

Numerical Investigation of Coolant-dependent Heat Transfer Performance in Jacketed Reactors

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Abstract

The thermal performance of jacketed reactors is strongly influenced by the thermophysical properties of the applied heat transfer fluid. While analytical methods provide rapid engineering estimates, they are often unable to describe local flow structures and temperature distributions within the jacket space. In the present study, a three-dimensional computational fluid dynamics (CFD) model was developed in ANSYS CFX to investigate the flow and heat transfer behavior of two commonly used coolant solutions: methanol-water and ethylene glycol-water mixtures. The numerical simulations were performed for two jacketed reactor geometries under identical thermal boundary conditions. The velocity field, temperature distribution, pressure drop, and heat transfer coefficient were evaluated and compared with previously published analytical calculations. The results showed that the methanol-based coolant provided higher heat transfer coefficients in both investigated geometries. The calculated differences between the two coolant solutions reached 23.0% and 20.7%, respectively, which is in good agreement with the trends predicted by the analytical model. The CFD simulations confirmed the main conclusions of the analytical investigation while providing additional insight into the underlying flow and temperature fields. The proposed methodology can support the comparative evaluation of heat transfer fluids and assist engineering decision-making during the thermal design of jacketed reactor systems.

Keywords

jacketed reactor, heat transfer coefficient, CFD

1 Introduction

The thermal behavior of jacketed reactors used in chemical and pharmaceutical engineering has a significant influence on process controllability, operational safety and energy efficiency. In processes involving heat-sensitive or exothermic reactions, the appropriate design of heat transfer between the reactor volume and the heat transfer medium is particularly important. Insufficient heat removal may lead to local overheating, deterioration of product quality or unfavorable operating conditions [1, 2].

Analytical and semi-empirical correlations are commonly used for the engineering estimation of heat transfer in reactor systems. These methods can be applied efficiently and provide preliminary estimates of key thermal quantities, such as the heat transfer coefficient and the heat transfer rate. Widely used correlations for convective heat transfer in internal flows include, among others, the Dittus–Boelter, Sieder–Tate and Gnielinski correlations [3–5]. For jacket-side heat transfer, more specific

correlations are also available for estimating the heat transfer coefficient on the jacket side of process vessels [6–8].

The main advantage of analytical methods is that they provide rapid estimates using a limited number of input parameters. However, these approaches are generally based on simplified geometrical assumptions, averaged flow quantities and idealized temperature distributions. Therefore, local flow structures, near-wall velocity and temperature gradients, and non-uniform temperature fields inside the jacket space can only be evaluated to a limited extent by analytical calculations.

Numerical flow simulation, especially computational fluid dynamics, provides a suitable tool for the more detailed analysis of flow and heat transfer processes in reactors and their heat transfer jackets. CFD simulations make it possible to determine the velocity field, temperature distribution, pressure field and the spatial variation of wall heat transfer characteristics. This is particularly

useful when the performance of two different heat transfer fluids must be compared under identical or nearly identical operating conditions [9].

The selection of the heat transfer fluid has a direct effect on the heat transfer coefficient, pressure drop and operating characteristics of the system. Methanol-water and ethylene glycol-water based solutions have different density, specific heat capacity, thermal conductivity and dynamic viscosity. Therefore, even under identical volumetric flow rate and temperature conditions, different jacket-side heat transfer and flow behavior can be expected [10–14]. Previous analytical investigations have shown that a considerable difference may occur between the jacket-side heat transfer coefficients obtained for the two coolants [15].

The objective of the present study is to perform a CFD-based investigation of an industrially motivated but generalized reactor heat transfer problem. The analysis considers two jacketed reactor geometries of different size. Methanol-water and ethylene glycol-water based coolants are compared under prescribed operating conditions. The main purpose of the study is not to determine final design values of the absolute heat transfer coefficients, but to demonstrate the relative difference between the two coolants and to evaluate how this difference appears in the velocity and temperature fields.

The numerical model presented in this paper was developed in ANSYS CFX [16]. The computational domain includes the coolant flow region in the reactor jacket and the wall surfaces relevant from the viewpoint of heat transfer. The model is used to evaluate the jacket-side flow patterns, temperature distribution, pressure drop and calculated heat transfer coefficients. The CFD results are compared with previous analytical calculations, with particular emphasis on the relative difference between the two investigated coolants.

2 Materials and methods

2.1 Investigated reactor system

The investigated system is a jacketed reactor configuration in which the coolant flows through a jacket space formed around the reactor body. Heat transfer takes place through the common wall between the reactor volume and the jacket-side coolant. Since the objective of the present analysis is to evaluate the heat transfer behavior of the coolant flowing in the jacket, the numerical model primarily considers the coolant flow domain, the heat transfer surfaces and the boundary surfaces relevant to environmental heat losses. The numerical investigation was carried out for two reactor geometries (Fig. 1 and Table 1).

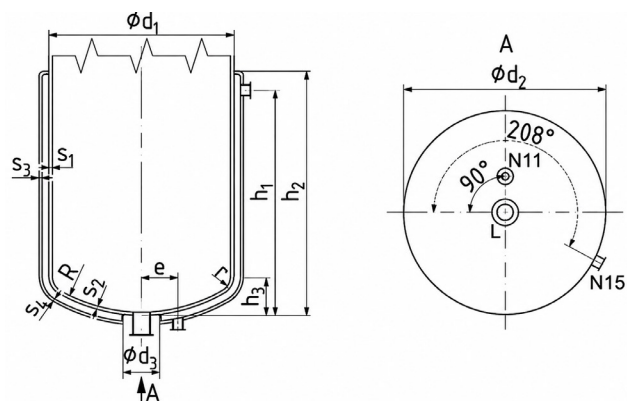


Fig. 1 Characteristic geometrical parameters of the investigated reactor configurations [15]

Table 1 Main geometrical parameters of the investigated reactor configurations [15]

Reactor	d_1	d_2	s_3	d_{N11}	h_2
Geometry A	1100	1100	6	51.2	1000
Geometry B	2000	2100	10	82.5	2500

The use of two geometries made it possible to examine whether the differences caused by the thermophysical properties of the coolants appear consistently in jacket spaces of different scale. Due to the industrial sensitivity of the original equipment, the geometrical details are presented in a generalized form in this paper, while retaining the main features required for the thermal and fluid flow evaluation.

Two coolants were compared in the simulations: a methanol-water based solution and an ethylene glycol-water based solution. Owing to their different thermophysical properties, different jacket-side heat transfer behavior is expected even under the same operating conditions. The inlet temperature of the coolant was identical in all cases, while prescribed volumetric flow rates were assigned to the two reactor geometries. In the CFD model, these volumetric flow rates were converted into mass flow rates using the density of the corresponding coolant at the inlet temperature.

At the inlet boundary, the mass flow rate and the coolant temperature were prescribed. At the outlet boundary, a pressure condition corresponding to atmospheric pressure was applied. On the reactor-side wall, the internal heat transfer from the reactor volume was represented by a simplified convective heat transfer boundary condition. On the external surfaces, heat exchange with the environment was taken into account by an external convective boundary condition. Since only limited operating and measurement data were available, some thermal parameters were defined based on engineering assumptions or literature data. Consequently, the interpretation of the results is primarily

comparative: the analysis focuses on the relative heat transfer behavior of the two investigated coolants.

The consistent transfer of heat flux between the jacket-side fluid domain and the reactor wall was of particular importance in the numerical model. The purpose of this treatment was to ensure numerical consistency between the heat flux supplied from the reactor-side wall and the heat absorbed by the coolant. The heat transfer coefficient was evaluated on the heat transfer surface between the reactor volume and the jacket space, because this surface directly determines the heat removal capability of the coolant.

2.2 Coolants and thermophysical properties

Two different coolant solutions were investigated in the numerical simulations: a methanol-water based solution and an ethylene glycol-water based solution. The comparison of these coolants is relevant because their thermophysical properties differ considerably, which directly affects the jacket-side heat transfer coefficient, the pressure drop and the thermal response of the system.

The inlet temperature of the coolant was kept identical in all investigated cases. Since only limited measurement data were available for the original industrial system, the thermophysical properties of the coolant solutions were defined using literature data and engineering assumptions. The same set of properties was applied consistently in the analytical and numerical evaluation, in order to make the comparison between the two coolants meaningful.

The methanol-water based solution has a lower dynamic viscosity than the ethylene glycol-water based solution. This difference is expected to influence the flow resistance and the wall heat transfer in the jacket space. At the same time, the two coolants also differ in density, specific heat capacity and thermal conductivity, which affects the Reynolds number, Prandtl number and the resulting convective heat transfer behavior.

The thermophysical properties used in the CFD simulations are summarized in Table 2.

Table 2 Thermophysical properties [15]

Coolant solution:	Density, [kg/m ³]	Specific heat capacity, [J/(kg K)]	Thermal conductivity [W/(m K)]	Dynamic viscosity [mPa s]
methanol-water based solution	1014	4011	0.445	7.18
ethylene glycol-water based solution	1067	3545	0.417	11.53

2.3 Computational domain and boundary conditions

The computational domain represented the coolant flow region in the jacket space of the investigated reactor configurations. The flow domain was generated from the jacket volume, while the solid walls were included to represent the heat transfer path between the reactor-side boundary and the coolant.

The same inlet temperature was applied for all coolant solutions and reactor geometries. The coolant entered the jacket space at an inlet temperature of $-16.1\text{ }^{\circ}\text{C}$. Prescribed volumetric flow rates were assigned to the two investigated geometries. For Geometry A, the inlet volumetric flow rate was $0.01443\text{ m}^3/\text{s}$, while for Geometry B it was $0.02564\text{ m}^3/\text{s}$. Since ANSYS CFX [16] requires the flow rate to be specified as mass flow rate at the inlet, the volumetric flow rates were converted into mass flow rates using the density of the corresponding coolant solution at the inlet temperature.

At the outlet boundary, a relative static pressure of 0 bar(g) was prescribed. The reactor-side heat transfer was represented by a convective thermal boundary condition. The temperature on the reactor side was assumed to be $25\text{ }^{\circ}\text{C}$, and the corresponding heat transfer coefficient was set to $500\text{ W}/(\text{m}^2\text{ K})$. Since the reactor contents were not included in the computational domain and no experimental data were available for the internal reactor-side heat transfer coefficient, this value was adopted as a representative engineering estimate for a liquid-filled, mechanically agitated industrial reactor. The same value was applied in all investigated cases to ensure that the comparison reflected only the influence of the coolant properties on the jacket-side heat transfer performance.

Heat exchange between the external jacket surface and the surroundings was also taken into account. The ambient temperature was set to $25\text{ }^{\circ}\text{C}$, and an external heat transfer coefficient of $10\text{ W}/(\text{m}^2\text{ K})$ was applied on the outer surfaces. All solid walls in contact with the coolant were treated as no-slip walls.

The applied boundary conditions are summarized in Fig. 2.

2.4 Interfaces and heat flux treatment

In the numerical model, the thermal connection between the coolant, the reactor wall and the external environment was defined through separate boundary and interface regions. Two main interface regions were distinguished. One of them was associated with the heat transfer wall

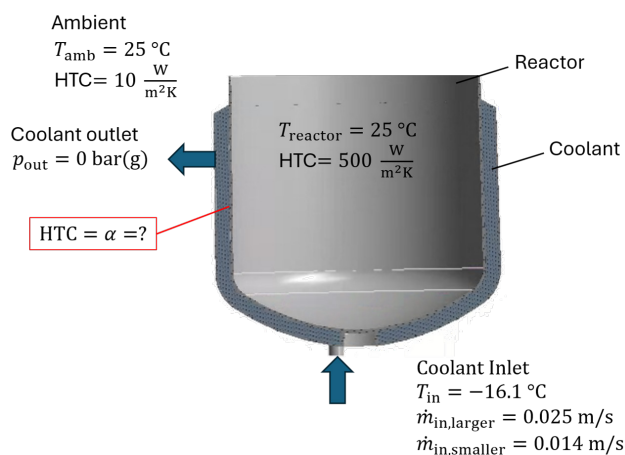


Fig. 2 Generalized jacketed reactor configuration and the main thermal boundary conditions

between the reactor volume and the jacket-side coolant, while the other represented the external side of the jacket exposed to the surroundings. The heat transfer coefficient was evaluated on the reactor-side heat transfer surface, because this surface directly determines the heat removal capability of the coolant. A conservative heat flux treatment was applied for the heat transfer between the solid and fluid domains. The purpose of this approach was to ensure numerical consistency between the heat transferred through the reactor wall and the heat absorbed by the coolant. This was particularly important in the present comparative study, since the reliable evaluation of the relative difference between the heat transfer coefficients of the two coolants requires that the heat flux transfer be treated in the same and energy-consistent manner.

The use of the conservative heat flux treatment reduces the possibility that energy imbalance errors arising from the numerical discretization at the solid-fluid connection influence the results. Consequently, the heat flux transferred through the wall and the heat flux absorbed in the fluid domain remain consistent with each other. The generalized locations of the interface regions and the main thermal boundary surfaces are illustrated in Fig. 3.

2.5 Mesh generation

The computational domain was discretized using an unstructured mesh consisting primarily of tetrahedral elements, while prismatic inflation layers were applied in the near-wall regions. The governing conservation equations were solved in ANSYS CFX [16] using a finite-volume approach.

The final mesh contained approximately one million elements, providing a reasonable compromise between numerical accuracy and computational cost. Local mesh

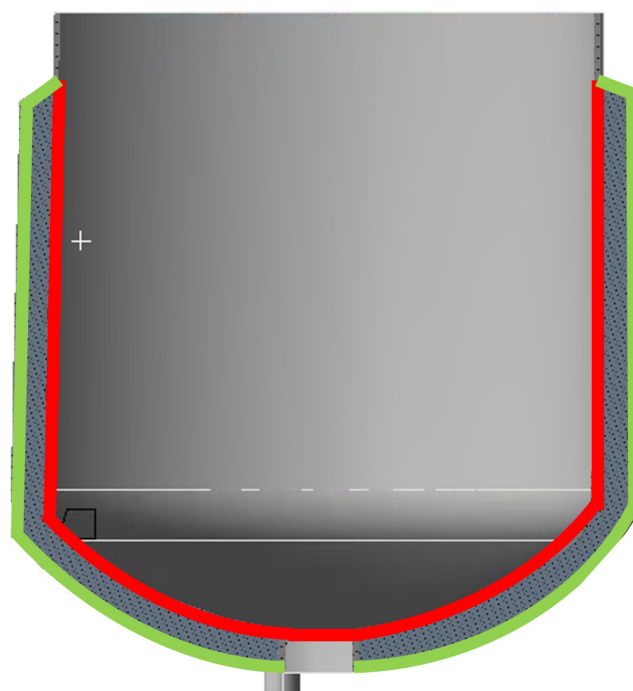


Fig. 3 Interface regions of the numerical model: green denotes the external ambient-side jacket surface, while red denotes the reactor-side heat transfer surface used for the heat transfer coefficient evaluation

refinement was applied in regions where higher velocity and temperature gradients were expected.

To improve the resolution of wall-bounded flow and heat transfer, 16 prismatic inflation layers with a growth rate of 1.2 were generated along the reactor wall. This mesh structure enabled a stable evaluation of the near-wall thermal behavior.

A mesh sensitivity study was performed for the smaller reactor configuration (Geometry A / AE630) by comparing the calculated heat transfer coefficient and pressure drop for different mesh resolutions. The results are summarized in Table 3. The predicted heat transfer coefficient and pressure drop became practically independent of the mesh density for meshes exceeding approximately 1.5 million nodes. Based on these results, the selected meshing strategy was also applied to the larger reactor geometry,

Table 3 Results of the mesh sensitivity study for Geometry A

Mesh	Node nr.	Pressure drop [Pa]	HTC [W/(m² K)]
Mesh 1	1 202 510	32 304	489
Mesh 2	1 324 451	34 154	502
Mesh 3	1 405 121	35 051	519
Mesh 4	1 500 417	36 333	526
Mesh 5	1 612 984	36 345	525
Mesh 6	1 743 646	36 384	526

providing a reasonable compromise between numerical accuracy and computational cost. A representative mesh detail is shown in Fig. 4.

2.6 Solver settings and turbulence model

The numerical simulations were performed in ANSYS CFX [16]. The calculations were carried out in steady-state mode using the pseudo-transient approach implemented in CFX. This setting made it possible to obtain the steady flow and heat transfer solution in a numerically stable manner.

The advection terms were discretized using the High-Resolution scheme, which provides a favorable compromise between numerical accuracy and stability. For the turbulence equations, a first-order discretization scheme was applied in order to support robust convergence. The maximum number of iterations was set to 500. The automatic timescale option was used with the Conservative length scale setting and a scale factor of 1.0 for both the fluid and solid domains.

Heat transport was modeled using the Thermal Energy formulation. Combustion and radiation effects were not included in the model, since the objective of the study was the comparative evaluation of coolant-side convective heat transfer and jacket-side thermal behavior. The heat flux transfer between the wall and the fluid was treated using a conservative heat flux approach, which ensured an energy-consistent thermal connection between the solid and fluid domains.

The turbulent flow was described using the standard ($k-\varepsilon$) turbulence model with scalable wall functions. This model was selected as a robust option for industrial internal flow simulations and provides adequate numerical

stability for comparative heat transfer analyses. Since the primary objective of the present study was the comparative evaluation of two different coolants under identical numerical conditions, the same turbulence model was consistently applied in all simulations to ensure that the observed differences originated solely from the thermo-physical properties of the investigated coolants. Although alternative turbulence models, such as the SST $k-\omega$, RNG $k-\varepsilon$, and realizable $k-\varepsilon$ models, may provide improved predictions of near-wall flow behavior, their evaluation was beyond the scope of the present study. The use of scalable wall functions enabled a consistent near-wall treatment for the applied mesh resolution.

The convergence of the simulations was assessed based on the RMS residuals and the stabilization of the monitored physical quantities. The target value for the RMS residuals was set to 10^{-4} . During the simulations, the heat transfer coefficient, the temperature difference between the inlet and outlet, the heat flux on the inner side of the jacket, the outlet mass flow rate and the system pressure were monitored. The solution was considered converged when the residuals decreased to the prescribed level and the monitored quantities no longer showed significant changes with further iterations.

3 Results and discussion

3.1 Convergence behavior

The reliability of the numerical solution was evaluated by monitoring both the residuals and the main physical quantities relevant to the present study. The convergence assessment was therefore not based solely on the residual curves, but also on the stabilization of the heat transfer coefficient, the jacket-side heat flux, the outlet mass flow rate, the system pressure and the temperature difference between the inlet and outlet.

The target value for the RMS residuals was set to (10^{-4}). During the initial stage of the iterations, the residuals decreased by several orders of magnitude and then reached a lower residual level with oscillatory behavior (Fig. 5). A periodic fluctuation can be observed especially in the mass conservation residual, while the residuals of the momentum equations show smaller-amplitude variations. This indicates that the solution did not converge in a fully monotonic residual sense; however, after the initial decay, no increasing trend or numerical instability was observed.

The iteration history of the heat transfer coefficient was an important additional convergence indicator, since the main objective of the study was to compare the heat

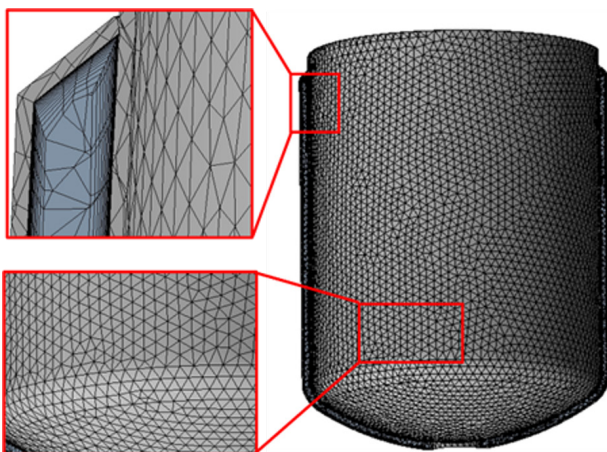


Fig. 4 Representative mesh detail showing the tetrahedral elements and near-wall prismatic inflation layers

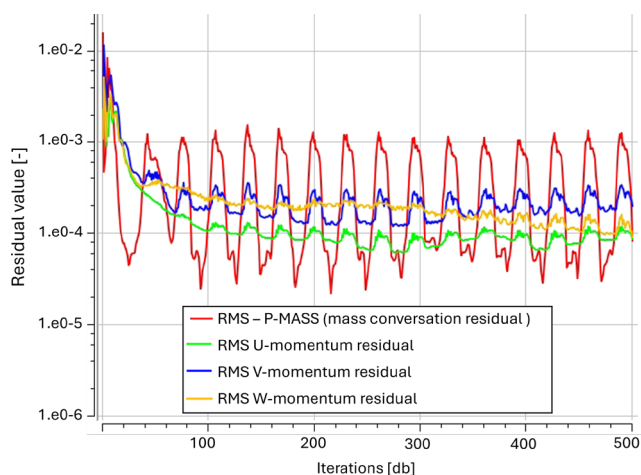


Fig. 5 RMS residual histories during the numerical simulation

transfer behavior of the two coolant solutions. The monitored heat transfer coefficient changed significantly at the beginning of the calculation and then gradually stabilized around an approximately constant value. On this basis, the near-wall heat transfer behavior can be regarded as steady from an engineering point of view.

Based on the convergence assessment, the simulations were considered suitable for comparative evaluation. Although oscillations remained in some residuals, the stabilization of monitored physical quantities confirmed that the obtained velocity, temperature and heat transfer results provide an appropriate basis for comparing the relative behavior of the two coolant solutions. The representative convergence histories of the residuals and the monitored heat transfer coefficient are shown in Fig. 6.

3.2 Flow field

The flow conditions inside the jacket space were investigated prior to the evaluation of the heat transfer performance, since the local velocity distribution has a significant influence on the convective heat transfer process.

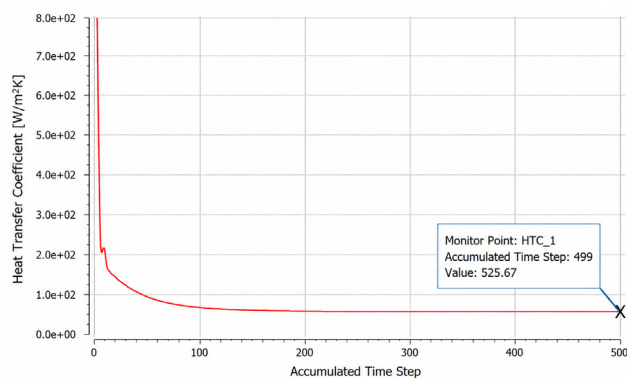


Fig. 6 Heat transfer coefficient history during the numerical simulation

Streamline visualization was employed to analyze the coolant motion and to identify the characteristic flow structures formed within the jacket.

Fig. 7 presents the three-dimensional flow patterns obtained for the investigated reactor geometries and coolant solutions. It can be observed that the coolant traverses the entire jacket volume and forms large-scale recirculation regions. These vortical flow structures are particularly pronounced in the larger reactor geometry. Based on the streamline distributions, no significant dead zones were identified that would exclude substantial portions of the heat transfer surface from the cooling process.

The cross-sectional streamline distributions are shown in Fig. 8. The highest local velocities occur in the vicinity of the inlet nozzle, where the flow accelerates due to the local geometrical constraints. After entering the jacket space, the coolant spreads circumferentially within the annular region and gradually moves toward the outlet section. The overall flow structures obtained for the methanol-based and ethylene-glycol-based coolants are similar.

Although local differences can be observed in the detailed streamline patterns, the global flow behavior remains essentially unchanged for the two coolant solutions. This suggests that the differences in the heat transfer performance discussed in Sections 3.3 and 3.4 are primarily related to the different thermophysical properties of the coolants rather than to significant changes in the overall flow structure.

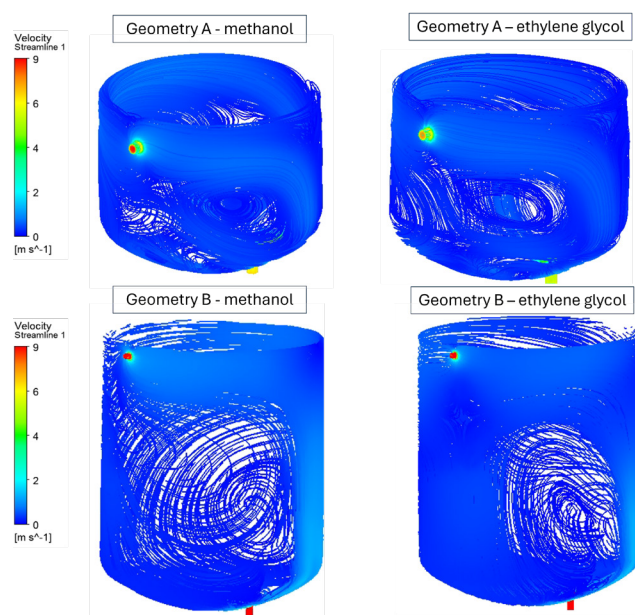


Fig. 7 Three-dimensional streamline representation of the coolant flow in the jacket space for the investigated reactor geometries and coolant solutions

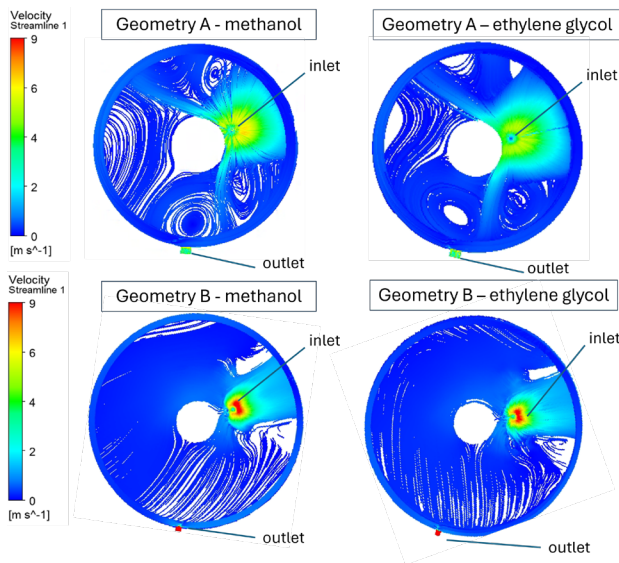


Fig. 8 Cross-sectional streamline distribution in the jacket space showing the inlet and outlet regions

Based on the calculated flow fields, both investigated reactor geometries provided adequate coolant distribution throughout the jacket space, creating favorable conditions for efficient heat transfer.

3.3 Temperature field

The temperature contours obtained for the investigated geometries and coolant solutions are presented in Fig. 9. In all cases, the lowest temperatures were observed near the inlet region, while higher temperatures developed along the flow path as the coolant absorbed heat from the reactor wall.

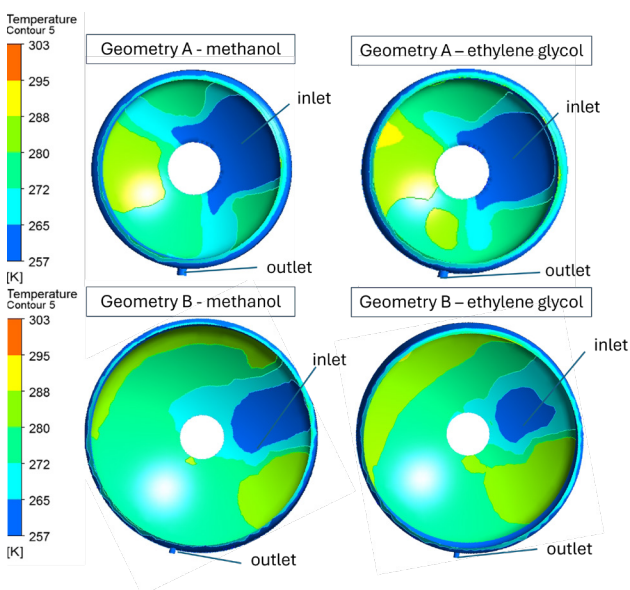


Fig. 9 Temperature contours in the jacket space for the investigated reactor geometries and coolant solutions

The temperature distributions are smooth and physically consistent, without significant numerical artifacts. Similar thermal patterns were obtained for both coolant solutions, indicating that the differences in heat transfer performance are primarily related to their thermophysical properties. Overall, both reactor geometries provided effective heat removal and adequate thermal communication between the reactor wall and the jacket-side coolant.

3.4 Comparison of heat transfer performance

The primary objective of the numerical simulations was to compare the heat transfer behavior of the methanol-based and ethylene-glycol-based coolant solutions. For this purpose, the pressure drop, mass flow rate, and heat transfer coefficient between the reactor wall and the jacket-side coolant were evaluated. A summary of the obtained results is presented in Table 4.

The numerical results indicate that the methanol-based solution provided higher heat transfer coefficients than the ethylene-glycol-based solution for both investigated reactor geometries. For Geometry A, the calculated heat transfer coefficient was $526 \text{ W/(m}^2 \text{ K)}$ for the methanol-based coolant and $405 \text{ W/(m}^2 \text{ K)}$ for the ethylene-glycol-based coolant. For Geometry B, the corresponding values were $508 \text{ W/(m}^2 \text{ K)}$ and $403 \text{ W/(m}^2 \text{ K)}$, respectively. These results demonstrate that the methanol-based coolant exhibits more favorable heat transfer characteristics under the investigated operating conditions.

The relative difference between the two coolant solutions reached 23.0% for Geometry A and 20.7% for Geometry B. Such differences can be considered significant from an engineering perspective, particularly in reactor systems where the efficiency of heat removal directly affects process controllability and operational safety.

With respect to pressure losses, the observed trends differed between the investigated geometries. For Geometry A, the methanol-based solution resulted in a higher pressure drop, whereas for Geometry B the ethylene-glycol-based solution produced a slightly higher

Table 4 Comparison of the CFD results for the investigated coolant solutions

Geometry	Coolant solution	Pressure drop [Pa]	HTC [$\text{W/(m}^2 \text{ K)}$]
Geometry A	methanol	36 333	526
Geometry A	ethylene g.	33 779	405
Geometry B	methanol	106 695	508
Geometry B	ethylene g.	110 259	403

pressure loss. This observation suggests that the pressure drop is influenced not only by the coolant properties but also by the local flow structures and the geometrical characteristics of the jacket space.

The numerical results were further compared with the analytical calculations presented in previous work [15] (Table 5). The analytical model predicted relative differences of 26.7% and 24.5% between the heat transfer coefficients of the two coolant solutions for Geometries A and B, respectively. Although the CFD simulations yielded somewhat smaller differences, both approaches led to the same engineering conclusion: the heat transfer performance of the investigated coolant solutions differs significantly under identical operating conditions.

It should be emphasized that the primary objective of the present study was not the determination of absolute design values for the heat transfer coefficient, but rather the comparative evaluation of the two coolant solutions. From this perspective, the CFD simulations confirm the main conclusions of the analytical calculations while providing additional insight into the underlying flow and temperature fields.

4 Conclusion

In the present study, the heat transfer performance of two coolant solutions was investigated for jacketed reactor configurations using computational fluid dynamics (CFD). The numerical model was developed in ANSYS CFX and enabled the detailed evaluation of the jacket-side flow field, temperature distribution, pressure drop, and heat transfer coefficient.

The calculated flow fields demonstrated that an adequate coolant distribution was achieved within the jacket space for both investigated geometries. The temperature contours showed smooth and physically consistent distributions without significant numerical anomalies, indicating stable heat transfer conditions throughout the simulations.

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Table 5 Comparison of analytical and numerical heat transfer coefficient differences

Geometry	HTC for methanol-water [W/(m ² K)]	HTC for ethylene glycol-water [W/(m ² K)]	Relative difference [%]
Geometry A - analytical	271	199	26.7
Geometry A - CFD	526	405	23.0
Geometry B - analytical	206	156	24.5
Geometry B - CFD	508	403	20.7

According to the numerical results, the methanol-based coolant provided higher heat transfer coefficients than the ethylene-glycol-based coolant in both reactor geometries. The relative difference between the two coolants reached 23.0% for Geometry A and 20.7% for Geometry B. These differences can be regarded as significant from an engineering point of view and may influence the thermal performance of industrial reactor systems.

A comparison of the analytical and numerical approaches showed that both methods led to the same overall conclusion: a considerable difference exists between the heat transfer performance of the investigated coolant solutions. While the analytical calculations provided a rapid engineering estimate, the CFD simulations offered additional insight into the underlying flow and temperature fields responsible for the observed behavior.

The results of the present work demonstrate that CFD can be successfully applied to the comparative evaluation of coolant performance in jacketed reactors. The developed methodology may support thermal analyses of industrial reactor systems and assist in the selection of suitable heat transfer fluids during engineering design and process optimization.

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