AmbarPro

High-Fidelity Modelling of Next-Generation Reactor Technologies

Thermal Management and Pressure-Drop Trade-offs in Cartridge-Based Reactors

An AmbarPro Whitepaper on Custom Process Modelling and Simulation

Executive Summary

Industrial decarbonisation is driving the development of advanced reactor concepts capable of handling highly exothermic catalytic processes with improved thermal control, higher conversion, and reduced pressure drop. Cartridge-based multitubular radial-flow reactors represent one such class of intensified reactor designs, combining short adiabatic reaction zones with distributed cooling stages to mitigate temperature excursions while maintaining compact geometries. However, the unconventional flow patterns, staged reaction–cooling sequences, and strong coupling between transport phenomena and reaction kinetics make these systems difficult to analyse using standard reactor models available in commercial process simulators.

This whitepaper presents a detailed modelling work of a cartridge-based multitubular radial-flow reactor, using methanol synthesis as an industrially relevant reference system. A high-fidelity, physics-based reactor model was developed to capture the coupled effects of reaction, intraparticle diffusion, heat transfer, and pressure drop across multiple cartridges arranged in series. The model resolves radial reaction within annular catalyst beds and axial cooling between cartridges, enabling a consistent description of temperature, composition, and pressure profiles throughout the reactor.

A sensitivity analysis on the number of cartridges per tube was performed to evaluate the impact of reactor staging on conversion, thermal behaviour, and hydrodynamic performance. The results illustrate the fundamental trade-offs inherent to cartridge-based reactor designs and demonstrate how detailed custom modelling can provide quantitative insight into design and operating decisions that cannot be assessed using simplified reactor representations.

AmbarPro Modelling Approach

The reactor model was developed using a fully custom, first-principles formulation developed to represent reactor configurations that fall outside the scope of standard plug-flow, fixed-bed, or radial-flow models. The approach integrates detailed reaction kinetics, multicomponent intraparticle diffusion, annular-bed hydrodynamics, and tightly coupled reaction–cooling sequences within a unified modelling framework.

By explicitly resolving geometry-dependent effects and transport–reaction interactions, the modelling approach enables predictive evaluation of temperature profiles, pressure drop, and conversion performance under industrially relevant conditions. This level of detail supports sensitivity analyses, design optimisation, and early-stage assessment of advanced reactor concepts where simplified models fail to provide sufficient insight.

Key Findings

- Increasing the number of cartridges improves methanol yield and carbon conversion per pass by moderating temperature excursions and enhancing catalyst utilisation.
- For sufficiently high cartridge counts, the reactor approaches quasi-isothermal operation, significantly reducing hot spots typical of highly exothermic fixed-bed systems.
- Improved thermal control is achieved at the expense of higher pressure drop, revealing a clear trade-off between heat management and hydrodynamic performance.
- Beyond a certain number of cartridges, further performance gains become marginal while pressure-drop penalties continue to increase, highlighting the need for design optimisation rather than simple scaling.
- The model captures the strong coupling between reactor geometry, reaction kinetics, heat removal, and pressure drop, enabling quantitative assessment of design and operating trade-offs.

Introduction & Background

The European Green Deal mandates that industrial sectors decarbonise their energy and process systems and achieve net-zero greenhouse gas emissions by 2050 [1]. This transition requires a progressive replacement of fossil fuels and fossil-based chemicals with sustainable, non-fossil alternatives. Among the various candidates, synthetic fuels have emerged as highly promising for large-scale industrial use. In particular, e-methanol produced from captured CO_2 and green hydrogen is receiving significant attention due to its favourable combustion characteristics and the wide range of derivatives it enables. Moreover, methanol synthesis from CO_2 does not require a reverse water-gas shift step, simplifying the overall process configuration.

Methanol is conventionally produced using two types of fixed-bed reactors: adiabatic and isothermal designs [2,3]. Adiabatic systems typically employ several reactors in series with intercooling—either via direct gas cooling or indirect water cooling. However, temperature gradients within adiabatic beds often lead to hot and cold spots, which can reduce reaction rates, accelerate catalyst deactivation, or promote undesired by-products. The quench reactor historically used by ICI (now Johnson Matthey) mitigates these effects by injecting cooling gas along a single catalyst bed, but the strong exothermicity of methanol synthesis quickly drives the temperature to equilibrium, limiting per-pass conversion. As a result, high recycle ratios are required, increasing reactant dilution and raising both operating and capital costs due to larger equipment.

Isothermal reactors, cooled by boiler feed water (as in the Lurgi steam-rising converter) or by a cooling gas, offer better thermal control. Yet when catalyst particles are packed inside tubes, radial heat transfer limitations restrict tube diameters to below roughly 40 mm [4], increasing construction costs and posing engineering constraints. Across both reactor concepts, industry faces persistent challenges related to pressure drop and effective heat removal.

To address these limitations, several alternative reactor geometries have been proposed. TOYO's MRF-Z® design incorporates a radial-flow fixed bed in which catalyst fills an annulus and heat is removed through vertical tubes within the shell, resulting in lower pressure drops compared to conventional beds [5]. Nevertheless, heat removal will become increasingly challenging with the new generation of catalysts, which are significantly more active than previous formulations. Kellogg Brown & Root introduced a spherical fixed-bed configuration that also reduces pressure drop [6].

A more recent innovation emerged with the 2014 patent by Davy Process Technology [4], now held by Johnson Matthey Davy Technologies. The design—commercially known as the CANS™ technology—introduces a multitubular reactor containing up to 200 cartridges per tube, with a cooling medium circulating on the shell side (see Figure 1). Each cartridge contains a ring-shaped catalyst container filled up with catalyst particles, enabling radial, adiabatic gas flow through the bed. After the reaction, the gas is collected, cooled against the tube wall, and directed downward to the next cartridge, repeating the reaction-cooling sequence. This staged configuration shortens the effective bed length, substantially reducing pressure drop while simultaneously enhancing heat-transfer performance—addressing two of the most significant bottlenecks in conventional fixed-bed reactor designs.

Although methanol synthesis is used here as the primary context, the reactor concept and modelling approach are broadly applicable to other highly exothermic catalytic processes such as Fischer-Tropsch synthesis (FTS), ammonia production, hydrogenation reactions, and related fixed-bed systems.

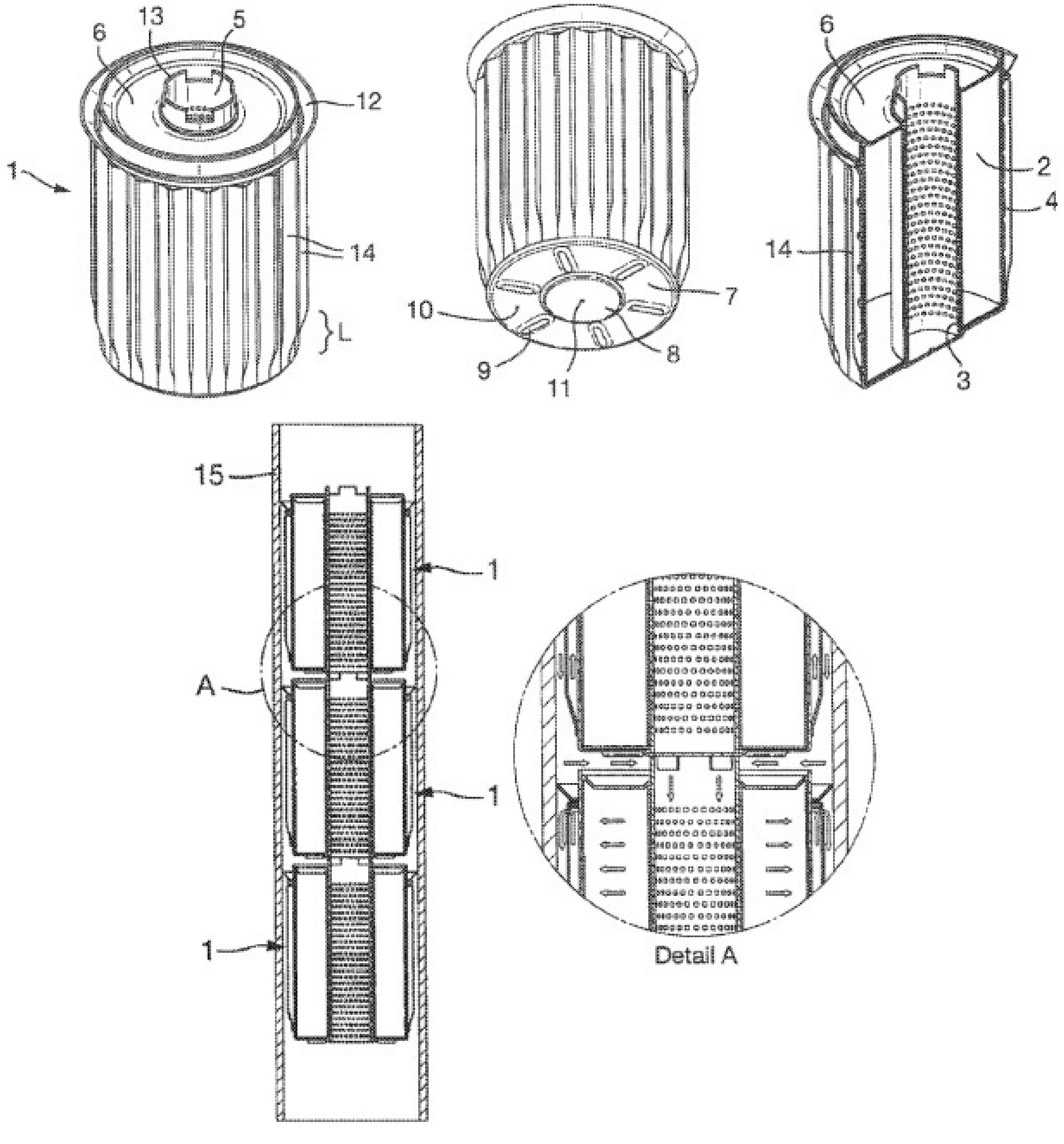

Figure 1. Schematic representation of an isolated CANS™ cartridge (top) and cross-sectional view of three CANS™ cartridges arranged within a tube (bottom) [4]

Motivation and Technical Challenges

The emergence of advanced reactor concepts—such as cartridge-based multitubular radial-flow configurations, spherical fixed beds, or monolithic reactors—offers a promising pathway to improve heat management, reduce pressure drop, and increase conversion efficiency in modern methanol synthesis. However, despite their potential, the industrial adoption of these technologies is significantly constrained by the absence of comprehensive, predictive reactor models capable of accurately representing their coupled transport, reaction, and thermal phenomena.

Limitations of Conventional Modelling Tools

Most industrial chemical processes rely on widely-used and well-characterised unit operations—compressors, reactors, distillation columns, heat exchangers, and others—that have been studied and designed for decades. As a result, process simulation tools (e.g., Aspen Plus, HYSYS, UniSim, gPROMS, ProMax) embed these units as standard modules with user-friendly models and straightforward configuration options. In contrast, cartridge-based reactors do not conform to any existing reactor class in these platforms. They exhibit distinct flow patterns, reaction-cooling sequences, and geometric features that cannot be adequately captured by the modelling frameworks embedded in conventional simulation environments. Therefore, their defining features —repeated reaction–cooling cycles, radial annular beds, multi-zone flow patterns, and geometric dependence—fall outside the capabilities of conventional plug-flow, CSTR, and generic radial-flow models. As a result, industry lacks rigorous design and decision-support tools to evaluate these reactors under realistic conditions, hindering innovation and slowing scale-up.

Typical reactor models assume either axial plug flow or simplified radial-flow behaviour. Cartridge-based radial-flow configurations, however, introduce geometric and hydrodynamic features that differ fundamentally from these assumptions. In particular, they involve:

- Radial gas flow through annular catalyst beds,
- Alternating reaction and cooling zones governed by cartridge geometry,
- Strong interactions between cartridge geometry, bed thickness, heat-removal capacity and temperature profiles,
- Localised catalyst loading that varies with the number and dimensions of cartridges, and
- The need to accurately predict pressure drop in annular fixed-beds, which differs substantially from conventional packed-bed correlations.

These characteristics demand geometry-specific, high-fidelity formulations that surpass the capabilities of standard fixed-bed reactor modules typically present in commercial process simulators.

Moreover, conventional reactor models treat reaction and cooling as separate or loosely coupled phenomena. In cartridge-based reactors, these processes occur in a tightly integrated sequence:

1. Radial flow and reaction inside each catalyst ring,
2. Gas collection and upward transport,
3. Direct cooling against tube walls with the gas flowing downward, and
4. Redistribution to the next cartridge.

Capturing this cyclic behaviour requires a unified framework in which mass, momentum, and energy balances are consistently linked across multiple zones. Existing tools rarely offer such coupled modelling capability without substantial customisation.

Furthermore, commercial process simulation tools have limited capacity to incorporate detailed and complex kinetics and intraparticle effects. Emerging catalyst systems for CO_2-to-methanol synthesis, Fischer-Tropsch Synthesis, and ammonia production exhibit complex kinetic behaviour, diffusion limitations, and heat-generation patterns. However, standard reactor models often rely on:

- Oversimplified macro-kinetic expressions,
- Neglect of intraparticle diffusion and effectiveness factors, and
- Limited support for multicomponent diffusion formulations or temperature-dependent transport properties.

Accurate performance prediction—particularly under high-activity catalyst regimes—requires rigorous multiscale reaction-diffusion descriptions that conventional tools do not natively support.

The absence of validated models creates uncertainty around the real-world feasibility and performance of cartridge-based reactors. This uncertainty affects:

- Feasibility studies,
- CAPEX/OPEX estimates,
- Catalyst loading and distribution strategies,
- Reactor design optimisation,
- Heat-removal and thermal-management design, and
- Integration with upstream and downstream process units

High-fidelity, physics-based models are therefore essential to support confident industrial decision-making and accelerate the commercialisation of advanced reactor technologies. In this context, custom, high-fidelity models are key to reduce technical and investment risk.

Modelling Framework and Numerical Implementation

Mathematical Model and Numerical Methods

To address the modelling gaps identified in the previous section, a dedicated high-fidelity reactor model was developed to accurately represent the transport, reaction, and thermal phenomena occurring within the CANS™ cartridge-based multitubular radial-flow reactors. The modelling framework integrates detailed descriptions of reaction kinetics, intraparticle diffusion, hydrodynamics, and heat transfer across all relevant regions of the reactor, ensuring a consistent and predictive representation of the sequential reaction-cooling cycles that characterise this technology. Figure 2 provides a longitudinal cross-section of a CANS™ cartridge, illustrating the distinct radial reaction zone and the subsequent cooling pathway, which must be modelled as two strongly coupled but physically different domains.

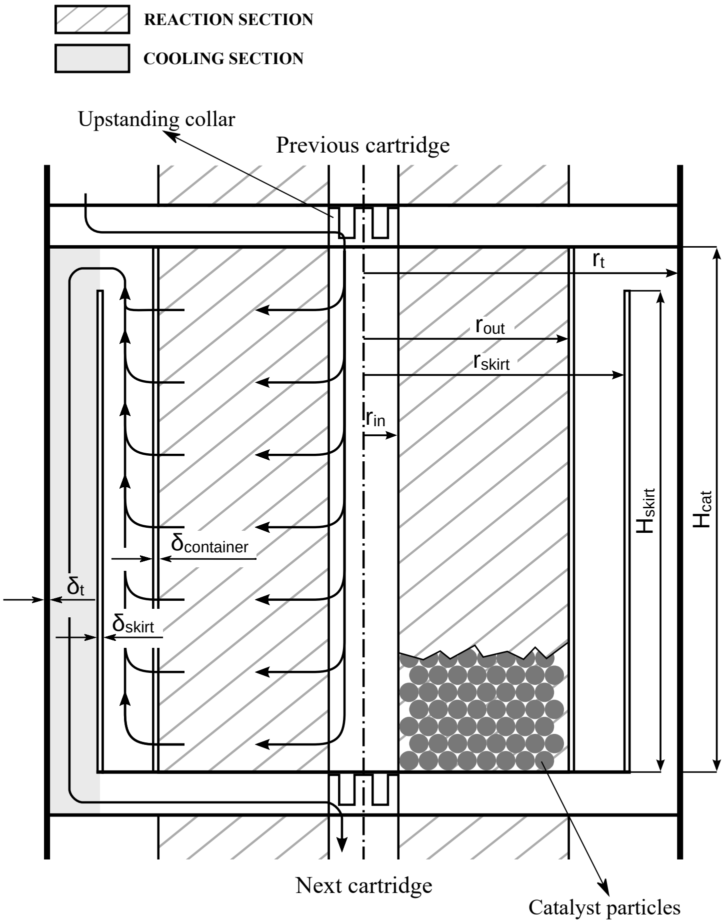

Figure 2. Longitudinal cross-section of a CANS™ cartridge [7]

Overall Modelling Framework

The reactor is decomposed into two fully coupled zones that repeat for each cartridge:

1. Reaction Section: Gas enters the inner void of the cartridge and flows radially outward through the annular catalyst bed, reacting adiabatically in contact with the catalyst particles.
2. Cooling Section: The reacted gas is collected, flows upward through the inner annulus, and subsequently cooled against the tube wall during its downward motion before entering the next cartridge.

Each of these sections is described using first-principles mass, momentum, and energy balances that capture the local behaviour of the reacting and non-reacting flows. The model is solved for every cartridge in series, enabling consistent propagation of temperature, composition, and flow profiles throughout the entire reactor length.

Reaction Section Modelling

Species conservation in the annular catalyst bed is described by a radial mass-balance equation that accounts for:

- Radial convective flow,
- Reaction rates for all chemical reactions,
- Stoichiometric coupling among species,
- Catalyst particle volume and bed density.

The molar flow variation of each species is expressed as a function of radial position within the catalyst bed, ensuring an accurate prediction of concentration gradients. The overall species mass balance is:

$$\frac{dF_i}{dr} = 2\pi r H_{cat} \rho_b \int_0^{V_p} \sum_{j=1}^{J} \nu_{i,j} r_j(s)\, dV_p$$

where F_i is the molar flow of species i, r is the radial dimension in the catalyst container, $r_j(s)$ is the reaction rate of reaction j at a distance s from the particle centre, $\nu_{i,j}$is the stoichiometric coefficient of species i in reaction j, $V_p$is the particle volume and ρ_b is the bed density.

To represent catalyst behaviour, a spherical intraparticle model is employed, coupling:

- Multicomponent diffusion,
- Reaction kinetics for all reactions,
- Local temperature-dependent diffusivities,
- Fickian diffusion and effective diffusivity models,
- Boundary conditions ensuring continuity between the particle surface and bulk gas.

The concentration of each species within the catalyst particle is defined by the mass continuity equation and the Fick's first law:

$$r_i(s)\,dV_p - d\left(J_i(s)\cdot A_p(s)\right) = 0$$

$$J_i(s) = -D_{e,i}\frac{dC_i}{ds}$$

where r_i is the total reaction rate of species i, J_i is the diffusion molar flux, C_i is the concentration of species i and a_p is the spherical superficial area. This multiscale formulation provides realistic estimates of effectiveness factors and diffusion-limited reaction zones—essential for modern high-activity catalysts.

The reaction section is assumed to be adiabatic at the boundaries of the catalyst container:

$$\frac{dH}{dr} = 0$$

This formulation enables the prediction of local hot-spot formation and its impact on catalyst performance without the need of calculating any heat of reaction, heat capacity or standard enthalpy of formation. This formulation takes advantage of the integrated environment where thermodynamic properties can be retrieved directly from Aspen Properties via Aspen Custom Modeler.

The momentum balance is defined as:

$$\frac{dP}{dr} = \frac{-1-\epsilon_b}{\epsilon_b^3}\left(4.2\left(\frac{1-\epsilon_b}{\mathrm{Re}_g}\right)^{\frac{1}{6}} + 150\frac{1-\epsilon_b}{\mathrm{Re}_g}\right)\frac{\rho_g u_g}{d_p}$$

where ρ_g is the gas density, d_p is the particle diameter, u_g is the superficial velocity of the gas and Re_g is the Reynolds number [8,9]. Each of the parameters involved in the momentum balance is estimated via specific correlations for annular packed beds.

Pressure drop across the radial packed bed is estimated via correlations for annular packed beds:

Cooling Section Modelling

The cooling section is described by a dedicated model that accounts for:

- Axial gas flow downward along the tube wall,
- Convective cooling against the wall surface,
- Heat conduction through the tube material,
- The imposed cooling-medium temperature on the shell side.

Mass composition is assumed constant through this region, while temperature variation is governed by a one-dimensional heat-transfer equation employing:

- Empirical correlations for annular heat-transfer coefficients,
- Temperature-dependent gas properties,
- Combined thermal resistances for gas, tube wall, and cooling medium.

It is assumed that the flow is fully developed in the cooling section. The temperature of the external surface of the tube wall (T_w) is assumed to be the same as that of the cooling media. The mass flow and compositions remain steady and equal to the inlet conditions along the entire cooling section. Additionally, the pressure drop in this section is neglected. The heat balance is as follows:

$$dH - dQ_{wall} = dH - UdA\left(T - T_w\right) = 0$$

The thermal resistance (UdA) is calculated with the definition presented by McAdams and Frost [10] and Steynberg et al. [11]:

$$\frac{1}{UdA} = \frac{\delta_t}{k_{steel}\, 2\pi\left(r_t + \delta_t/2\right) dz} + \frac{1}{h\, 2\pi\, r_t\, dz}$$

Model Parameters and Physical Property Methods

Relevant physical and transport properties—such as thermal conductivity, viscosity, diffusion coefficients, etc.—are manually implemented using temperature-dependent correlations from literature sources. Effective diffusivities are calculated using a combination of bulk binary diffusivities and Knudsen diffusion to capture pore-scale limitations. Heat-transfer coefficients are determined using established correlations for turbulent flow in annular ducts.

Both reaction section and cooling section use consistent thermodynamic models to ensure mass and energy conservation. Additionally, the vapour-liquid equilibrium and other physical properties —such as bulk densities, enthalpies, etc.—are directly retrieved from Aspen Properties through Aspen Custom Modeler.

Numerical Implementation

The complete model is implemented in a high-performance simulation environment capable of solving large systems of coupled differential and algebraic equations. The full CANS™ reactor model is therefore constructed programmatically by:

1. Defining the number of tubes in the shell and other reactor parameters.
2. Specifying the number of cartridges per tube and the cartridge geometry.
3. Replicating the single-cartridge model for each cartridge.
4. Enforcing continuity equations across all cartridge interfaces.
5. Solving the entire set of coupled equations simultaneously.

This approach allows the number of cartridges to act as a reactor-level design parameter, enabling rapid sensitivity analyses and scale-up studies.

The set of equations for each section in the cartridge are implemented and solved as follows:

- The reaction section in the catalyst ring is solved using Aspen Custom Modeler's 2nd-order backward finite-difference discretisation. The governing mass and energy balances are formulated along the radial direction of the annular bed, and the resulting system of coupled algebraic equations is integrated simultaneously with the intraparticle reaction-diffusion phenomena. This approach provides numerical stability and accuracy under the strong temperature and concentration gradients characteristic of highly exothermic methanol and Fischer–Tropsch synthesis reactions.
- The intraparticle reaction-diffusion phenomena are solved using the finite-volume method (FVM), assuming uniform catalyst and bulk-gas temperature. Species compositions vary along the particle radius, and a mass balance is applied to each differential control volume. Diffusive fluxes are evaluated at the control-volume interfaces, and the resulting discretised equations are solved to obtain the radial concentration profiles and effectiveness factors.
- The cooling section is modelled and solved using the FVM. The energy balance is discretised across the cooling annulus, with heat fluxes computed at the control-volume faces to capture the strong coupling between wall heat transfer and the downward gas flow. This formulation enables accurate prediction of temperature moderation between cartridges and ensures numerical robustness across a wide range of operating conditions.

The model was coded in Aspen Custom Modeler (ACM) V14 and used the Peng-Robinson equation of state for property calculations, reflecting its established applicability to methanol synthesis and Fischer-Tropsch synthesis systems. The FVM mesh resolution was adjusted and optimised to enable fast simulations without compromising accuracy.

Case Study Setup

To demonstrate the capabilities of the modelling framework described in the previous section, a representative case study was conducted using the methanol synthesis process as the reference system. The CANS™ reactor model—consisting of a detailed single-cartridge representation replicated across multiple cartridges and tubes—was simulated under industrially relevant operating conditions.

Although methanol synthesis is used here as the demonstration platform, the same modelling approach is directly applicable to a wide range of catalytic processes, including Fischer-Tropsch synthesis, ammonia production, hydrogenation reactions, and other exothermic fixed-bed systems that exhibit strong coupling between heat management, transport phenomena, and reaction kinetics.

The case study is adapted from the case presented by Yusup et al. [12] and also used by Leonzio [13] to study different kinetic models. Table 4 of Yusup et al.'s work [12] shows the feed conditions and composition. The geometry of the cartridge-based radial-flow reactor is adapted from the conventional reactor geometry to keep the same catalyst loading (see Table 1). A sensitivity analysis was performed on the number of cartridges to evaluate its impact on the results. The height of each cartridge corresponds to the total reactor length divided by the number of cartridges per tube.

Table 1. Reactor geometry and design parameters

Parameter	Units	Value
Total catalyst loading	kg	35,778.5
Catalyst density	kg/m3	1,100
Tube diameter	m	0.1
δ_t	mm	3.2
r_{in}	m	0.0183
r_{out}	m	0.0432
r_{skirt}	m	0.0675
δ_{skirt}	mm	1
$\delta_{container}$	mm	0.3
d_p	mm	0.5
Number of tubes		1521
Reactor length	m	7.26
H_{cat}/H_{CANS}		0.95
T_w	° C	250

Within the reactor, the following three reversible reactions take place in presence of Cu-Zn-Al catalysts:

$$\mathrm{CO}+2\,\mathrm{H_2} \rightleftarrows \mathrm{CH_3}$$

$$\mathrm{CO_2}+\mathrm{H_2} \rightleftarrows \mathrm{CO}+\mathrm{H_2O}$$

$$\mathrm{CO_2}+3\,\mathrm{H_2} \rightleftarrows \mathrm{CH_3OH}+\mathrm{H_2O}$$

Two different kinetics are evaluated in this work: the original Van der Graaf kinetics [14] and the refitted version proposed by Bisotti et al. [3], the latter providing predictions more consistent with industrial data. The corresponding kinetic rate expressions for those reactions are taken from Graaf et al. [14] (see Eqs. 1, 2 and 3), while equilibrium constants are reported in the work of Graaf et al. [15].

$$r_1=\frac{k_1 K_{CO}\left(P_{CO}P_{H_2}^{1.5}-P_{CH_3OH}/\left(P_{H_2}^{0.5}K_{P1}^{0}\right)\right)}{\left(1+K_{CO}P_{CO}+K_{CO_2}P_{CO_2}\right)\left(P_{H_2}^{0.5}+\left(K_{H_2O}/K_{H_2}^{0.5}\right)P_{H_2O}\right)} \tag{1}$$

$$r_2=\frac{k_2 K_{CO_2}\left(P_{CO_2}P_{H_2}-P_{H_2O}P_{CO}/K_{P2}^{0}\right)}{\left(1+K_{CO}P_{CO}+K_{CO_2}P_{CO_2}\right)\left(P_{H_2}^{0.5}+\left(K_{H_2O}/K_{H_2}^{0.5}\right)P_{H_2O}\right)} \tag{2}$$

$$r_3=\frac{k_3 K_{CO_2}\left(P_{CO_2}P_{H_2}^{1.5}-P_{CH_3OH}P_{H_2O}/\left(P_{H_2}^{1.5}K_{P3}^{0}\right)\right)}{\left(1+K_{CO}P_{CO}+K_{CO_2}P_{CO_2}\right)\left(P_{H_2}^{0.5}+\left(K_{H_2O}/K_{H_2}^{0.5}\right)P_{H_2O}\right)} \tag{3}$$

The model was parametrised to allow variation of the number of cartridges per tube and the total number of tubes, enabling a systematic assessment of their impact on reactor behaviour. Operating conditions and feed compositions were taken from industrial methanol synthesis data.

The simulations were carried out to evaluate key performance metrics, including:

- Carbon conversion per pass,
- Methanol yield,
- Temperature profiles through reaction and cooling zones,
- Pressure drop across each cartridge and the full reactor,
- Thermal behaviour and approach to quasi-isothermal operation,
- Sensitivity of performance to the number of cartridges.

These indicators provide insight into the fundamental trade-offs in compact multitubular designs and enable evaluation of the CANS™ configuration relative to conventional fixed-bed reactors.

Results and Performance Evaluation

The simulations provide a detailed picture of how the CANS™ multitubular reactor behaves under different design configurations and operating conditions. Results are presented as a function of the number of cartridges per tube—a key design variable that controls the sequence of reaction–cooling cycles and therefore the thermal and hydrodynamic characteristics of the system.

Methanol Yield and Carbon Conversion

Figure 3 (top) shows that increasing the number of cartridges leads to an improvement in methanol yield and carbon conversion per pass for both kinetic models. This enhancement arises from:

- More frequent temperature moderation
- Reduced severity of hot spots
- More uniform catalyst utilisation

However, beyond approximately 20–25 cartridges, the marginal benefit diminishes, and the reactor approaches quasi-isothermal performance. In this regime, additional cartridges provide minimal improvement in conversion because the reaction-cooling cycles become more frequent than necessary to maintain optimal temperature profiles.

The refitted Van der Graaf kinetics consistently predicts higher methanol production, aligning with observations from industrial practice.

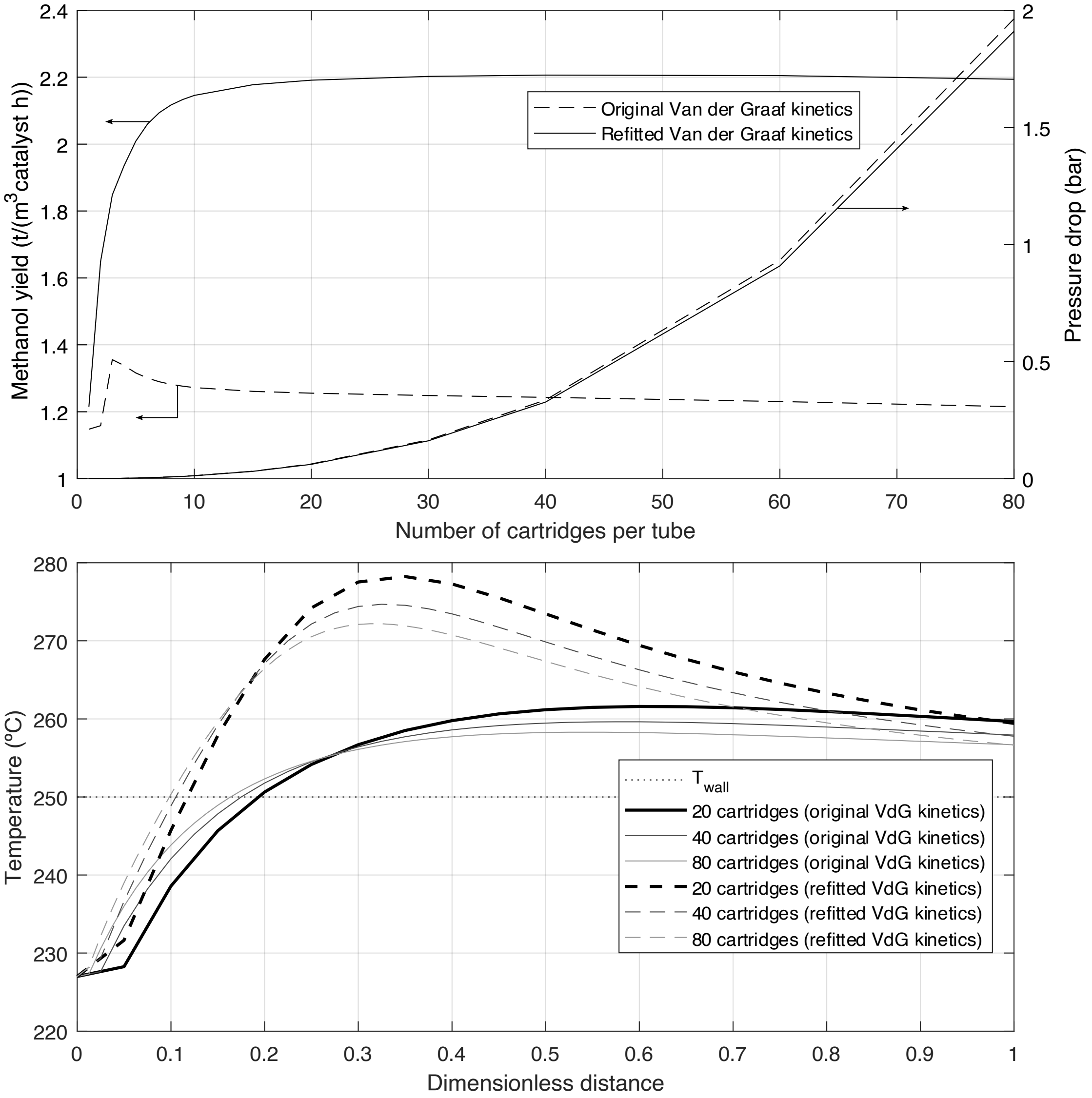

Figure 3. Methanol yield and pressure drop vs number of cartridges per tube (top) and temperature profiles along the reactor (bottom) [7]

Temperature Profiles and Thermal Behaviour

Figure 3 (bottom) illustrates the evolution of temperature along the reactor axis for different cartridge counts. Key observations include:

- Few cartridges (e.g., 1–3): pronounced temperature excursions and high peak temperatures.
- Intermediate cartridge counts (e.g., 10–15): moderated temperature swings with improved heat management.
- High cartridge counts (≥ 20): nearly flat temperature profiles, indicating quasi-isothermal operation.

The results confirm that the CANS™ architecture fundamentally alters heat management by distributing reaction heat across multiple short adiabatic zones separated by efficient cooling intervals.

Pressure Drop Behaviour

As expected, Figure 3 (top) shows that increasing the number of cartridges increases the effective bed thickness, leading to higher pressure drops. This trade-off is central to the reactor's design:

- Low cartridge counts → low ΔP but poorer thermal control
- High cartridge counts → good heat management but higher ΔP

The model thus enables a rigorous multi-objective evaluation, balancing conversion, heat removal, catalyst utilisation, and hydrodynamics.

Comparison with Conventional Reactors

For equal catalyst loading, the CANS™ configuration delivers:

- Higher methanol yield per unit catalyst mass
- Lower or comparable pressure drop depending on cartridge count
- Improved temperature control due to distributed cooling
- Flexibility in design optimisation, since cartridge number is a tunable parameter

These results indicate that CANS™ reactors can significantly outperform conventional multitubular fixed beds while enabling finer thermal control and improved operational stability. These benefits are further enhanced when recycle loops are incorporated into the process design.

Applicability Beyond Methanol

While methanol synthesis is used as the demonstrator, the model and findings translate directly to other high-heat-release catalytic processes, including:

- Fischer-Tropsch synthesis
- Ammonia synthesis
- Methanation
- Shift reactions
- Oxidation reactions (e.g., maleic anhydride and ethylene oxide formation)
- Exothermic gas-phase hydrogenations

In all such systems, the ability to alternate reaction and cooling in tightly controlled sequences offers strong potential advantages in selectivity, safety, and catalyst longevity.

Conclusions

A comprehensive high-fidelity modelling framework for cartridge-based multitubular radial-flow reactors was developed by AmbarPro. The model integrates detailed descriptions of reaction kinetics, intraparticle diffusion, hydrodynamics and heat transfer, enabling a rigorous representation of the strongly coupled reaction-cooling cycles that define the behaviour of these reactors. By combining first-principles equations, specialised correlations for annular fixed beds and advanced numerical methods, AmbarPro provides capabilities that conventional simulation tools cannot adequately represent.

The case study, based on industrial methanol synthesis, demonstrates how AmbarPro enables the development of advanced custom reactor models that deliver predictive insight into performance under realistic operating conditions. The results highlight the existence of a clear trade-off between methanol yield, temperature moderation and pressure drop as the number of cartridges is varied. Specifically, increasing the number of cartridges enhances conversion and favours a quasi-isothermal operation but also leads to higher pressure drop. Above a certain number of cartridges, performance improvements diminish while hydrodynamic penalties increase, underscoring the need for optimisation rather than straightforward maximisation of cartridge number. These findings confirm that CANS™-type reactors can deliver significantly higher catalyst productivity than conventional multitubular designs when appropriately configured.

Although methanol synthesis was used as the reference system for validation, the modelling approach is directly applicable to other highly exothermic catalytic processes, including Fischer-Tropsch synthesis, ammonia synthesis, gas-phase hydrogenations and other systems in which heat removal and pressure-drop constraints critically influence performance. The generality of the formulation and the modular construction of the reactor model make it suitable for scale-up studies, process optimisation, feasibility assessments and preliminary techno-economic evaluations.

The modelling and numerical techniques applied in this study are representative of the type of custom reactor models developed by AmbarPro for complex process units where standard simulation approaches fail to provide sufficient insight. These high-fidelity custom reactor models are essential to unlock the full potential of emerging reactor technologies such as CANS™. Additionally, it reduces design uncertainty, supports informed investment decisions, and accelerates the transition toward more efficient and carbon-neutral chemical manufacturing.

References

[1] European Commission, The European Green Deal, European Commission, Brussels, 2019.

[2] G. Bozzano, F. Manenti, Efficient methanol synthesis: Perspectives, technologies and optimization strategies, Progress in Energy and Combustion Science 56 (2016) 71–105. https://doi.org/10.1016/j.pecs.2016.06.001.

[3] F. Bisotti, M. Fedeli, K. Prifti, A. Galeazzi, A. Dell'Angelo, F. Manenti, Impact of Kinetic Models on Methanol Synthesis Reactor Predictions: In Silico Assessment and Comparison with Industrial Data, Ind. Eng. Chem. Res. 61 (2022) 2206–2226. https://doi.org/10.1021/acs.iecr.1c04476.

[4] T.D. Gamlin, Process for the synthesis of methanol, (2014).

[5] K. Ohsaki, J. Zamma, Y. Kobayasi, H. Watanabe, Chemical process and apparatus therefor, (1982).

[6] F. Hartig, F.J. Keil, Large-scale spherical fixed bed reactors: modeling and optimization, Ind. Eng. Chem. Res. 32 (1993) 424–437. https://doi.org/10.1021/ie00015a005.

[7] F. Sauerhöfer-Rodrigo, M. Rodríguez, I. Díaz, Modelling of a Cartridge-based Fixed Bed Radial Flow Reactor for Methanol Synthesis, in: Computer Aided Chemical Engineering, Elsevier, 2024: pp. 337–342. https://doi.org/10.1016/B978-0-443-28824-1.50057-0.

[8] E. Erdim, Ö. Akgiray, İ. Demir, A revisit of pressure drop-flow rate correlations for packed beds of spheres, Powder Technology 283 (2015) 488–504. https://doi.org/10.1016/j.powtec.2015.06.017.

[9] J.A. Tallmadge, Packed bed pressure drop—an extension to higher Reynolds numbers, AIChE Journal 16 (1970) 1092–1093. https://doi.org/10.1002/aic.690160639.

[10] W.H. Mcadams, T.H. Frost, Heat Transfer by Conduction and Convection II- Liquids FLowing through Pipes, J. Ind. Eng. Chem. 14 (1922) 1101–1104. https://doi.org/10.1021/ie50156a002.

[11] Fischer-Tropsch Reactors, in: Studies in Surface Science and Catalysis, Elsevier, 2004: pp. 64–195. https://doi.org/10.1016/S0167-2991(04)80459-2.

[12] S. Yusup, N.P. Anh, H. Zabiri, A simulation study of an industrial methanol reactor based on simplified steady-state model, Ijrras 5 (2010) 213–222.

[13] G. Leonzio, Mathematical modeling of a methanol reactor by using different kinetic models, Journal of Industrial and Engineering Chemistry 85 (2020) 130–140. https://doi.org/10.1016/j.jiec.2020.01.033.

[14] G.H. Graaf, H. Scholtens, E.J. Stamhuis, A.A.C.M. Beenackers, Intra-particle diffusion limitations in low-pressure methanol synthesis, Chemical Engineering Science 45 (1990) 773–783. https://doi.org/10.1016/0009-2509(90)85001-T.

[15] G.H. Graaf, P.J.J.M. Sijtsema, E.J. Stamhuis, G.E.H. Joosten, Chemical equilibria in methanol synthesis, Chemical Engineering Science 41 (1986) 2883–2890. https://doi.org/10.1016/0009-2509(86)80019-7.