fitted kinetic constants; the absolute rate scale, therefore, requires verification against a reported experimental condition. Second, the PR–SRK comparison is only a property-method sensitivity test and was not benchmarked against experimental benzene–cumene VLE data; it therefore does not validate the reacting mixture at 3.54 MPa. Third, pressure drop was prescribed rather than predicted, and the nominal two-phase inlet requires a dedicated horizontal two-phase packed-bed hydraulic closure before hydraulic performance can be claimed. Fourth, no coupled nonisothermal reactor–coolant calculation with a finite overall HTC was performed; thermal feasibility is inferred only from the isothermal duty profile and the post-processing heat-flux screen. The reactor-only cost index likewise does not constitute a plantwide total annual cost (TAC) analysis. Within these bounds, the workflow supports a transparent and reproducible preliminary reactor-length screening rather than a definitive industrial reactor design.

4 | Conclusions

A criteria-based Aspen HYSYS V15 analysis was conducted to evaluate isothermal PFR lengths of 6–10 m for cumene synthesis. The assessment included a PR apparent-rate reference, three secondary-reaction multipliers, an SRK property-method sensitivity, and a reversible Han–LHHW model-form comparison. Under the refined base apparent-rate formulation, the 8 m candidate satisfied the specified conversion, cumene-yield, and outlet-composition criteria relative to the corresponding 10 m reference. Propene conversions of 99.9427% and 99.9895% were obtained at 8 and 10 m, respectively. This apparent-rate 8 m result, however, was model dependent and does not establish a grid-independent minimum reactor length.

The common-grid Han–LHHW calculations produced a substantially different result. Propene conversion increased from 14.8113% at 6 m to only 28.3644% at 10 m. Over the same range, net cumene yield based on propene feed increased from approximately 0.1373 to 0.2458 mol mol^{−1} propene feed, whereas net cumene selectivity decreased from 0.9273 to 0.8666 mol mol^{−1} propene reacted, and the outlet DIPB mole fraction increased from 0.002562 to 0.009621. None of the tested Han–LHHW cases satisfied the minimum conversion criterion. Consequently, no defensible minimum reactor length can be selected from the 6–10 m Han–LHHW screen, and 10 m represents only the upper bound of

the investigated range. Because the operating temperature and pressure exceed the fitted range of the Han kinetics, these results constitute a model-form robustness test rather than validation of the catalyst or kinetic parameters.

For the apparent-rate reference calculations, halving the axial spacing from 0.025 to 0.0125 m changed total duty by only 0.003301% at 8 m and 0.001650% at 10 m. In contrast, the maximum segment-average heat flux changed by 6.499% and 6.935%, respectively. The global heat-removal calculation may therefore be used as a preliminary screening result, but local grid independence and cooling-system feasibility are not established. Similarly, the applied pressure drops are prescribed model boundary conditions rather than predictions from a validated two-phase packed-bed hydraulic correlation; hydraulic equivalence and pumping-power savings are, therefore, not claimed.

The principal conclusion is that the inferred reactor-length decision is governed primarily by kinetic-model form. A final design decision requires kinetic parameters validated at the intended operating conditions, extension of the Han–LHHW calculations beyond 10 m or reconsideration of the operating conditions, further local-grid refinement, and coupled thermal and two-phase hydraulic models. Until these requirements are satisfied, the apparent-rate 8 m result should be retained only as a model-specific reference rather than a validated reactor-length recommendation.

Nomenclature

Symbols

A	heat-transfer area, m ² (Equations 18–20a–c)
A	pre-exponential factor in the Han parameter expression $A \exp(b/T)$, parameter-dependent units (Table 1A)
b	temperature parameter in the Han expression $A \exp(b/T)$, K
C_i	molar concentration of component i , kmol m ^{−3}
$C_{p,CW}$	specific heat capacity of cooling water, kJ kg ^{−1} K ^{−1}
D_{ads}	LHHW competitive-adsorption denominator, –
D_o	external tube diameter, m

E	equivalent HYSYS Arrhenius energy parameter, kJ kmol^{-1}
F_i	molar flow rate of component i , kmol h^{-1}
f_2	secondary-rate multiplier, –
I_C	relative purchased-equipment cost index, –
k_i, k'_2	kinetic constants/apparent rate coefficient, model-dependent units
K_i	adsorption constant, $\text{concentration}^{-1}$
L	reactor length, m
$\dot{m}_{CW}$	hypothetical cooling-water mass flow rate, kg h^{-1}
n	equipment-cost scaling exponent, –
N_t	number of parallel tubes, –
Q, Q_j	heat-removal duty; Q_j denotes segment duty, kJ h^{-1} or MW
q''	segment-average heat flux, W m^{-2} or kW m^{-2}
R	universal gas constant, $\text{kJ kmol}^{-1} \text{K}^{-1}$
r_i	liquid-phase volumetric reaction rate, $\text{kmol m}^{-3} \text{s}^{-1}$
S	net cumene selectivity, –
T	temperature, K or $^{\circ}\text{C}$
U_o	external-area-based overall heat-transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
V	reactor volume, m^3
w_1, w_2	Han–LHHW reaction rates, $\text{kmol m}^{-3} \text{s}^{-1}$
x_i	mole fraction of component i , –
X	propene conversion, –
Y	net cumene yield, –
z	axial position, m
ΔF_i	molar-flow change of component i , kmol h^{-1}
ΔP	prescribed reactor pressure drop, kPa
ΔT_{CW}	cooling-water temperature rise, K
ΔT_{lm}	log-mean temperature difference, K
Δz	axial segment length, m

Greek Variables

Δ	difference or change
ε_b	interparticle bed void fraction, –
ρ	density, kg m^{-3}

Subscripts

1, 2	reaction/pathway index
ads	adsorption
avail	available
B	benzene
bulk	bulk density
CW	cooling water
D	DIPB

i	component or reaction index, as applicable
I	isopropylbenzene (cumene)
in	inlet
j	axial segment
lm	log mean
o	external-area basis
out	outlet
P	propene
p	constant-pressure property
r	reactor
req	required
sens	sensitivity case
solid	solid density

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The authors have nothing to report.

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

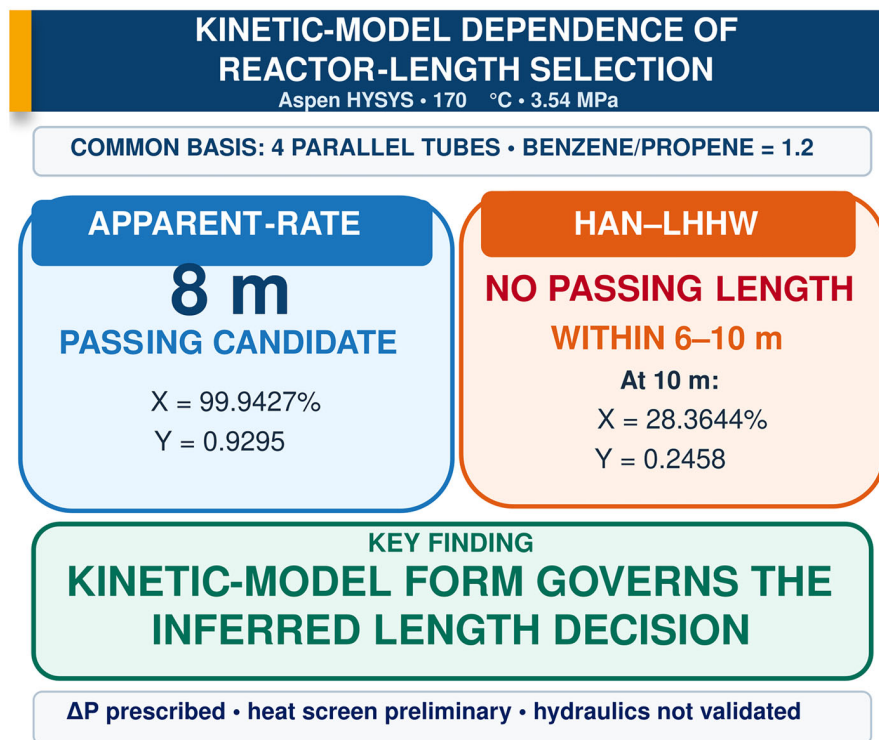
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Kinetic-model dependence of cumene-PFR length selection

An auditable Aspen HYSYS workflow shows that reactor-length screening for cumene synthesis is highly sensitive to kinetic-model form. The apparent-rate model supports a shorter candidate relative to its reference, whereas the reversible Han-LHHW formulation yields no passing length in the investigated range. Thermal and hydraulic results remain preliminary screening-level assessments.

Screening of Isothermal Plug-Flow Reactor Length for Cumene Synthesis Using Aspen HYSYS

Rudy Agustriyanto ✉, Puguh Setyoprato, Edy Purwanto, Aloisiyus Yuli Widiyanto

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ABSTRACT

An auditable Aspen HYSYS workflow was developed to screen isothermal plug-flow reactor length for cumene synthesis at a benzene-to-propene molar ratio of 1.2 and to test the robustness of the resulting length decision. An apparent-rate model was compared with a reversible Langmuir–Hinshelwood–Hougen–Watson (LHHW) formulation, whereas Peng–Robinson and Soave–Redlich–Kwong were assessed as property-method alternatives. The apparent-rate formulation supported a shorter candidate relative to its reference case, whereas the Han–LHHW model-form test yielded no passing length within the investigated range. Reactor-length inference was, therefore, strongly kinetic-model dependent, and the thermal and hydraulic results remain preliminary screening quantities rather than validated design predictions.

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement



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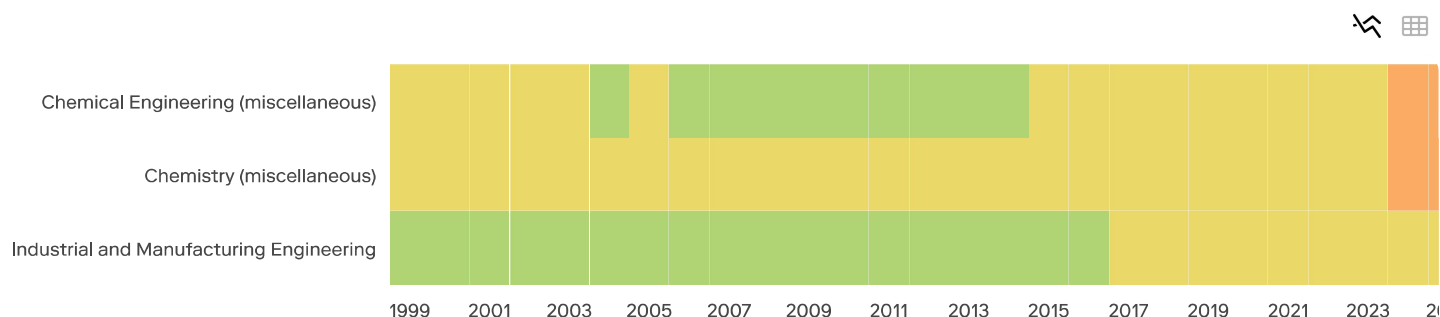
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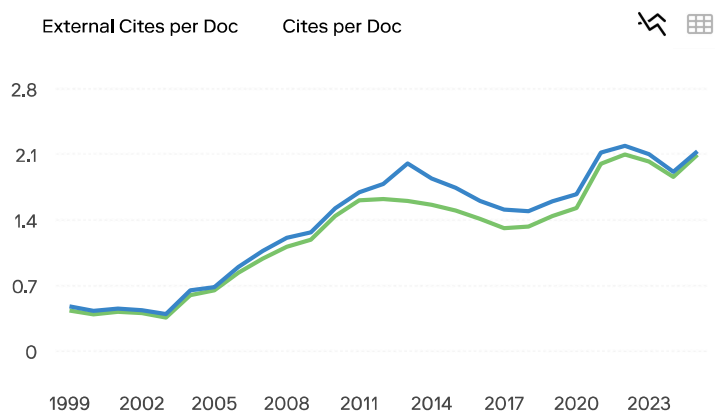
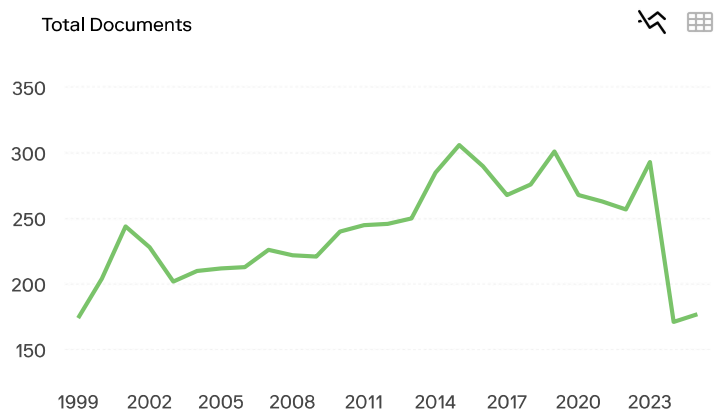
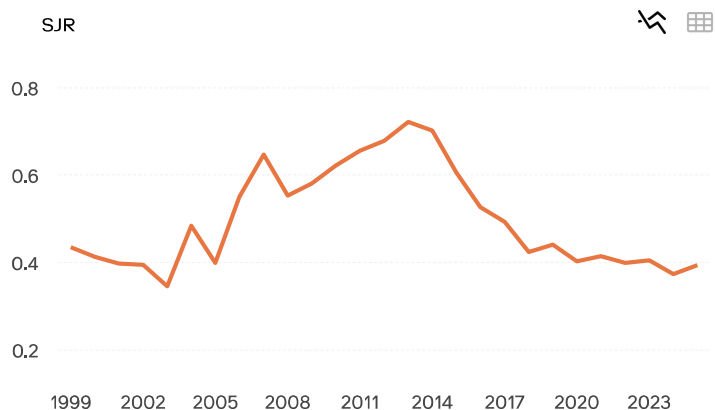
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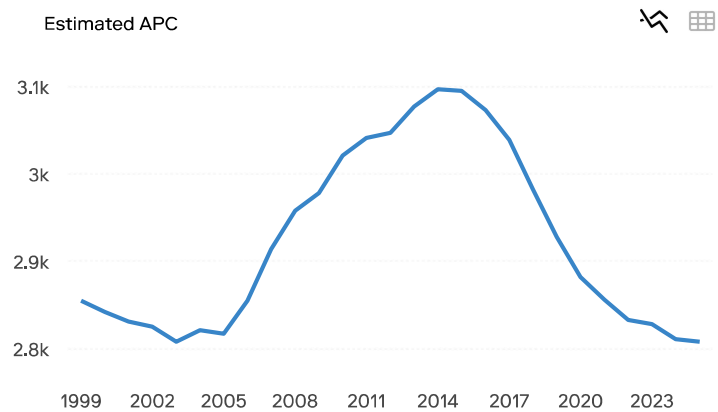
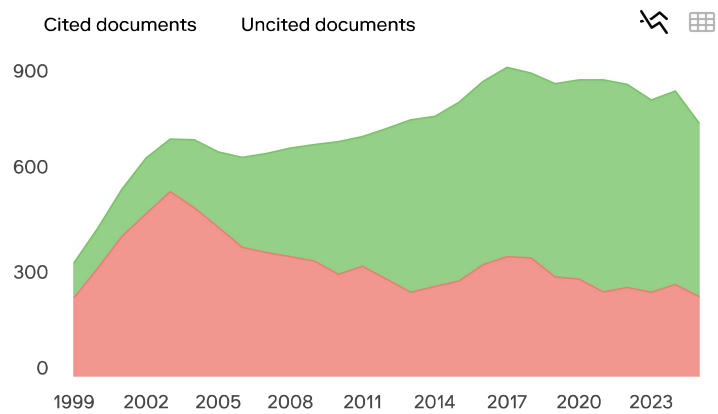
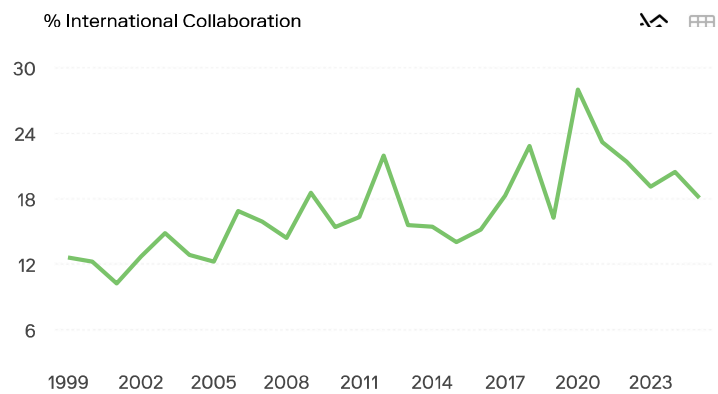
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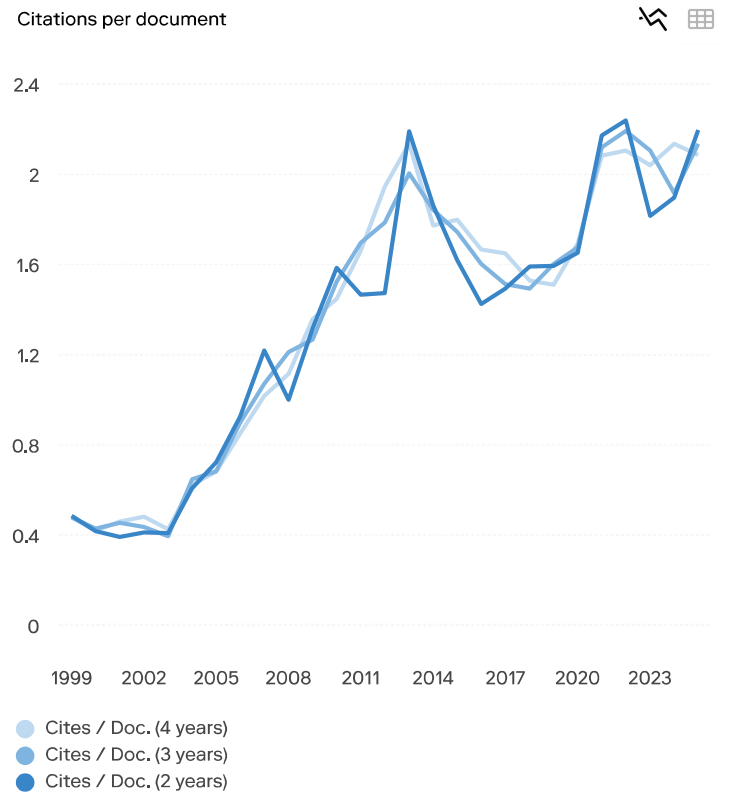
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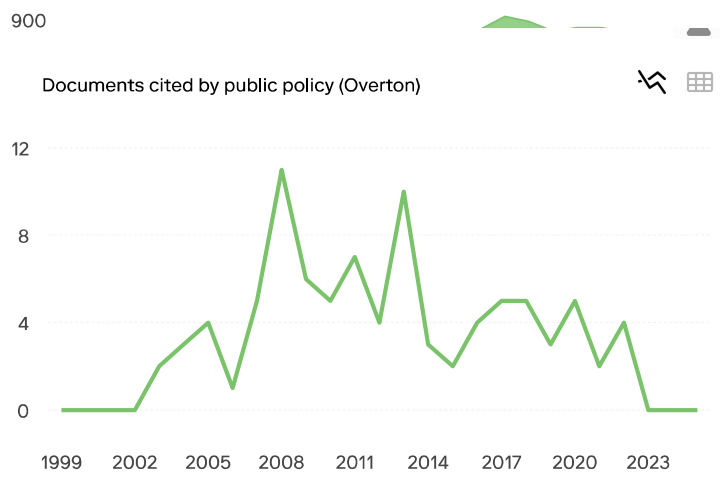
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Different methods have been proposed in the world to produce biodiesel. The most important factors affecting the type of process are the type of feed used and the capacity of the process.

The problem of reactive distillation can be studied using various methods, including feasibility, simulation, modeling, design and empirical studies in laboratory and pilot. A

combination of these methods will provide the right solution. One of the most important aspects of predicting the behavior of these systems is the model used to design and simulate the process of reactive distillation.

The present work aims to find the more preferable reactive distillation and downstream separation process following a process simulation approach to obtain a pure biodiesel fuel 99 wt. %. The currently most efficient distillation models considered, i.e., alkali and heterogeneous catalysts, for biodiesel. Productions were compared to determine the most cost-effective process. Pure soybean oil was used as process feedstock due to its low free fatty acids content (less than 0.3%); which prevents the need of a pre-treatment process. The two processes are compared based on a detailed economic analysis

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