

A Molecular-Structure-Based Framework for Fouling Monitoring in Air-Cooled Heat Exchangers

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ARTICLE INFO

Article Type

Original Research

Article History

Received: April 17, 2026

Revised: May 13, 2026

Accepted: May 13, 2026

ePublished: June 20, 2026

ABSTRACT

This study aims to develop an intelligent and integrated framework for the predictive monitoring of the performance of air-cooled heat exchangers in refinery applications. The main innovation lies in the simultaneous and systematic investigation of the impact of fluid molecular structure (focusing on hydrocarbon branching) and dynamic operating parameters within a data-driven approach. To this end, a real heat exchanger was configured using simulation software and technical data. Ten hydrocarbon compounds with linear, two-branched, and three-branched structures were selected, and for each compound, one hundred operational scenarios were executed by varying key parameters, including inlet temperature, inlet flow rate, and fouling coefficient. Quantitative findings revealed that altering the molecular structure to longer branched forms significantly increased pressure drop by 2.25 to 3 times under a constant fouling coefficient, resulting in a decrease in heat exchanger performance. This indicates that changes in fluid structure (e.g., branching) have a substantial impact on exchanger performance. Additionally, sensitivity analysis using the Sobol method identified the inlet flow rate as the most influential parameter on exchanger performance, with an index of 0.8086. Accordingly, the operational output of the research is a predictive monitoring framework based on data analysis models, which, by defining three levels of performance indicators (optimal, requiring monitoring, and critical), facilitates early detection of fouling and optimal maintenance planning. The implementation of this system could enhance the reliability of heat exchangers and achieve significant cost savings in operational expenses by reducing unplanned shutdowns.

Keywords: Predictive maintenance, Air-cooled heat exchanger, Hydrocarbon structure, Intelligent monitoring

How to cite this article

Motamedi M., Mahjoub Sh., Azimifar F., Abdollahi A., A Molecular-Structure-Based Framework for Fouling Monitoring in Air-Cooled Heat Exchangers. *Modares Mechanical Engineering*; 2026;26(09):689-696.

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چارچوبی برای پایش رسوب در مبدل‌های هواخنک بر پایه‌ی ساختار مولکولی

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چکیده

این پژوهش با هدف توسعه یک چارچوب هوشمند و یکپارچه برای پایش پیش‌بینانه عملکرد مبدل‌های هواخنک پالایشگاهی انجام شد. نوآوری اصلی، بررسی همزمان و سیستماتیک تأثیر ساختار مولکولی سیال (با تمرکز بر شاخه‌بندی هیدروکربن‌ها) و پارامترهای عملیاتی پویا در قالب یک رویکرد داده‌محور است. برای این منظور، یک مبدل واقعی با استفاده از نرم‌افزار شبیه‌سازی و داده‌های فنی پیکربندی شد. ده ترکیب هیدروکربنی با ساختارهای خطی، شاخه‌ای دوگانه و سه‌گانه انتخاب و برای هر یک، یکصد سناریوی عملیاتی با تغییر پارامترهای کلیدی شامل دمای ورودی، دبی ورودی و ضریب رسوب اجرا شد. یافته‌های کمی نشان داد که تغییر ساختار مولکولی به شاخه‌ای بلندتر یک ضریب رسوب ثابت، افت فشار را ۲/۲۵ تا ۳ برابر افزایش می‌دهد که افت عملکرد مبدل را به همراه دارد و نشان می‌دهد تغییر ساختار سیال (مثلاً شاخه‌ای شدن) تأثیری مهمی بر عملکرد مبدل دارد. همچنین تحلیل حساسیت با روش سوپول، دبی سیال ورودی را با شاخص ۰/۸۰۸۶ به عنوان مؤثرترین پارامتر بر عملکرد مبدل شناسایی کرد. بر این اساس، خروجی عملیاتی تحقیق، یک چارچوب پایش پیش‌بینانه مبتنی بر مدل‌های یادگیری ماشین است که با تعریف سه سطح شاخص عملکردی (بهبود، نیازمند نظارت و بحرانی)، امکان شناسایی زود هنگام رسوب و برنامه‌ریزی بهینه نگهداری را فراهم می‌کند. پیاده‌سازی این سیستم می‌تواند قابلیت اطمینان مبدل‌ها را افزایش داده و از طریق کاهش توقف‌های ناخواسته، صرفه‌جویی قابل‌توجهی در هزینه‌های عملیاتی ایجاد نماید.

اطلاعات مقاله

نوع مقاله

مقاله پژوهشی

تاریخچه مقاله

دریافت: ۱۴۰۵/۰۱/۲۸

بازنگری: ۱۴۰۵/۰۲/۲۳

پذیرش: ۱۴۰۵/۰۲/۲۳

ارائه آنلاین: ۱۴۰۵/۰۳/۳۰

کلیدواژه‌ها: نگهداری پیش‌بینانه، مبدل حرارتی هواخنک، یادگیری ماشین، ساختار هیدروکربنی، پایش هوشمند

نحوه ارجاع به این مقاله

معتمدی مجید، محبوب شعیب، عظیمی فر فرهاد، عبدالهی علی، چارچوبی برای پایش رسوب در مبدل‌های هواخنک بر پایه‌ی ساختار مولکولی، مهندسی مکانیک مدرس. ۷۹۷-۶۸۹: ۲۶(۰۹): ۱۴۰۵

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1- Introduction

Air-Cooled Heat Exchangers are essential components in the cooling systems of the oil refining industry, playing a vital role in ensuring energy efficiency. Nonetheless, their performance is frequently hindered by a major challenge known as fouling. This phenomenon creates thermal resistance layers on heat transfer surfaces, which not only diminishes the rate of heat exchange but also leads to a significant increase in pressure drop. Consequently, this raises the electrical energy consumption of fans and pumps, potentially resulting in unplanned and costly production stoppages. While there are standard monitoring and control systems available, they often fail to accurately forecast the onset of operational crises due to the intricate changes in fluid properties, especially within refinery settings.

A substantial body of literature has explored the mechanisms of fouling and strategies for mitigating it. A considerable number of studies have examined the influence of operational parameters such as mass flow rate, temperature, and flow velocity on fouling propensity, and have proposed mitigation strategies, including chemical additives, periodic cleaning, and temperature control [2-5].

Nevertheless, much of the existing work relies on simplified assumptions regarding the thermophysical properties of fluids or on maintaining constant operating conditions. In real refinery processes, however, process streams are complex hydrocarbon mixtures whose properties are highly sensitive to chemical composition and can exhibit substantial variability [6-8].

The main gap in the existing literature is the insufficient attention to the role of the fluid's molecular structure as a fundamental factor governing changes in thermophysical properties and fouling phenomena. While previous studies have predominantly focused on surface-level variables such as temperature and pressure, recent research indicates that molecular architecture (e.g., the degree of branching of hydrocarbon chains) exerts a deep impact on viscosity, thermal conductivity, and the phase behavior of the fluid [9-11]. This is particularly relevant for air-cooled heat exchangers, where air cooling can induce temperature fluctuations that lead to phase changes or abrupt variations in the properties of branched fluids, thereby promoting faster fouling compared with linear fluids. The neglect of this structural factor in current monitoring models results in predictive errors and reduced effectiveness of maintenance strategies [12].

To address this gap, the current study proposes a novel data-driven anticipatory monitoring framework. The central premise is that understanding operational dynamics without accounting for the fluid's molecular structure is not complete. In this study, hydrocarbons with different molecular architectures (linear and branched) are modeled in a real air-cooled heat exchanger using Aspen Plus simulation to capture the fluid behavior. Subsequently, a Global Sensitivity Analysis (GSA) using Sobol' and Morris methods is employed to quantify the relative importance of operational parameters and thermophysical properties on fouling and pressure drop. The results establish a design basis for an intelligent monitoring system capable of detecting patterns associated with changes in molecular structure, providing early maintenance alerts, and improving energy efficiency [13, 14].

2- Problem statement

Air-cooled heat exchangers, as key equipment in process industries—especially refineries—play an indispensable role in ensuring process efficiency, managing energy consumption, and maintaining uninterrupted production. Nonetheless, their performance deteriorates over time under the influence of multifaceted factors, resulting in progressive efficiency decline and, ultimately, unplanned outages. In addition to fluctuations in operational parameters such as mass flow rate, temperature, and pressure, a fundamental yet comparatively underexplored determinant of performance degradation is the molecular structure of the process fluid. In real

operating environments, hydrocarbon fluids are complex mixtures whose molecular structure can vary from simple linear to branched and highly intricate architectures. Evidence indicates that this molecular structure directly influences the rheological and thermophysical properties of the fluid and affects fouling patterns and heat transfer in the exchanger. Conventional maintenance and monitoring approaches, which are often based on fixed schedules or simple empirical rules, lack the capability to predict the combined effects of these factors. These approaches typically overlook the complex interplay between fluid structure and operating conditions. Moreover, many prior studies have focused on pure fluids or simple mixtures, and there is a lack of an integrated analytical framework that simultaneously accounts for molecular structure and the dynamics of operating conditions. The absence of such a framework hampers accurate forecasting of performance trends, timely detection of suboptimal patterns, and intelligent planning for preventive maintenance. In response to this challenge, the central problem of the current study is the development of an integrated, data-driven analytical approach. Aiming to fill the gaps in the literature, this study uses systematic simulations across varied conditions and builds a comprehensive database of operational scenarios and diverse molecular formulations, thereby enabling the development of predictive models and the deployment of an intelligent monitoring system for exchanger performance.

In refinery air-cooled heat exchangers processing complex hydrocarbon mixtures, fouling is a multi-mechanism phenomenon. In this study, the fouling layer is specifically defined as physical/crystallization fouling (primarily driven by the precipitation of heavy organic fractions such as waxes and asphaltenes due to localized temperature drops) combined with particulate deposition. The molecular architecture of the fluid—specifically hydrocarbon branching—directly influences the mixture's rheological behavior, cloud point, and local viscosity, which in turn governs the deposition rate. To model the dynamic growth of the fouling thermal resistance (R_f) over time, the classical Kern-Seaton degradation model is adopted, representing the competitive balance between the deposition rate (\dot{m}_d) and the fluid-induced removal/shear-induced suppression rate (\dot{m}_r):

$$\frac{dR_f}{dt} = \dot{m}_d - \dot{m}_r \quad (1)$$

The deposition rate (\dot{m}_d) is formulated as a function of the local mass flux (G) and the temperature-dependent solubility/viscosity profiles governed by the molecular structure:

$$\dot{m}_d = x_f G \exp\left(-\frac{E_a}{R_g T_{int}}\right) \quad (2)$$

where x_f is the fouling precursor concentration, E_a is the activation energy, R_g is the universal gas constant, and T_{int} is the fluid-solid interfacial temperature. Conversely, the removal rate (\dot{m}_r) is driven by the fluid's wall shear stress (τ_w), which scales directly with the structural viscosity modifications caused by molecular branching:

$$\dot{m}_r = C_r \frac{\tau_w}{\rho_f \nu_f} x_f \quad (3)$$

where τ_w is the fluid wall shear stress, ρ_f is the fluid density, ν_f is the kinematic viscosity, and C_r is an empirical removal coefficient.

3- Problem-solving approach

Traditional performance-management methods for heat exchangers rely on simple empirical rules and have proven inadequate for predicting the complex behavior of such systems. Accordingly, this study adopts a data-driven framework to analyze intricate datasets and simulate the system's nonlinear behavior. The core model of this research is derived from a real-world, air-cooled, forced-convection heat exchanger located in an Iranian refinery. As illustrated in Figure 1, hot fluid with a specified inlet temperature (T_i) and known

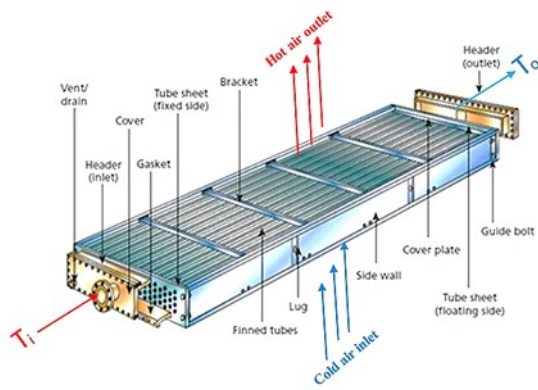


Fig. 1 Schematic diagram of the heat exchanger and boundary conditions

properties such as pressure and density is injected through the inlet header into a bundle of finned tubes arranged in several parallel rows [1]. The material and all geometric dimensions of these tubes are specified.

Cooling of the process fluid inside the tubes occurs via forced air flow generated by blowers; the fans direct the air from bottom to top over the exchanger, and the cooled fluid is collected at the outlet header at temperature T_o . The inlet air temperature equals the ambient temperature, and both inlet and outlet air temperatures are measurable. Given the Reynolds numbers and the geometry, both the flow regime of the process fluid inside the tubes and the airflow over the tubes are treated as turbulent, and the air flow is assumed incompressible due to small pressure variations. This model was developed using comprehensive technical data of the exchanger and the properties of the base fluid, and its validity was established by comparing simulation results with actual refinery operating data. To generate the data required for training intelligent models, extensive operational scenarios were defined by systematically varying key parameters (e.g., inlet fluid temperature, mass flow rate, and fouling factor) and by accounting for ambient air temperature under varying seasonal conditions. Simulations of these scenarios were conducted for ten hydrocarbon blends with different molecular structures (linear, branched, and cyclic), ultimately producing a comprehensive database. These data serve as the primary input for developing predictive models aimed at forecasting the exchanger's future performance from real-time operational data and identifying conditions requiring maintenance. Thus, this framework provides a foundation for transitioning from fixed-schedule maintenance to predictive and intelligent maintenance strategies.

3-1- Data Extraction and Model Development

In the first step, all precise technical specifications of a readily available air-cooled heat exchanger at the refinery, including the tube-bundle geometry (length, diameter, and tube-bundle arrangement type), fin specifications (type, dimensions, geometry, material), process fluid properties (viscosity, density, specific heat capacity, and the base convective heat transfer coefficient for hydrocarbon base conditions), and operating conditions (design pressure, allowable pressure drop, and temperature range) were extracted from the main datasheet. Given that the process fluid remains in the liquid phase from inlet to outlet with no phase change, the process fluid was assumed to be incompressible. Both the air side and the process-fluid side flows were assumed to be steady (fully developed). Based on the above combined conditions, an initial design was performed using ASPEN software, and a baseline model of the exchanger was developed for simulation. Validation of the baseline model was carried out by comparing the initial-model results with actual refinery operating data under baseline conditions (pure hydrocarbon). The mean absolute percentage error for key parameters, including the outlet temperature difference and the heat-transfer rate, as

Table 1 Model Validation Against Operational Data (Baseline Case).

Parameter	Actual	Present (Simulated)	Unit	Relative Error (%)
Process Fluid Outlet Temp.	93	92.99	°C	0.01
Heat Transfer Rate	14773	13684.8	kW	7.37

Table 2 Binary and Ternary Mixture Compositions.

Mixture	$C_{50}H_{102}$ (wt.%)	$C_{50}H_{102}-N1$ (wt.%)	$C_{50}H_{102}-N2$ (wt.%)
SA	100	0	0
SB	0	0	100
SC	0	100	0
SD	70	0	30
SE	70	30	0
SF	50	0	50
SG	50	50	0
SH	40	30	30
SI	60	20	20
SJ	30	30	40

Table 3 Key Operational Parameter Ranges for Simulation.

Parameter	Variation Range	Unit	Change Step
Mass Flow	10 ~ 20	kg/s	1
Inlet Fluid	260 ~ 355	°C	5
Initial	0.00000 ~ 0.00008	m^2K/W	0.00005
Inlet Air	-20 ~ 43	°C	3

summarized in Table 1, was less than 10%, thereby confirming the model's accuracy.

3-2- Molecular Property Modifications of the Fluid

Base fluid (reference) in this study was pure linear hydrocarbon sample, $C_{50}H_{102}$, designated as category S_A . To modify the fluid properties at the molecular level, three main strategies were employed. Step 1 — Structural modification from linear to branched hydrocarbons: Branches were introduced by converting hydrocarbons from linear to branched forms, designated as categories S_B and S_C . Properties such as viscosity (which influences the primary sticking mechanism of deposited droplets to the heated surface) and cloud point (which influences nucleation and crystal growth of deposits within the fluid volume) were altered.

Step 2 — Variation in fluid composition with dual-structural molecules: By incorporating molecules with dual structural motifs from category S_D to category S_G , the rheological behavior (properties such as viscosity, elasticity, and non-Newtonian fluid behavior) and the convective heat transfer of the targeted fluid were examined to identify an optimum balance between heat-transfer efficiency and resistance to fouling/deposition.

Step 3 — Introduction of triple-structural molecules: Structures from category S_H to category S_J were engineered so that thermodynamic and transport properties were adjusted to achieve a favorable balance between two conflicting objectives: enhanced heat transfer and reduced deposition (fouling).

Ten hydrocarbon mixtures, ranging from category S_A to category S_J , with pure hydrocarbon composition $C_{50}H_{102}$, short-branched ($C_{50}H_{102}-N_2$), and long-branched ($C_{50}H_{102}-N_1$) dual- and triple-structured molecules, commonly encountered in refinery processes, were named and considered as indicated in Table 2.

3-3- Design of Operational Scenarios

For each of the ten hydrocarbon mixture cases under investigation, one hundred operational scenarios were defined by simultaneously varying key parameters including inlet temperature, inlet flow rate, and fouling factor on the process fluid side. The temperature of the air passing through the heat exchanger via fans was considered in proportion to different seasons of the year. To accurately examine the effect of hydrocarbon branching on fluid behavior and heat exchanger performance, all simulations were performed assuming a constant flow rate for the air stream and under conditions of no (negligible) fouling formation on the air side, as per Table 3.

For each case comprising the operational scenarios and hydrocarbon mixtures, simulations were conducted in the software environment, and the required output parameters were recorded. In total, one thousand samples were obtained, forming a database in a matrix format of dimensions 24*1000. The results from analyzing the database obtained from the simulations serve as a solid foundation for developing models capable of predicting system behavior and heat exchanger performance in real-time. Data-driven approaches and analyses have been proposed as efficient alternatives to traditional thermodynamic models, enabling them to simultaneously account for various molecular compositions and operational conditions, and extract complex patterns between molecular structure and fluid behavior. Using these models, predictive maintenance can be effectively implemented in real-world conditions.

4- Discussion and Results Analysis

The primary objective is to investigate the simultaneous effect of fluid molecular structure and operational parameters on heat exchanger performance and to provide a framework for predictive monitoring. For this purpose, various analytical methods, including scatter plot analysis, correlation matrices, and sensitivity analysis, were employed.

4-1- Detailed Data Analysis and Performance Patterns

The data analysis results clearly demonstrate that increased molecular branching in hydrocarbons has a direct impact on reducing heat transfer and increasing pressure drop in heat exchangers. The physical mechanism behind this performance degradation can be justified as follows:

The branched structure of molecules, particularly long chains, significantly increases the dynamic viscosity (μ) by disrupting the smooth movement of molecules relative to each other and relative to the tube wall. Assuming other parameters remain constant, this leads to a reduction in the Reynolds number (R_c) and a weakening of the turbulent regime. Since the convective heat transfer coefficient (h) in turbulent flow is significantly higher than in laminar flow, the shift in flow regime results in a substantial decrease in the heat transfer rate.

Furthermore, the three-dimensional and bulky structure of branched molecules, by increasing voids and disorder in molecular arrangement, reduces the thermal conductivity (k) of the fluid. Simultaneously, the increased viscosity thickens both the hydrodynamic and, consequently, the thermal boundary layers. These thicker layers act as thermal insulation. Even under turbulent conditions, higher viscosity dampens turbulent eddies more rapidly, reducing the intensity of transverse mixing, which also negatively affects heat transfer.

For a deeper understanding of the relationship between molecular structure and fouling phenomena, it should be noted that while branched structure theoretically reduces the potential for physical fouling (wax) by lowering cloud points, in the high-temperature range of the present study (260 to 355°C), the dominant mechanism shifts towards thermo-chemical reactions (such as polymerization and coking).

In summary, this chain of effects—including increased viscosity, reduced thermal conductivity, weakened turbulence, and intensified chemical fouling—leads to an increase in overall thermal resistance and a significant drop in the heat transfer rate (Q).

4-1-1- Classification of Performance Patterns

Preliminary data analysis based on scatter plots has identified three distinct performance patterns that can form the basis of a predictive maintenance system. As shown in Table 4, this classification includes the groups "Optimal," "Requires Monitoring," and "Critical."

Table 4 Heat Exchanger Performance Classification

Performance Group	Performance Group	Key Characteristics
Optimal	Optimal	High heat transfer, low ΔP
Requires Monitoring	Requires Monitoring	Moderate performance loss, low MTD
Critical	Critical	High ΔP , abnormal outlet T

Table 5 Heat Exchanger Performance Comparison for Different Mixtures (Constant Fouling, $R_f = 0.0001 \text{ m}^2 \cdot \text{K}/\text{W}$).

Scenario	LMTD Range (°C)	ΔP Range (bar)	ΔP Ratio (vs. S_A)	Fluid Composition
S_A	124.7 - 193.0	0.16 - 0.31	Reference	Pure Base (Reference)
S_B	127.5 - 198.0	0.46 - 0.90	2.87 - 3.00	Short-Branched
S_C	127.5 - 197.9	0.46 - 0.89	2.87 - 2.97	Long-Branched
S_D	129.0 - 195.1	0.38 - 0.68	2.19 - 2.37	70% Base, 30% Short-Branched
S_E	130.4 - 195.1	0.38 - 0.68	2.19 - 2.37	70% Base, 30% Long-Branched
S_F	125.5 - 195.8	0.37 - 0.71	2.19 - 2.29	50% Base, 50% Short-Branched
S_G	125.5 - 195.7	0.37 - 0.71	2.19 - 2.29	50% Base, 50% Long-Branched
S_H	125.8 - 196.1	0.38 - 0.74	2.19 - 2.38	40% Base, 30% Long, 30% Short
S_I	125.9 - 195.5	0.36 - 0.68	2.19 - 2.25	60% Base, 20% Long, 20% Short
S_J	126.0 - 196.4	0.39 - 0.78	2.43 - 2.51	30 %Base, 30% Long, 40% Short

Optimal (Primary) Group: Comprises base (pure) fluids with appropriate flow rates, high heat transfer, and low pressure drop.

Requires Monitoring (Secondary) Group: Typically involves semi-branched fluids exhibiting moderate performance degradation, requiring continuous monitoring of parameters such as effective mean temperature difference (MTD).

Critical (Warning) Group: Pertains to highly branched fluids associated with high pressure drop and abnormal outlet temperatures, necessitating immediate maintenance actions.

4-1-2- Quantifying the Effect of Molecular Structure on Fouling

To gain a more precise understanding of the impact of "fluid structure change" on heat exchanger performance and to demonstrate that this performance degradation is independent of the fouling level, it is necessary to eliminate the influence of other confounding factors. In Table 5, the fouling factor (R_f) for all scenarios is set to a constant, low value of $0.0001 \text{ m}^2 \cdot \text{K}/\text{W}$. This controlled approach allows us to isolate and examine the pure effects of fluid composition and molecular structure (branching) on pressure drop and heat transfer, ensuring that the observed differences are attributable to the fluid itself (inherent properties such as viscosity, density, and thermal conductivity) rather than to varying degrees of fouling.

Analysis of the data in Table 5 reveals a very clear trend. In the base case (S_A), where the fluid has a linear structure, the pressure drop ranges from 0.16 to 0.31 bar. In contrast, the use of branched fluids (S_B) and (S_C) causes a significant increase in pressure drop, reaching a range of 0.46 to 0.90 bar; this figure is, on average, three times higher than the base case. This substantial increase in pressure drop, with no change in the fouling factor, confirms that a branched molecular structure alone—solely through altering thermophysical properties (such as increasing viscosity)—can severely impact heat exchanger performance.

Beyond pressure drop, variations in LMTD (Log Mean Temperature Difference) also indicate that complex molecular structures disrupt the cooling process by altering the heat balance conditions. These findings quantitatively demonstrate that ignoring molecular structure in monitoring models will lead to significant errors in predicting heat exchanger performance.

Table 6. Pearson Correlation Matrix of Key Performance Parameters.

Parameter	Heat Transfer	Inlet Temp.	Flow Rate	Viscosity	Fouling Resistance	Pressure Drop
Heat Transfer	1.000	0.685	0.721	-0.564	-0.432	-0.345
Inlet Temperature	0.685	1.000	0.123	-0.234	0.345	0.289
Fluid Flow Rate	0.721	0.123	1.000	-0.189	-0.210	-0.156
Outlet Viscosity	-0.564	-0.234	-0.189	1.000	0.298	0.412
Fouling Resistance	-0.432	0.345	-0.210	0.298	1.000	0.323
Pressure Drop	-0.345	0.289	-0.156	0.412	0.323	1.000

4-2- Correlation Matrix Analysis

This matrix is obtained by calculating the Pearson correlation coefficient "r" (which has a value between +1 and -1). A value of +1 indicates a perfect direct relationship, -1 indicates a perfect inverse relationship, and zero indicates the absence of a linear relationship between the two variables. This analysis helps identify hidden patterns among variables and prevents multicollinearity (correlation among independent variables) in modeling.

To identify hidden linear relationships between variables and prevent collinearity in modeling, the Pearson correlation coefficient ("r") was calculated for key parameters. A summary of the results is presented in Table 6.

Strong Correlations ($|r| > 0.5$):

The results indicate that fluid mass flow rate ($r = 0.721$) and inlet temperature ($r = 0.685$) have the strongest positive correlation with the heat transfer rate; this means that increasing these two parameters leads to improved performance. Conversely, viscosity ($r = -0.564$) has an inverse correlation with heat transfer, confirming its obstructive role in the heat exchange process.

Moderate Correlations ($0.3 < |r| < 0.5$):

Analysis of the relationships shows that fouling resistance ($r = -0.432$) has a negative correlation with heat transfer, and viscosity ($r = 0.412$) has a direct correlation with pressure drop. A key and somewhat unexpected finding is the positive correlation between inlet temperature and fouling resistance ($r = 0.345$). While engineering intuition suggests fouling decreases with rising temperature (due to lower viscosity), this finding indicates that at high temperatures for complex branched fluids, thermo-chemical mechanisms become dominant, and temperature transforms into a fouling-enhancing factor.

Weak Correlations ($|r| < 0.3$):*

The relationship between fluid flow rate and inlet temperature is very weak ($r = 0.123$), suggesting that these two parameters can be controlled independently in the model.

4-2-1- Mechanistic Interpretation of the Temperature-Fouling Relationship

Analysis of the results reveals a complex and often nonlinear correlation between fluid temperature and fouling rate. A precise understanding requires special attention to the thermodynamic mechanisms of solubility and the rheological properties of the fluid. In hydrocarbon fluids, the fouling phenomenon results from changes in the solubility of heavy components such as paraffins and asphaltenes. Specifically, as the fluid temperature decreases along the exchanger or due to operational fluctuations, the solubility of paraffinic compounds in the liquid phase decreases. When the fluid/wall temperature falls below the Cloud Point or Wax Appearance Temperature (WAT), these compounds become saturated, separate as solid crystals, and, by moving towards the colder wall, form the fouling layer. This mechanism explains why crossing the saturation point and temperature reduction are the primary triggers for fouling initiation.

However, increasing the temperature within certain ranges can have a reverse, cleaning effect. This occurs if the fluid or wall temperature rises sufficiently to exceed the melting point of the deposited crystals,

triggering a re-dissolution process. This softens the fouling layer, causes it to lose its adhesive strength, and leads to its detachment by the shear stress of the flowing fluid—a phenomenon that justifies the dual role of temperature as both a fouling enhancer and reducer.

Beyond temperature, the molecular structure of hydrocarbons plays a fundamental role in determining the temperature thresholds and flow characteristics of the deposit. Molecules with a linear structure (n-alkanes) can arrange themselves in an orderly manner, forming a stable crystalline network at higher temperatures and exhibiting a higher cloud point. This leads to the onset of fouling at higher temperatures. In contrast, the presence of side branches in branched structures creates steric hindrance, disrupting the necessary order for crystalline network formation and lowering the cloud point, which helps delay fouling initiation.

Furthermore, linear structures, due to their high potential for entanglement, lead to high viscosity and the formation of a fouling layer with high adhesive strength and mechanical integrity, making it difficult to remove. Conversely, branched structures, functioning similarly to a rolling bearing and reducing internal friction, decrease fluid viscosity and create a more porous, weaker fouling layer.

This layer offers less resistance to fluid shear stress, increasing the likelihood of self-cleaning. Therefore, the observation in Table 5 that some mixtures (branched) exhibit lower pressure drop is justifiable and defensible based on these explanations.

4-2-2 Effect of Molecular Structure on Cold vs. Hot Fouling Mechanisms

To gain a deeper understanding of fouling behavior, the effects of molecular branching must be differentiated for the two primary fouling mechanisms: "cold fouling" (also known as 'gumming' or 'wax deposition') and "hot" or "reactive fouling". This is because molecular structure plays a dual and contrasting role in these two mechanisms.

In the cold fouling mechanism, where the primary driver is phase separation due to temperature reduction below the saturation point, molecules with a linear structure (n-alkanes) can easily align with each other due to their simple geometry. This leads to the formation of regular, dense crystalline networks. Consequently, this results in fouling at higher temperatures (higher cloud point), creating a hard, encrusted layer on the wall.

Conversely, the presence of side branches creates steric hindrance, preventing the orderly arrangement of molecules. This causes the fouling structure to become amorphous and porous rather than crystalline and hard. This translates to a lower onset temperature for fouling and the formation of a deposit with reduced adhesion and a higher tendency for self-cleaning.

In contrast, in the hot or reactive fouling mechanism, which typically occurs at high temperatures due to chemical bond scission, oxidation, and polymerization, the role of branches can be negative. Branched molecules are more prone to undesirable chemical reactions. The carbon-hydrogen bonds at tertiary positions (where branches are located) have lower bond dissociation energies. This facilitates the generation of free radicals and polymerization, leading to the formation of hard chemical (e.g., coke) and asphaltenic deposits that are difficult to remove from the wall surface.

Therefore, while branches are beneficial in preventing cold fouling, they increase the potential for reactive fouling at very high temperatures. This behavioral contradiction highlights the need for precise thermal management of branched fluids to avoid the temperature regimes conducive to hot chemical reactions.

4-3- Validation and Sensitivity Analysis

In the study of complex engineering systems, sensitivity analysis serves as a powerful tool for identifying influential parameters. In this research, two complementary methods, Sobol and Morris, were employed. The Sobol method quantifies the contribution of each

parameter to the output variance by calculating first-order (S_1) and total (S_T) sensitivity indices. The Morris method evaluates the direction and magnitude of effects using μ and μ^* indices.

For a visual and comparative assessment of these results, Figure (2) presents a comprehensive overview of the role and impact of each key parameter on heat exchanger performance, utilizing both methods. The inlet fluid mass flow rate was identified as the most influential parameter, exhibiting the highest total Sobol index ($S_T = 0.80$) and Morris index ($\mu^* = 26.5$). This finding is entirely consistent with its strong positive correlation with heat transfer ($r = 0.721$) from the correlation matrix. Following this, the inlet temperature ranked second, with corresponding indices of $S_T = 0.78$ and $\mu^* = 18.74$, which aligns with its significant correlation with heat transfer ($r = 0.685$).

These results are significant for two primary reasons. First, they confirm that operational parameters take precedence over intrinsic fluid properties (such as viscosity, with $S_T = 0.189$) in the real-time control of system performance. Second, they provide a practical guideline for intelligent monitoring systems; the primary focus of such a system should be directed towards supervising the inlet flow rate and temperature, as variations in these parameters have the most immediate impact on system efficiency.

In contrast, viscosity, despite exhibiting a moderate negative correlation with heat transfer ($r = -0.564$), holds a lower ranking in the sensitivity analysis ($S_T = 0.189$, $\mu = 4.36$). This indicates that the influence of molecular structure on exchanger performance is indirect and manifests over the long term, primarily through its effect on fouling rather than through direct, instantaneous control.

4-4- Comparison of Results with Previous Studies

The findings of this research align with and, in some aspects, complement the existing literature. Regarding the impact of molecular structure, the current results—indicating increased viscosity and reduced heat transfer in branched fluids—confirm and quantify the findings of Gudala et al. [12]. Furthermore, the precedence of operational parameters (inlet flow rate and temperature) in controlling heat exchanger performance is consistent with the conclusions of Crittenden and Yang [7].

The primary innovation of this article lies in the **quantitative integration of these factors within a data-driven framework**. This approach bridges the existing gap between fundamental molecular-level studies and the practical operational requirements of the industry.

4-5- Scope Limitations and Simplifying Assumptions

While the established molecular-structure-based framework demonstrates high fidelity, its current practical application is bounded by the following simplifying assumptions and limitations:

- **Steady-State Thermal-Hydraulics:** The numerical engine assumes steady-state and single-phase liquid flow within the tube bundle. Transient hydraulic surges, cyclic operational swings, and localized two-phase flow regimes (such as micro-vaporization) are not accounted for.
- **Hydrocarbon Composition Limits:** The generated database is built upon ten representative hydrocarbon structures ranging from linear to three-branched configurations (SA to SJ matrix). Extremely heavy fractions, resins, or highly heteroatom-rich crude segments may require recalibration of the physical property models.
- **Uniform External Environment:** The air-side cross-flow velocity and ambient temperature distributions are assumed to be uniform across the face of the tube bundle. In actual refinery operations, environmental factors like wind direction, ambient crosswinds, and thermal plume recirculation can introduce spatial non-uniformities that alter localized deposition rates.

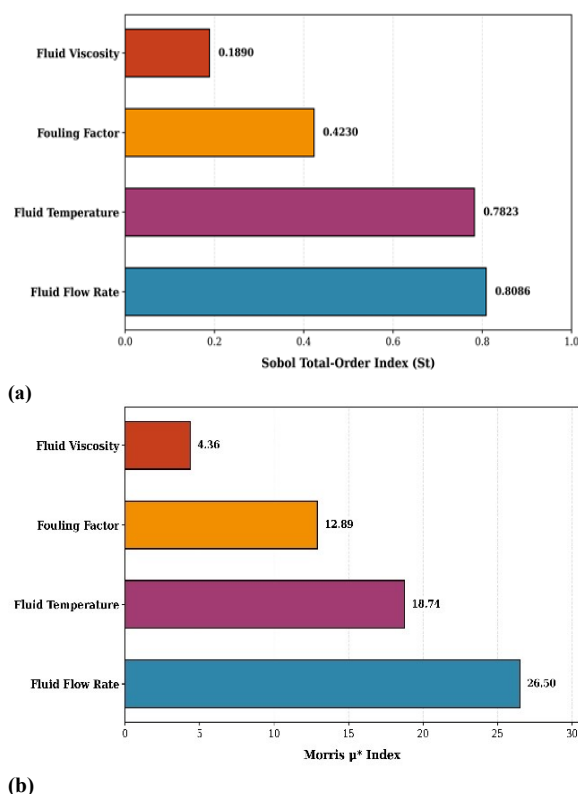


Fig. 2 Comparative sensitivity analysis of key performance parameters using (a) Sobol and (b) Morris indices

5- Summary and Conclusion

In this research, the aim was to develop a data-driven framework for the predictive monitoring of air-cooled heat exchangers, focusing on the combined effects of fluid molecular structure and operational parameters. The results from systematic simulations and sensitivity analyses demonstrated that changing the fluid structure from linear to long-branched configurations leads to an increase in pressure drop by approximately 2.5 to 3 times. This effect is also observable in the constant fouling coefficient, highlighting the profound impact of molecular structure on thermophysical properties (increased viscosity and decreased thermal conductivity) and the weakening of turbulence regimes. Based on the overall indices from sensitivity analysis (Sobol and Morris), the "input mass flow rate" and "input temperature" were identified as the most significant factors in determining performance and fouling formation, underscoring the priority of monitoring operational parameters over the intrinsic properties of the fluid. Furthermore, a more detailed investigation revealed that, in complex branched fluids, the input temperature plays a dual role; at high temperatures (260 to 355 degrees Celsius), despite the expectation of reduced fouling due to lower viscosity, chemical-thermal fouling mechanisms dominate, turning temperature into an exacerbating factor for fouling.

The main innovation of this paper is the introduction of an integrated simulation-data-driven framework that, for the first time, establishes a link between molecular structure and dynamic operational parameters. This framework facilitates the transition from fixed, reactive maintenance strategies to predictive maintenance by defining monitoring index levels. However, this study is subject to limitations such as the assumption of constant air flow rates, the use of software models to estimate properties of branched fluids, and the lack of precise considerations for chemical reactions and time-dependent phenomena like corrosion, which necessitates final validation through implementation on long-term operational data from a real heat exchanger.

In terms of practical application, the key accomplishment of this study lies in converting the findings from numerical and sensitivity analyses into a functional framework for Distributed Control Systems (DCS). By utilizing four identified functional groups (optimal, requiring monitoring, warning, and critical), a detailed alarm logic system can be designed that archives data in optimal status, draws the operator's attention to subtle changes in monitoring status, restores heat exchanger performance through automatic corrective commands (such as adjusting fan speeds) in warning status, and issues immediate stop and wash alerts in critical status. This strategy, leveraging sensitivity data and continuous monitoring of transitions between performance levels, enables preventive maintenance and precise planning of periodic services, thereby preventing unexpected production shutdowns. Ultimately, using this classification as a decision-making algorithm bridges the gap between advanced analysis and real-world refinery operations, ensuring safety, reducing maintenance costs, and boosting energy efficiency by transforming raw data into strategic information.

Nomenclature

P	Pressure (bar)
R_f	Fouling Factor ($m^2 \cdot K/W$)
ε	Thermal Effectiveness
\dot{m}	Mass Flow Rate (kg/s)
T	Temperature ($^{\circ}C$)
MDT	Logarithmic Mean Temperature Difference ($^{\circ}C$) LMTD
Δ_P	Pressure Drop (bar)
U	Overall Heat Transfer Coefficient ($kW/m^2 \cdot K$)
A	Heat Transfer Area (m^2)
C_p	Specific Heat Capacity ($kJ/kg \cdot K$)
C_r	Capacity Ratio (C_{min}/C_{max}) (-)
r	Pearson Correlation Coefficient (-)
r	Absolute Pearson Correlation Coefficient (-)
μ	Dynamic Viscosity ($mPa \cdot s$)
ρ	Density (kg/m^3)
k	Thermal Conductivity
Re_c	Reynolds Number (-)
Q	Heat Transfer Rate (kW)

Ethics Approval:

The scientific content of this article is the result of the authors' research and has not been published in any Iranian or international journal.

Conflict of Interest:

The authors declare no conflict of interest.

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