

# The Comprehensive Evaluation of the Coke Formation and Catalyst Deactivation in the Propane Dehydrogenation Reactor: Computational Fluid Dynamics Modelling

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ARTICLE INFO	ABSTRACT
<p><b>Article History:</b> Received: 12 July 2022 Revised: 14 October 2022 Accepted: 18 October 2022</p> <p><b>Article type:</b> Research</p> <p><b>Keywords:</b> CFD Modeling, Coke Formation, Deactivation, Hot Spots, Propane dehydrogenation</p>	<p>A numerical evaluation was performed to find out the impact of bed geometry on the catalyst deactivation and propane dehydrogenation efficiency by consideration of the coke formation in the reactor. Furthermore, the temperature distribution and propane conversion along the reactor were studied. The governing equations with appropriate initial and boundary conditions were solved numerically, while two different bed arrangements (i.e. rectangular and parallelogram) were evaluated to find the optimized geometry in order to avoid the creation of hot spots. Findings indicated that parallelogram arrangement causes more conversion percentage owing to more axial as well as the radial mixing of reactants compared to the rectangular arrangement. Moreover, the obtained numerical results revealed that the optimum operating temperature to achieve the maximum conversion is 550 °C. As the temperature rises from 450 °C to 650 °C, the conversion of propane increases from 68.15% to 99.51%, during the reactor length. When the temperature exceeds above the optimum operating temperature, hot spots are created due to coke formation and also accumulation of coke on the catalyst bed surface that will lead to the deactivation of catalysts. The results of this work can be useful to examine the effects of operating conditions to better understand physical and chemical phenomena occurring in the propane dehydrogenation reactor.</p>

## Introduction

Propylene ( $C_3H_6$ ) is well-known as an important petrochemical feedstock that is used for the fabrication of precious products such as polypropylene, acrylonitrile, cumene, propylene oxide, acrylic acid polypropylene, and acrylonitrile [1-3]. Over the past two decades, by the increasing request for propylene derivatives caused increasing in the propylene production demand. In this regard, different production techniques have been studied and developed [2,4]. Although the dehydrogenation of propane ( $C_3H_8$ ) to propylene is a common and effective commercialized process, it suffers from some limitations including thermodynamic restrictions on conversion, strong endothermicity, side reactions, and coke formation [5-8].

Owing to the thermodynamics restrictions, high conversion percentage needs high temperatures which rises energy consumption. In this condition, the probability of coke formation increases owing to high temperature [9]. The coke formation leads to catalyst deactivation as well as creation of hot spots [10]; Hence, catalytic bed must be regenerated

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periodically to remove the deposited carbon which imposes serious unit operating cost. It is worth noting that in the case of hot spots being closer to the reactor wall, serious damages will arise [11,12]. Accordingly, finding the optimized operating temperature is an essential step in the propane dehydrogenation process to overcome the mentioned limitations [13, 14].

The empirical studies for finding optimum conditions require high operating time, and consume much reagents which imposes high cost to the process [15-17]. Hence, theoretical modeling based on the reaction kinetics, transport phenomena, operating conditions, and geometrical considerations could be a cost-effective approach for prediction of reactor behavior [18]. Kamlesh Ghodasara et. al. [19] developed a mathematical modeling for catalytic propane dehydrogenation using moving bed reactor while the reactor efficiency was assessed as a function of operating parameter. In their research, different geometries were studied through the optimization of operating parameters, while propane conversion was examined as the response. Bijan Barghi et. al. [20] proposed a mathematical model for propane dehydrogenation using an industrial catalyst to describing catalyst deactivation. Their findings showed that the addition of water and methanol as oxygenated additives could enhance the propane conversion, while the coke formation is reduced. Seyed M. Miraboutalebi et. al. [11] presented a numerical model for the kinetics of propane dehydrogenation using a radial-flow reactor. Pt-Sn/Al<sub>2</sub>O<sub>3</sub> was applied as the catalyst while the catalyst activity and propane conversion were evaluated as the responses. Their obtained numerical results revealed that the catalyst activity was highly time dependent. Antonio Ricca et. al. [2] used a mathematical approach for modelling of a membrane-assisted propane dehydrogenation process, while catalyst activity and stability were considered as responses at two operating temperatures. Their Findings indicated a good agreement between experimental data and the results of proposed kinetic model. Yun Jin et. al. [5] developed one-dimensional, steady-state model for propane dehydrogenation process. A hollow fiber membrane reactor was used, whereas the membrane area, fiber length, and flow rate were selected as the operational parameters. The obtained modeling results revealed that the optimum propylene selectivity was found to be 91% at operating temperature of 1000 °C when propane conversion reaches 58%.

Although different modeling and correlations have been assessed for the prediction of propane conversion and temperature gradient during the propane dehydrogenation process, such correlations have disadvantages in terms of insufficient accuracy [20-25]. Therefore, this work focuses on the application of computational fluid dynamics (CFD) technique for the examination of propane dehydrogenation reactor involving reactor geometry, momentum, mass transfer, heat transfer, and the reactions. Besides experimental studies, successful implementation of CFD technique have been developed to evaluate overall reactor performance and coke deposition behaviors. Behnam and Dixon [26] examined the local carbon formation in the steam methane reforming process using a 3D-CFD model. Their proposed model showed a non-uniform a descending carbon formation rate from the heated tube wall to the tube center. Xuesong Yang et. al. [27] established a particle-resolved model for investigation of the coke formation. It was reported that the coke formation and catalyst deactivation are higher near the reactor wall. Claudio Antonio et. al. [28] investigated the influence of hydrodynamics on the activity and selectivity. Their findings showed that the optimum temperature was 453 °C, while the process efficiency increased from 6.0% to 6.7% for the 2D proposed model, and from 6.0% to 7% for the 3D proposed model. Furthermore, the selectivity increased from 20% to 26% and 21% for the 2D and 3D models, respectively. Gopal Manoharan and Buwa [29] developed a CFD model to understand the impact of various catalytic geometries on the catalyst deactivation. Their research highlighted the quantitative relationship between the catalytic structure and the overall reactor performance.

The creation of changes in the bed structure leads to changes in transport rates, and the of catalyst loading in the reactor. The present work provides a developed model of transport in packed bed reactors, and helps to a better understanding of the influence of reactor bed geometry on the reactor efficiency. and thereby aids in selecting the optimal configuration.

The present work provides a comprehensive evaluation to prediction of the product conversion, catalyst deactivation as well as creation of hot spots across the catalytic bed, with reduction in the time and cost of the analysis. Different catalytic bed arrangements were modeled to prediction of the product conversion, catalyst deactivation as well as temperature distribution across the bed. The finite element procedure was applied to solve all governing equations including momentum, mass, and energy with appropriate initial and boundary conditions along with the side reactions simultaneously. It worth noting that few mathematical and CFD models have been presented in the recent literature on the catalyst deactivation and the creation of hot spots, while in this work an appropriate model has been proposed for investigation of propane dehydrogenation system behavior. Generally, current model covers many lacks of previously reported modeling.

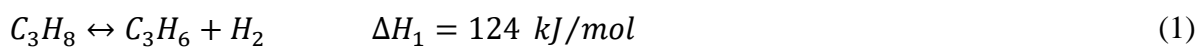
## Model Development

### Geometrical Model

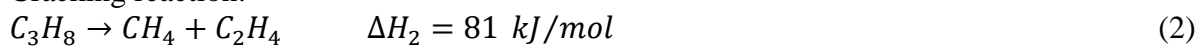
A two-dimensional CFD model was applied to evaluation the impact of temperature variations on the coke deposition and catalyst deactivation in the propane dehydrogenation reactor. An axial symmetry model was used to simulation of a fixed bed reactor with length of 0.15 m and diameter of 0.02 m, while the bed was filled by spherical catalysts with a diameter of 0.001 m. The feed was entranced from the bottom of the reactor, passing through the catalytic bed and after conversion to the product exited the reactor. The plug flow model was considered to describe the occurring chemical reactions. The geometry of catalytic bed reactor for different bed geometries is illustrated in Fig. 1a.

### Reaction kinetics

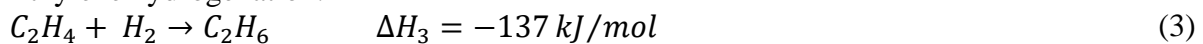
Since the propane dehydrogenation reaction is an endothermic equilibrium limited reaction, the high temperatures and low pressures are desirable in order to increasing the yield reaction. However, it is important to mention that high temperatures can cause undesirable side reactions which produce unwanted products. Hence, finding optimized temperature is very necessary for such process. The process reactions are mentioned as follows which [Reaction. 1](#) is the main, while others are side reactions [30].



Cracking reaction:



Ethylene hydrogenation:



The proposed reaction rates for main and side reactions were provided as follows [11]:

$$-r_1 = \frac{k_1 \left( P_{C_3H_8} - \left( \frac{P_{C_3H_6} P_{H_2}}{k_{eq}} \right) \right)}{1 + \left( \frac{P_{C_3H_6}}{k_{C_3H_6}} \right)} \quad (4)$$

$$-r_2 = k_2 P_{C_3H_8} \quad (5)$$

$$-r_3 = k_3 P_{C_2H_4} P_{H_2} \quad (6)$$

where,  $r_i$  ( $\frac{kmol}{m^3.s}$ ) is the reaction rate,  $k_i$  ( $s^{-1}$ ) is the reaction rate constant, and  $P_i$  is the partial pressure of species. The reaction rate is given based on reactor volume. The fixed bed volume fraction was considered 0.65.

### Deactivation Model

The deactivation model was selected based on the rate of coke formation during the process (versus the time). The deactivation was estimated as follows [19, 20]:

$$\frac{dC_c}{dt} = \frac{dC_m}{dt} \quad (7)$$

where  $C_m$  is the coke concentration in monolayer described as follows [11]:

$$C_m = C_{max}^2 \left( \frac{k_{1c}t}{1 + C_{max}k_{1c}t} \right) \quad (8)$$

The catalyst activity reduction due to monolayer–multilayer coke formation was estimated as follows [23]:

$$\alpha = (1 - \alpha_1 C_m)^2 \quad (9)$$

where  $\alpha_1$  indicates that the primary active surface, while  $C_m$  is the coke production rate due to reaction.

The reaction constants were calculated based on the Arrhenius equation chemical kinetics as follows [31]:

$$k_1 = k_{01} \exp\left[\frac{-E_{a1}}{R\left(\left(\frac{1}{T}\right) - \left(\frac{1}{T_0}\right)\right)}\right] \quad (10)$$

$$k_2 = k_{02} \exp\left[\frac{-E_{a2}}{R\left(\left(\frac{1}{T}\right) - \left(\frac{1}{T_0}\right)\right)}\right] \quad (11)$$

$$k_3 = k_{03} \exp\left[\frac{-E_{a3}}{R\left(\left(\frac{1}{T}\right) - \left(\frac{1}{T_0}\right)\right)}\right] \quad (12)$$

$$k_{C_3H_6} = k_0 \exp\left[\frac{-\Delta H}{R\left(\left(\frac{1}{T}\right) - \left(\frac{1}{T_0}\right)\right)}\right] \quad (13)$$

$$k_{eq} = k_{0e} \exp\left[\frac{-E_{eq}}{R\left(\left(\frac{1}{T}\right) - \left(\frac{1}{T_0}\right)\right)}\right] \quad (14)$$

$$k_{1c} = k_{01c} \exp\left[\frac{-E_{a1c}}{RT}\right] \quad (15)$$

$$k_{2c} = k_{02c} \exp\left[\frac{-E_{a2c}}{RT}\right] \quad (16)$$

The reaction kinetic parameters and their values are presented in [Table 1](#).

**Table 1.** The values of kinetic parameters [11,23].

Parameter	Value	Unit
$k_{01}$	0.5242	(mmol/gr. min. bar)
$k_{02}$	0.00465	(mmol/gr. min. bar)
$k_{03}$	0.000236	(mmol/gr. min. bar)

$k_0$	3.46	(mmol/gr. min. bar)
$k_{0e}$	35.50	(mmol/gr. min. bar)
$E_{a1}$	34.57	(kJ/mol)
$E_{a2}$	137.31	(kJ/mol)
$E_{a3}$	154.54	(kJ/mol)
$E_{eq}$	35.50	(kJ/mole)
$\Delta H$	-85.817	(kJ/mol)
$\alpha_1$	813	g catalyst/g coke
$C_{max}$	0.000682	mg coke/mg catalyst
$k_{01c}$	234	mg coke/mg catalyst
$E_{a1c}$	38.43	kJ/mole
$k_{02c}$	0.00000145	mg coke/mg catalyst
$E_{a2c}$	125.51	kJ/mol

A “sequential steady-state solutions” technique has been used to compute the time-dependent manner of deactivating catalyst particles. Nevertheless, this simplified approach was very costly due to computation time. It should be noticed that more accurate modeling would be even more expensive, as the system of equations is very stiff, owing to the slow diffusion inside the catalysts particles. For assessment of the coke formation inside the catalyst particles, the time evolution of the carbon deposits was tracked by running a steady-state simulation. In this procedure, computation is performed at base case (un-deactivated) conditions to gain the initial local carbon deposition rates ( $r_{i0}$ ). After that, over a time interval, the accumulating local carbon is calculated. Generally, the deactivation rate is estimated as follows [29]:

$$r_i = r_{i0} \exp(-\alpha C_c) \quad (17)$$

The Eq. 17 is applied to modify the reaction rates with fresh catalyst  $r_{i0}$  to give the reaction rates after 1 min.  $C_c$  (kmol/m<sup>3</sup>) denotes the accumulated coke concentration on the catalyst. The CFD simulation was done at the steady-sated condition for a further 1-min time period with the new reaction rates to gain the increased values of  $C_c$  and the process was then repeated.

## Governing Equations

The kinetic equations of the main and side reactions along with the governing transport phenomena equations including momentum, mass and energy with appropriate initial and boundary conditions were solved numerically.

### Momentum transfer

The continuity and Navier-Stokes equations were applied throughout the reactor domain to description of the flow of fluids as follows [27]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (18)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F} \quad (19)$$

where,  $\rho$  ( $\frac{kg}{m^3}$ ) is density,  $u$  (m/s) is the velocity vector,  $P$  (Pa) is the total pressure,  $I$  denotes the identity matrix, and  $F$  ( $\frac{N}{m^3}$ ) is the volumetric force vector.

### Mass transfer

The mass transfer for each species throughout the reactor domain was given as follows [27]:

$$\rho \frac{\partial \omega_i}{\partial t} - \nabla \cdot \left( \rho D_{i,j} \nabla \omega_i + \rho D_{i,j} \frac{\nabla M_n}{M_n} - \rho \omega_i \sum_k \frac{M_i}{M_n} D_{i,j} \nabla X_k \right) + \rho (\mathbf{u} \cdot \nabla) \omega_i = 0 \quad (20)$$

where,  $D_{i,j}$  ( $\frac{m^2}{s}$ ) is the diffusion coefficient of species.

### Heat transfer

Energy balance equation throughout the reactor domain can be considered as follows [27]:

$$\rho C_P \frac{\partial T}{\partial t} + \rho C_P \mathbf{u} \cdot \nabla T + \nabla \cdot (-k \nabla T) = 0 \quad (21)$$

where,  $C_P$  ( $kJ/kg \cdot K$ ) refers to the specific heat and  $k$  ( $W/m \cdot k$ ) denotes the thermal conductivity. The rate of production/consumption for all chemical components was obtained using the stoichiometry of the reactions while the heat production term was calculated by multiplying the reaction rate in the heat generated by each reaction.

### Solution technique

The proposed CFD model was solved using finite element procedure. All partial differential equations including mass transfer, momentum and energy equations were solved simultaneously with appropriate initial and boundary conditions. The numerical simulation was made with unstructured grids composed of approximately 163,000 nodes (including 1,156,000 tetrahedral cells by consideration the independency of their solution). Additionally, a higher density of elements was created in the regions close to the particles and the reactor wall. The convergence was certified by checking the scaled residuals to a criterion of  $10^{-4}$  for the continuity and momentum, and  $10^{-5}$  for the concentration factors. [Fig. 2a](#) shows the diagram of the sequence of steps which is used in this study. As can be seen, a comprehensive evaluation has been performed including the pre-processing, simulations, results post-processing, and visualization. The boundary conditions were provided as follows:

At the reactor inlet:  $C_i = C_{i0}$ ,  $T = T_0$ ,  $u = u_0$

At the reactor outlet: *Convective flux*,  $p = p_0$

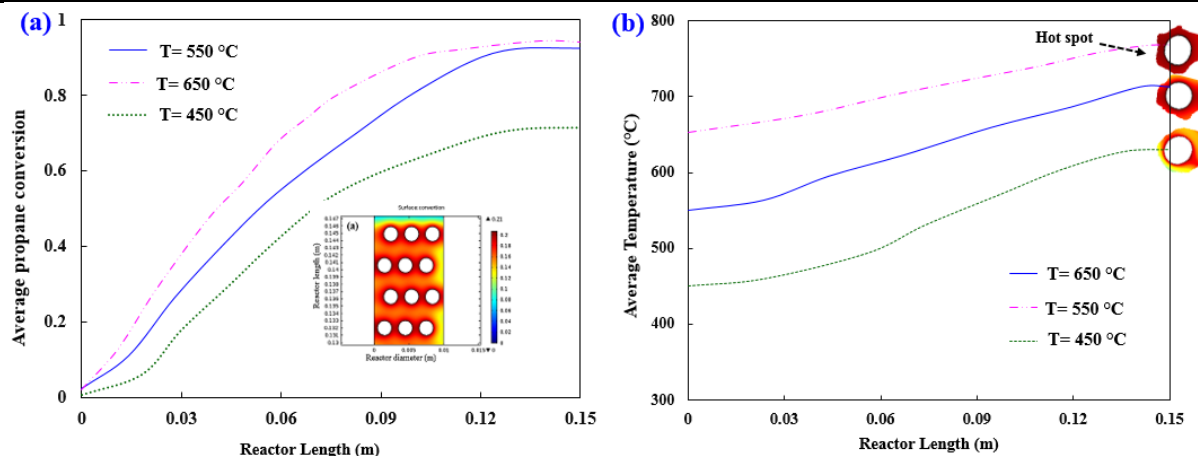
Axial symmetry:  $\frac{\partial C_i}{\partial r} = 0$ ,  $\frac{\partial T}{\partial r} = 0$

At the wall:  $\frac{\partial C_i}{\partial r} = 0$ ,  $-K \frac{\partial T}{\partial r} = U (T - T_c)$ ,  $u=0$

The negligible internal mass- and energy-transport limitations were considered inside the catalyst particles. Furthermore, negligible external mass and heat transfer resistances were assumed at the surface of the catalyst particles. Moreover, the ideal gas law was supposed to describe the behavior of the gas phase inside the reactor.

### Results and discussion

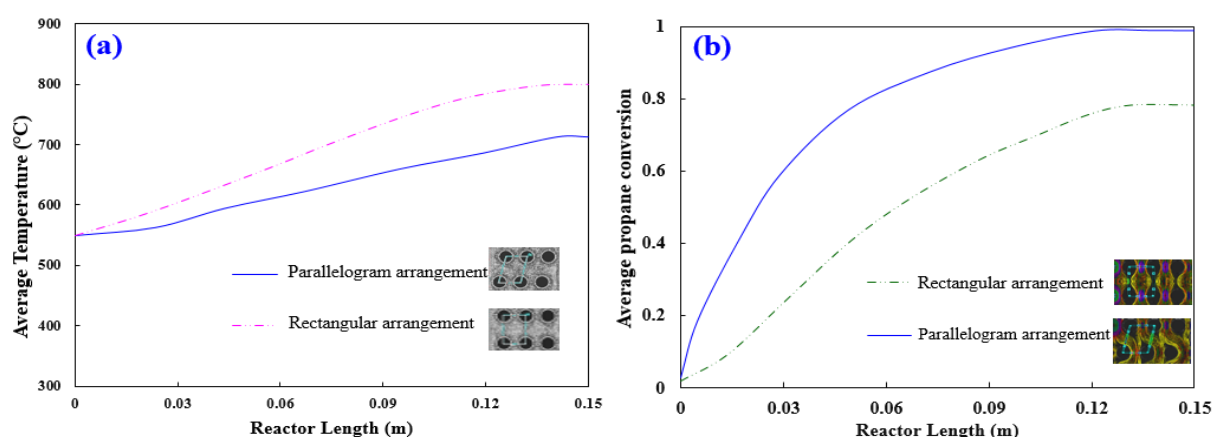
The evaluation of the temperature effect on the propane conversion revealed that higher operating temperatures lead to increasing propane conversion owing to the endothermic reaction ([Fig. 1a](#)).



**Fig. 1.** The average propane conversion (a) and the average temperature (b) along the reactor obtained from the proposed CFD model

In fact, both reaction rates and species diffusivities are depending on temperature, hence increasing the temperature affects the propane conversion significantly. However, it should be noted that excessive temperature in the reactor has some disadvantages such as creating hot spots in the catalyst bed which leads to the deactivation and ultimately destruction of the catalysts. In this condition, the system requires a catalyst revive cycle which imposes serious unit operating costs, and in the case of that hot spots being closer to the reactor wall, serious damages will arise. Moreover, high temperature means a magnification of side reactions that causes reduction of product purity. In this regard, finding the optimized temperature is an essential step in the propane dehydrogenation process. Typically, the impact of the operating temperature on the average temperature across the catalyst bed (Fig. 1b) indicated that the higher operating temperature causes high temperature variation in the reactor length. Findings indicated that maximum operating temperature to achieve the highest conversion without formation of hot spots is 550 °C. The temperature gradually increases from the reactor entrance and heat accumulation causes temperature rise especially in the final catalyst rows. When the operating temperature exceeds the optimum value, temperature rises on the catalyst surface which creates hot spots, especially in the final part of the reactor that will cause catalyst destruction as well as damage to the reactor structure.

A comparison of the average temperature for both bed geometries is shown in Fig. 2a.

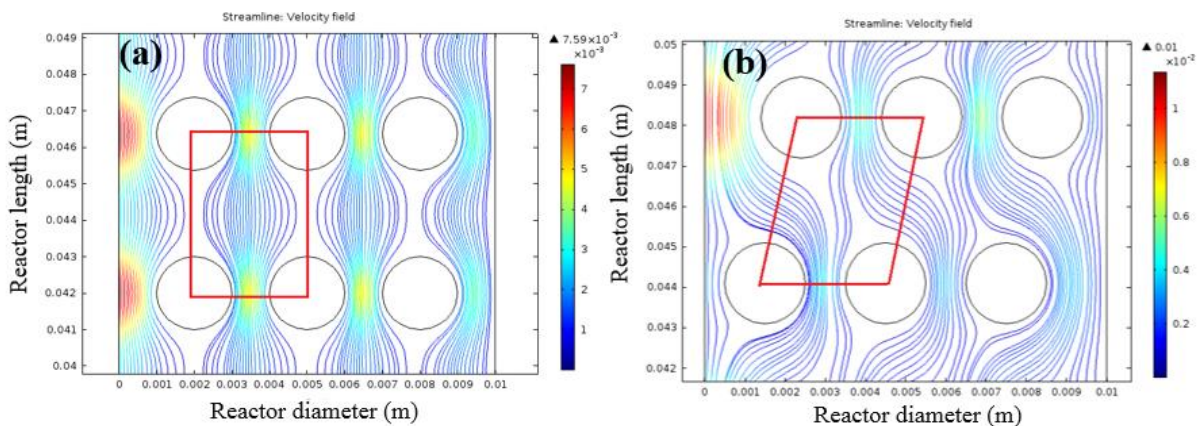


**Fig. 2.** Average temperature (a) and the average propane conversion (b) across the reactor at optimum condition (T=550 °C), obtained from the proposed CFD model

The different temperature gradient observed during the reactor length for rectangular and parallelogram arrangements shows an increase in the accumulated coke due to continuous

creation of coke for both bed geometries. As can be seen, the rate of increased temperature is considerably higher for the rectangular arrangement which can be related to the accumulated coke. The accumulated coke decreases on the end part of the reactor length for both geometries. This is owing to decreasing in the reaction rates caused by less desirable. Findings can be analyzed as follows: rectangular arrangement contains higher accumulated coke compared to the parallelogram arrangement which is owing to the higher reaction rates as a result of better flow distribution. In other words, the parallelogram arrangement creates better mixing which improves the conversion rate. The investigations to find the optimum catalyst bed arrangement revealed that the parallelogram arrangement significantly increases propane conversion in compare to the rectangular arrangement (Fig. 2b) which would be related to the flow pattern through the bed.

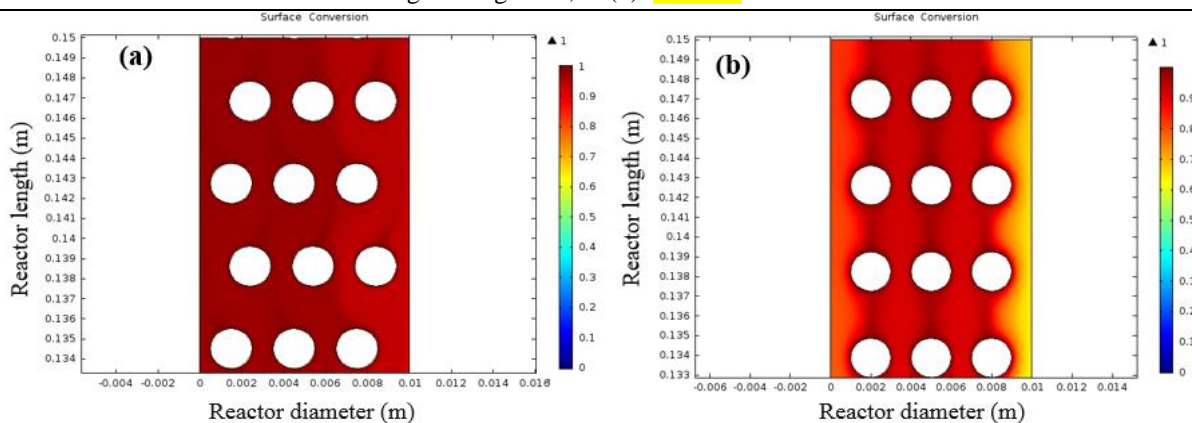
In the case of the rectangular arrangement, reactants flow axially among the catalysts particle, while in the parallelogram arrangement the reactants flow both axially and radially due to obstacles in their path. Under this condition, more mixing is occurred compared to the rectangular arrangement and consequently leads to more interactions between the reactants (Fig. 3). The obtained results for propane conversion at different parts of the reactor indicated that by crossing the catalytic bed conversion was increased gradually until reaches the maximum at reactor outlet owing to the consumption of raw materials. Temperature gradients in different parts of the reactor at optimal operating temperature revealed that the temperature increases throughout the reactor. At the entrance of the reactor the heat is used to improve the reaction rate due to the endothermic reaction and by crossing the catalytic bed, the reaction rate gradually decreases owing to the consumption of raw materials. Therefore, the existing heat results in increasing the temperature at the end of the reactor.



**Fig. 3.** Streamlines of the velocity field in the catalytic bed at optimum condition ( $T=550\text{ }^{\circ}\text{C}$ ). (a): rectangular arrangement, (b): parallelogram arrangement, obtained from the proposed CFD model

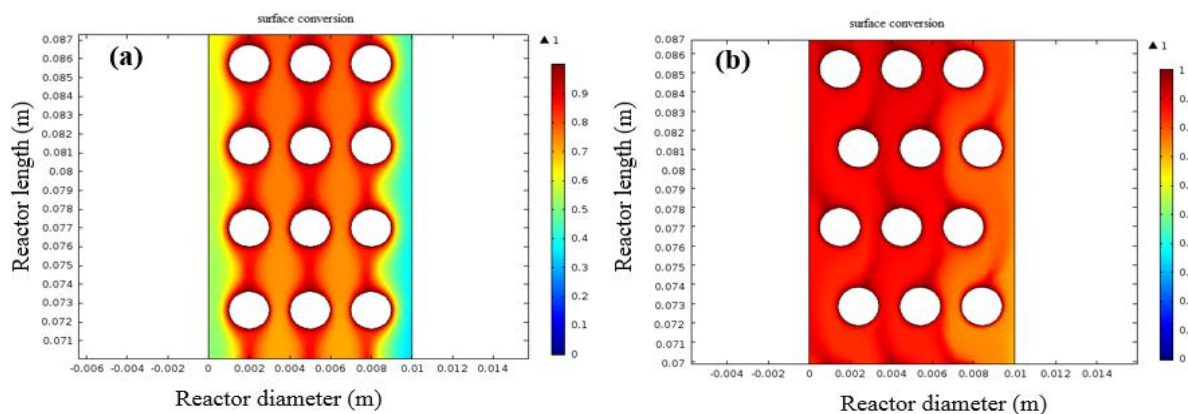
The comparison of the propane conversion for both bed geometries under the same conditions shows that parallelogram arrangement beings more efficiency (Fig. 4). As can be seen, in the parallelogram arrangement the conversion is formed more uniform, while rectangular arrangement causes less product purity.





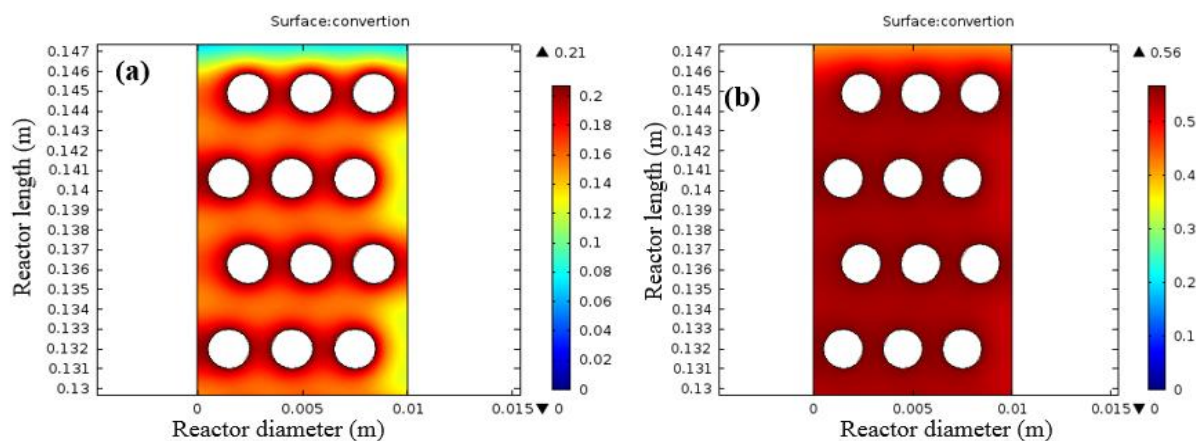
**Fig. 4.** The propane conversion at the reactor height of 0.15 m at optimum condition ( $T=550\text{ }^{\circ}\text{C}$ ). (a): parallelogram arrangement, (b): rectangular arrangement

In the rectangular arrangement, the conversion rate is very slow at the entrance of reactor, while using the parallelogram arrangement the conversion rate was improved because of better mixing as well as good distribution of the reactants in the reactor (Fig. 5).

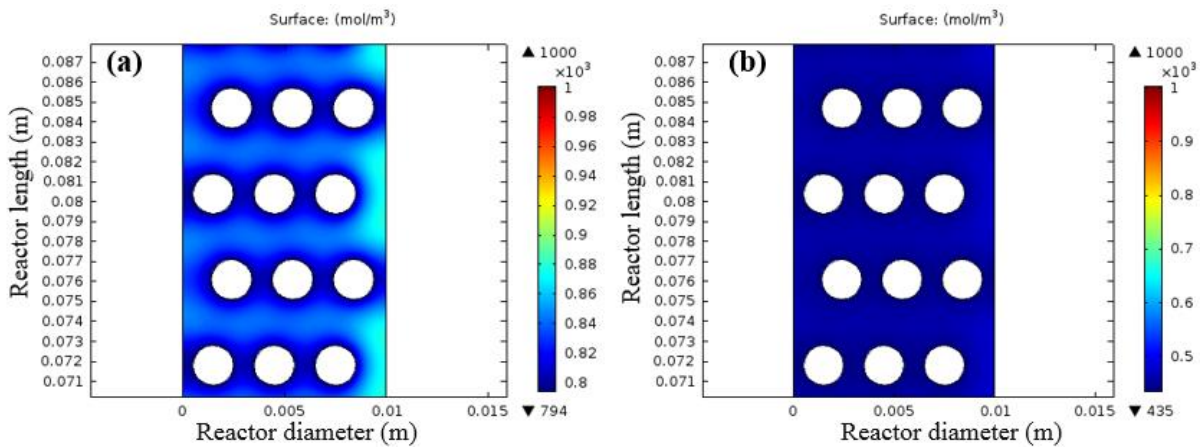


**Fig. 5.** The propane conversion at the reactor height of 0.087 m at optimum condition ( $T=550\text{ }^{\circ}\text{C}$ ). (a): rectangular arrangement, (b): parallelogram arrangement

The deactivation model results demonstrated that due to the coke formation on the catalytic bed and consequently, deactivation of the catalysts active surfaces the propane conversion falls by half the usual amount (Fig. 6). Moreover, the propane concentration gradient across the reactor length at different times indicated that the conversion rate is more uniform using the parallelogram arrangement (Fig. 7). The reaction rate was higher near the catalyst surfaces. As time increases, owing to more carbon deposition and consequently higher deactivation rates, the reaction rate is reduced. In fact, the coke deposition directly affects the catalytic bed activity.

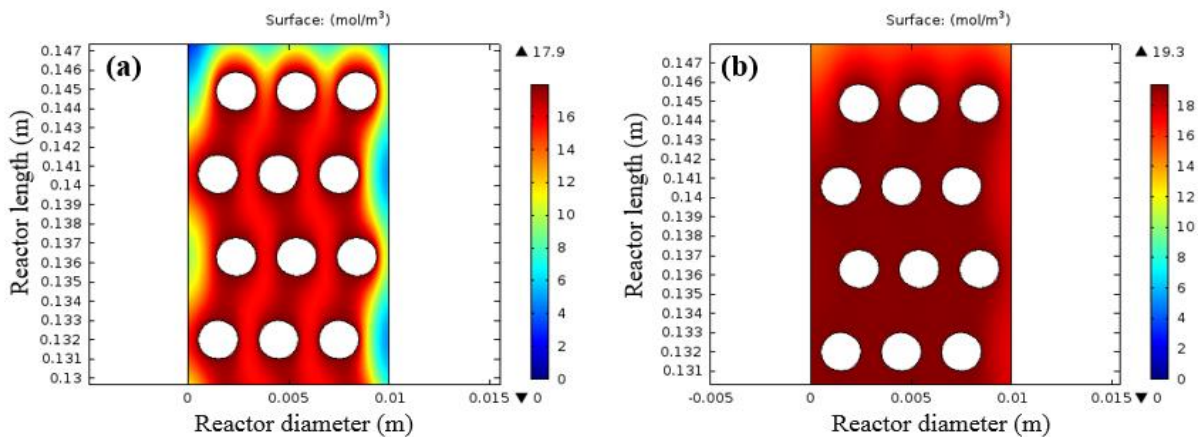


**Fig. 6.** The propane conversion at the reactor height of 0.147 m for parallelogram arrangement at optimum condition ( $T=550\text{ }^{\circ}\text{C}$ ), (a): at the time of 1600 s, (b): at the time of 400 s



**Fig. 7.** The propane concentration at the reactor height of 0.087 m for parallelogram arrangement at optimum condition ( $T=550\text{ }^{\circ}\text{C}$ ), (a): at the time of 1600 s (b): at the time of 400 s

The carbon concentration gradient across the reactor length at different times (Fig. 8) revealed that at first, high propane concentration causes more coke formation, while by reduction in the propane concentration during the process, coke formation rate decreases.



**Fig. 8.** The carbon concentration at the reactor height of 0.15 m at optimum condition ( $T=550\text{ }^{\circ}\text{C}$ ). (a): parallelogram arrangement and the time of 400 s, (b): parallelogram arrangement and the time of 1600s

The variation of the coke formation rates versus the time at different reactor temperatures is represented in Fig. 9. An extreme impact of the reaction temperature is seen. At  $550\text{ }^{\circ}\text{C}$ , after longer times on stream the coke formation rate maintains at a constant value, hence this temperature is an optimum condition.

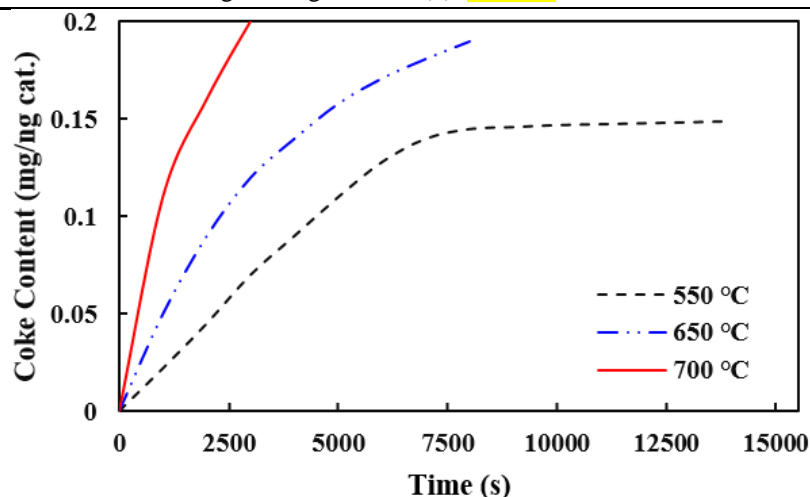


Fig. 9. Coke content versus time at different reactor temperatures

The propane conversion percentage across the reactor length for parallelogram arrangement with and without deactivation model was studied (Fig. 10) and the obtained results showed that propane dehydrogenation process modeling is very unreasonable regardless of the coke production reaction, and so it is very necessary to consider the deactivation equation in the process modeling.

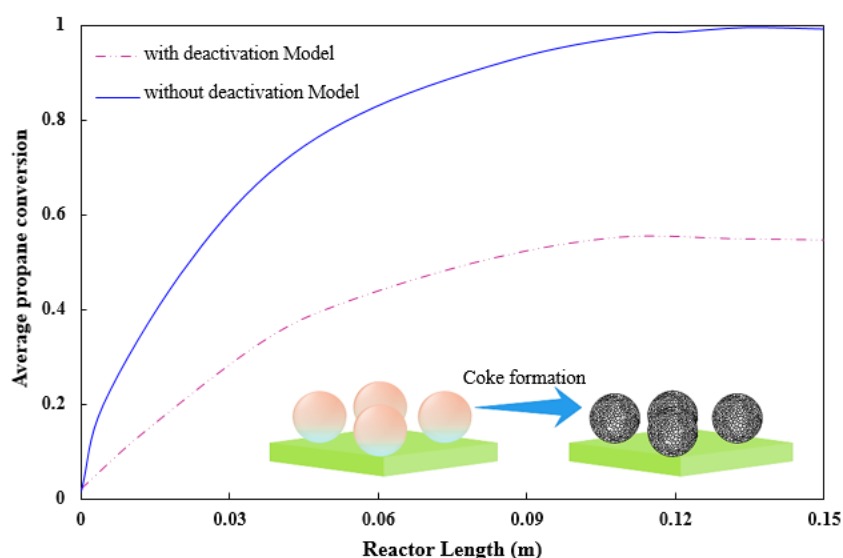


Fig. 10. The comparison of the propane conversion percentage along the reactor at optimum condition ( $T=550$  °C), with and without deactivation model

The tracer test was carried out to investigate the mixing performance of both bed configurations. The tracer with a specified mass fraction was initially patched at the reactor inlet, while a transient CFD simulation was used to analysis of the improvement of mixing performance. The simulation results for both bed arrangements were depicted using Fig. 11. It can be concluded that the parallelogram arrangement causes more mixing inside the reactor.

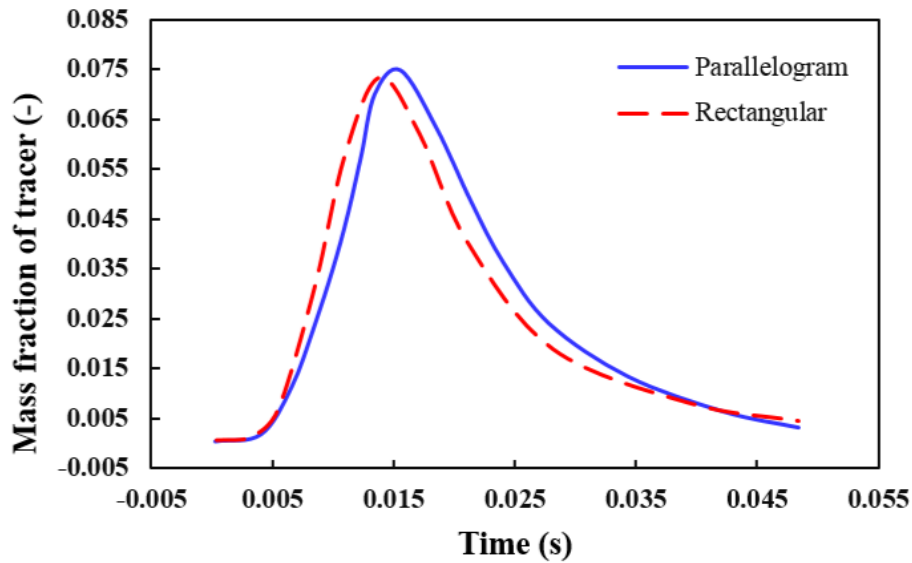


Fig. 11. The tracer test for both bed configurations

Validation of the model was evaluated using experimental data from Hamel et al [32]. Fig. 12 shows the propylene selectivity (%) versus propane conversion (%) for both proposed model results and empirical data. The propane conversion ( $X$ ) and propylene selectivity ( $S$ ) were obtained as follows [33]:

$$X (\%) = \frac{F_{propane}^{In} - F_{propane}^{Out}}{F_{propane}^{In}} \times 100 \quad (22)$$

$$S (\%) = \frac{F_{propylene}^{Out}}{F_{propane}^{In} - F_{propane}^{Out}} \times 100 \quad (23)$$

where  $F$  denoted the molar flow. As can be seen in Fig. 12, the difference between experimental data and proposed model results is within 10% which confirms the validation of the proposed model.

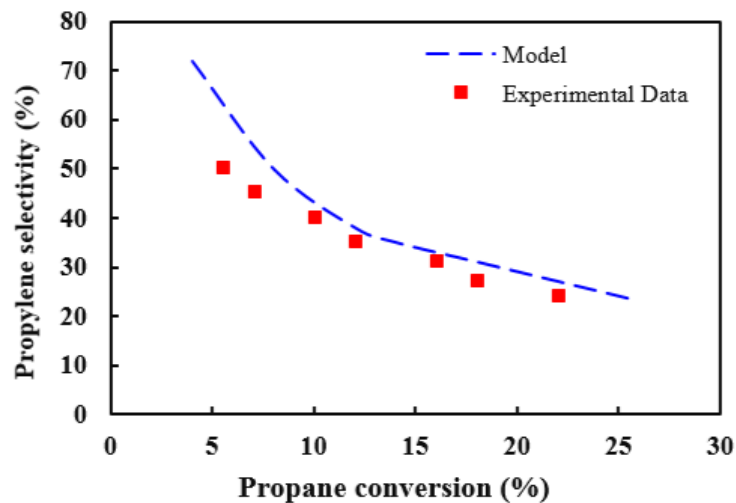


Fig. 12. The proposed model validation: comparison of the obtained models results vs. experimental data

## Conclusion

A CFD model was applied to analysis of the catalytic bed reactor for propane dehydrogenation process. The effect of operating temperature on the propane conversion, creation of hot spots, and deactivation of the bed was evaluated. Findings revealed that higher operating temperatures lead to increasing propane conversion owing to the endothermic reaction. However, it should be noted that excessive temperature in the reactor has some disadvantages such as creating hot spots in the catalyst bed which leads to the deactivation and ultimately destruction of the catalysts. Accordingly, the optimal operating temperature to achieve the highest conversion without the formation of hot spots was found at 550 °C. To comprehend further the differences in temperature variation for different bed geometries, a comparison of the temperature distribution on the catalyst surfaces was performed. Findings indicated that the propane conversion decreases exponentially which is related to the increase in catalyst deactivation with the reactor length. The rectangular arrangement brings faster deactivation of the catalysts compared to the parallelogram arrangement. This phenomenon is more detrimental to the catalyst volume near the reactor wall as it may create local spots which is a serious danger for wall failure

## Acknowledgment

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## Nomenclature

$C_i$	The chemical concentration of species ( $\frac{mol}{m^3}$ )
$C_m$	The coke concentration in monolayer ( $\frac{mol}{m^3}$ )
$C_P$	The specific heat ( $kJ/kg. K$ )
$D_i$	The diffusion coefficient of species ( $\frac{m^2}{s}$ )
$F$	The volumetric force vector ( $\frac{N}{m^3}$ )
$I$	The identity matrix
$k$	The thermal conductivity ( $W/m. k$ )
$k_i$	The reaction rate constant ( $s^{-1}$ )
$P$	The total pressure ( $Pa$ )
$P_i$	The partial pressure of species ( $Pa$ )
$R_i$	The reaction rate ( $\frac{kmol}{m^3.s}$ )
$T$	The absolute temperature ( $K$ )
$u$	The velocity vector (m/s)
$X_{C_3H_8}$	Propane conversion
$\alpha$	Catalyst activity
$\rho$	Density ( $\frac{kg}{m^3}$ )
$\mu$	The dynamic viscosity ( $\frac{Ns}{m^2}$ )

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