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Research Article

Numerical investigation of sulfur trioxide decomposition in microchannel heat exchangers

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ABSTRACT

Due to global increasing in the energy demand and the need to reduce greenhouse gases, hydrogen is considered as an important energy carrier. In this work, numerical modeling of sulfur trioxide decomposition in the sulfur-iodine cycle in micro-channel heat exchangers has been considered. Different baffles shapes have been investigated. Results show by using these baffles in the flow path, the rate of decomposition increases. The highest decomposition percentage of 91.84% was obtained for the alternative design for the channel with asymmetric rectangular baffles. Also, the effect of the operating conditions such as the direction of inlet fluid flow, the inlet temperature of the helium channel and the type of reaction heat supply gas have been investigated. Results show that in the model with counter-current flow, the molar decomposition of sulfur trioxide is about 7% and the thermal performance coefficient is about 31% more than the parallel flow. Also, by increasing the inlet temperature of the helium flow, by about 18% compared to the base model, the molar sulfur trioxide decomposition increases by about 32%. But there is an about 21% reduction in the thermal performance coefficient. This study can provide a useful consideration of the effective parameters on the performance of a high temperature heat exchanger which worked as a sulfuric acid decomposer for hydrogen production within the sulfur-iodine thermochemical cycle.

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INTRODUCTION

With the development of human societies, the need of human beings for transportation and vehicles has increased, so consequently the consumption of fuel, especially fossil fuels such as gasoline and diesel, is increasing exponentially [1]. Hydrogen is one of the most essential commercial commodities and is known as an economical fuel source. In recent years, the use of hydrogen gas as a fuel for vehicle power, heating, electricity generation, and some industrial affairs has been given priority [2]. The primary challenge for increasing hydrogen use is its cost of producing, storing and transporting, which in the following, we will focus on its production issue.

Hydrogen can be produced by various processes, such as from non-renewable sources or by water splitting [3].

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The most common processes for producing hydrogen from non-renewable sources are the reforming process (especially methane reforming). However, this method produces pollution along with the production of hydrogen. Hydrogen production by water splitting is possible from two methods: water electrolysis and thermochemical cycle. Electrolysis requires low temperatures but is not economically justified due to its low hydrogen production and high cost of electricity consumption. Since 1980, more than 200 thermochemical cycles have been studied, the best of which is the sulfur-iodine thermochemical cycle, abbreviated as the sulfur-iodine cycle. In the sulfur-iodine cycle, all reactants and products are reproduced and recycled. This cycle requires heat and water at the inlet, and its outlet is pure oxygen and hydrogen. The three reactions exist in the sulfur-iodine cycle:

$$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4 \quad (1)$$

$$2HI \rightarrow I_2 + H_2 \quad (2)$$

$$H_2SO_4 \rightarrow SO_3 + H_2O \quad (3)$$

Equation (3) is the most important reaction of the sulfur-iodine cycle [4]. Sulfuric acid is one of the most important products of industrial units. The decomposition reaction of sulfuric acid includes two steps.

$$H_2SO_4 \rightarrow SO_3 + H_2O \quad (4)$$

$$SO_3 \rightarrow SO_2 + 0.5\ O_2 \quad (5)$$

Equation (4) decomposes completely at temperatures above 450 °C and occurs very rapidly. Reaction (5), the decomposition reaction of sulfur trioxide, is a reaction with favorable kinetics. Decomposition of sulfur trioxide requires a high temperature, which can be provided by clean energy sources such as solar and atomic energy. Sulfur trioxide decomposes slowly at high temperatures, and a suitable catalyst must be used accelerate the decomposition process [5]. However, this reaction (Equation (5)) can lead to lower temperatures inside the catalyst particle. So, some researchers have considered this viewpoint [6-7]. Pathak and Upadhyayula [6] studied the catalysts for this reaction. They studied the activity of various catalysts (noble, non-noble, complex metal, supported and unsupported metal oxide). They considered the effect of preparation methods, temperature, flow rate, inlet composition, and pressure.

In other works, simulation and optimization of sulfuric acid decomposition process had been investigated. Gao et al. [8] had experimentally and numerically studied this process for hydrogen production. They measured the kinetic factor of sulfuric acid decomposition reaction in experimental section. In the modelling section, the thermal-hydraulic characteristics and the parameters of chemical reaction had been predicted. Their results showed good agreement. In another work, done by Sujeesh et al. [9], modeling and optimization of packed bed reactor for sulfuric acid decomposition. They experimentally studied the effect of flow rate, wall temperature and with two catalyst loadings. A two-dimensional model was considered. In their model, fluid flow, heat transfer, and species transport with reaction in the porous domain were investigated. They found the suitable performance of this reaction in this reactor, which can be helpful for optimization study.

On the other hand, the overall efficiency of the process depends on the rate of decomposition of sulfur trioxide. One of the factors, which is affected on the efficiency of the reaction, is the residence time of the reactant in the reactor [10]. The design of sulfur trioxide decomposer is one of the main challenges in the development of hydrogen production. Microchannel heat exchangers have baffles with different arrangements in the fluid flow path, which affect the molar decomposition of sulfur trioxide by changing the residence time [11]. Because the sulfur trioxide decomposition is a surface reaction, the contact surface between the stream and the channel wall is an essential parameter in the decomposition rate [12].

Many researches had been studied on the sulfuric acid decomposers based on different issues such as the structures and efficiencies of hydrogen production. One of these studies is Ginosar›s work [12]. They used three different catalysts. The influence of exposure on the reaction conditions was considered. Their results showed that the catalyst with higher surface area leads to the higher activity of catalyst, but their deactivation will be rapidly. Pt/TiO_2 catalyst had a lower surface area catalyst. In another work studied by Nagarajan et al. [13] a particular type of heat exchanger was studied. In their study, the temperature of wall is constant which one is measured experimentally. Different types of pellets in the packed bed region were used. The decomposition percentage of sulfur trioxide is considered. In the other their work [2], four different types of fins had been numerically simulated under three different arrangements and proposed a proper design scheme.

In the study done by Sun et al. [14], the design of the decomposer and its pipeline have been studied. Their design is based on a shell-and-tube heat exchanger with a bayonet heat exchanger as the core. They also investigated the heat transfer in their system. They were numerically simulated this system with accounting the phase change of sulfuric acid and the decomposition reaction. They found that the decomposition fraction of sulfuric acid decreases with the enhancement of the flow rate. Also, the sulfuric acid decomposition rate increases and then, with increasing the velocity, it will be stable [15]. Gao et al. [16] focused on the temperature profile, phase change, and chemical reactions of sulfuric acid in this system. The evaporation-condensation model was used to simulate the different stages of the phase change process.

In some other works, the effect of the geometry with different fins or grooves have been considered on the fluid flow and heat transfer, different shape such as: rectangular and semi cylindrical [17], wavy [18] and some other types [19-21]. In the study by Zhu et al. [19], microchannel heat sinks with grooves were studied. The effect of the channel geometry on the performance of this system was considered. Five different types of structures were designed. These different structures were compared, and the optimum structure was determined. Their results showed that the arrangement of the grooves on walls can be affected on performance. Wang et al. [20] found that the use of ribs will induce high-flow disturbances and a blocking-flow effect, so, heat transfer can be improved, although, the pressure drop increases. Their results show that the system with grooves can be more enhanced in heat transfer and smaller pressure drop related to the system with ribs. With consideration of related studies, it can be found that a comprehensive study in various conditions (different operational and geometrical conditions) is needed to better study of the performance of the system.

In this study, sulfur trioxide decomposition in the microchannel heat exchangers has been considered. the thermal performance coefficient, which studied the effect of frication factor and Nusselt number together, was considered in different conditions in this work. In the base model, the rectangular baffles were used. The location of these baffles (only on the bottom wall, asymmetric baffles on the upper and lower walls) were compared. At the next step, the effect of some operating parameters such as the direction of the fluid flow in microchannels, the temperature of each inlet streams, and some geometrical parameter (different baffle shapes) on the molar decomposition of sulfur trioxide had been investigated.

CFD MODELING

The modeling method is based on Computational Fluid Dynamics (CFD). CFD is the analysis of systems involving fluid flow, heat transfer, and associated phenomena, such as chemical reactions, based on computer simulations. The structure of the CFD program is a numerical method, so fluid flow problems can be solved using this method [22]. CFD modeling and simulation is as a valuable tool for modeling of some processes. There are different studies done by CFD modeling [23-24].

Geometry of the system

Figure 1 shows the base model of a micro-channel heat exchanger. There are three sections in this microchannel heat exchanger: a helium passage channel, a reaction channel and the middle part between these channels made of silicon carbide to transfer heat from the hot helium channel to the reaction channel. The direction of the inlet flow in these channels is counter-current. The height of the helium and reaction channel is 0.85 mm and 0.424 mm, respectively. In this base model, 20 rectangular baffles were located on the walls. The height of the rectangular baffles is 0.2 mm and their width is 0.1 mm. Also, the distance between the baffles is 0.3 mm. The location of the baffles has been considered in this work. Figure 2 shows a schematic view of the baffle location.

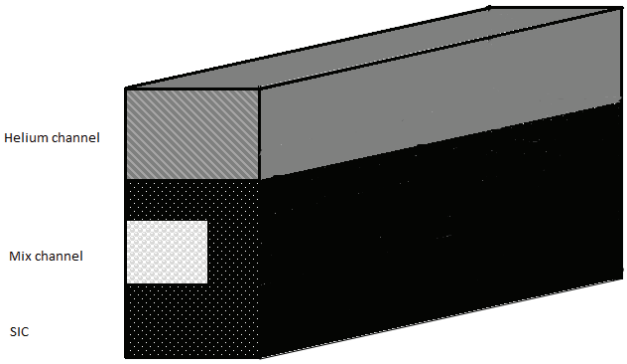


Figure 1. Schematic view of three sections of the microchannel heat exchanger.

a) b)

Figure 2. Location of baffles, (a) only on the bottom wall, (b) asymmetric baffles on the upper and lower walls.

Governing Equations

The mathematical model of steady state flow in a microchannel heat exchanger is described using the Navier-Stokes three-dimensional flow equations, which include a set of partial differential equations (PDE) for the equations of continuity, momentum, energy, and species transfer which are expressed in Equations (6) to (11). The governing equations are as follows [25]:

Continuity equation:

$$\frac{\partial}{\partial \mathrm{x}}(\rho\vartheta_{\mathrm{x}}) + \frac{\partial}{\partial \mathrm{y}}(\rho\vartheta_{\mathrm{y}}) + \frac{\partial}{\partial \mathrm{z}}(\rho\vartheta_{\mathrm{z}}) = 0 \quad (6)$$

Momentum equation:

$$\rho(v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}) = -\frac{\partial p}{\partial x} + \mu[\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}] \quad (7)$$

$$\rho(v_x\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} + v_z\frac{\partial v_x}{\partial z}) = -\frac{\partial p}{\partial y} + \mu[\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}] \quad (8)$$

$$\rho(v_x\frac{\partial v_z}{\partial x} + v_y\frac{\partial v_z}{\partial y} + v_z\frac{\partial v_z}{\partial z}) = -\frac{\partial p}{\partial z} + \mu[\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}] \quad (9)$$

Energy equation:

$$\rho\hat{\mathrm{C}}_{\mathrm{P}}\left(\vartheta_{\mathrm{x}}\frac{\partial \mathrm{T}}{\partial \mathrm{x}} + \vartheta_{\mathrm{y}}\frac{\partial \mathrm{T}}{\partial \mathrm{y}} + \vartheta_{\mathrm{z}}\frac{\partial \mathrm{T}}{\partial \mathrm{z}}\right) = \mathrm{k}\left[\frac{\partial^2 \mathrm{T}}{\partial \mathrm{x}^2} + \frac{\partial^2 \mathrm{T}}{\partial \mathrm{y}^2} + \frac{\partial^2 \mathrm{T}}{\partial \mathrm{z}^2}\right] + \mathrm{S_h} \quad (10)$$

Species transfer equation:

$$\rho\left(\vartheta_x\frac{\partial Y_A}{\partial x} + \vartheta_y\frac{\partial Y_A}{\partial y} + \vartheta_z\frac{\partial Y_A}{\partial z}\right) = \rho D_{AB}\left[\frac{\partial^2 Y_A}{\partial x^2} + \frac{\partial^2 Y_A}{\partial y^2} + \frac{\partial^2 Y_A}{\partial z^2}\right] + S_c \quad (11)$$

In above equations, ρ, μ, k, C_p, and D_{AB} are mixture density, viscosity, thermal conductivity, specific heat at constant pressure, and diffusion coefficient, respectively. The density was calculated using the ideal gas law for an incompressible flow. Other parameters were calculated by equations (12-15) based on kinetic Theory. The diffusivity of the mixture (D_{AB}) was calculated using the Chapman–Enskog kinetic theory. S_h is the heat of the reaction and S_c is the net production rate by chemical reaction.

In the helium channel, the Continuity, momentum and energy equations (Equations 6-10) are solved. There is no reaction in this channel. The term heat of reaction (S_h) in equation (10) is zero due to the lack of reaction in the helium channel. In the reaction channel, in addition to those equations (Equations 6-10), the species transfer equation (Equation 11) is also established. In the middle part, only the energy equation (Equation 10) is solved. In this part, due to the lack of the reaction, the heat term of reaction (S_h) in Equation (10) is zero.

$$\mu = \sum_i \frac{x_i\mu_i}{\sum_j x_j\emptyset_{ij}} \quad (12)$$

$$\emptyset_{ij} = \frac{\left[1+\left(\frac{\mu_i}{\mu_j}\right)^{\frac{1}{2}}\left(\frac{Mw_j}{Mw_i}\right)^{\frac{1}{4}}\right]^2}{\left[8\left(1+\frac{Mw_j}{Mw_i}\right)\right]^{\frac{1}{2}}} \quad (13)$$

$$k = \sum_i \frac{x_i k_i}{\sum_j x_j\emptyset_{ij}} \quad (14)$$

$$C_P = \sum_i Y_i C_{Pi} \quad (15)$$

The wall surface reaction model is done on the wall of the reaction channel and is implemented to determine the mole fractions of SO_3, SO_2 and O_2. The reaction rate was obtained by using the Arrhenius equation and the reaction is first order reaction (Equations 16 -17) [26].

$$K = Ae^{\left(\frac{-Ea}{RT}\right)} \quad (16)$$

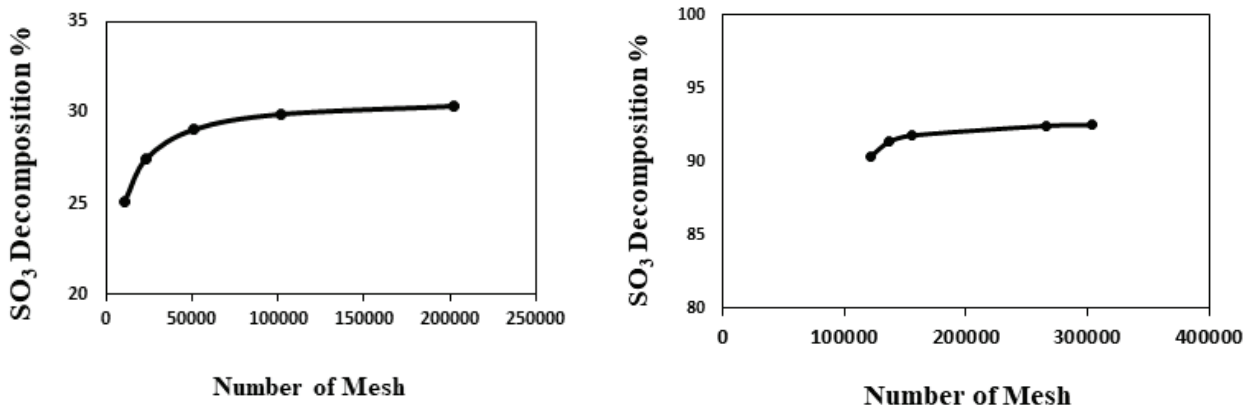
$$Rrxn = -KCso3 \quad (17)$$

Where E_a is the activation energy (equals to 3.267 * 10^7 J/kmol) and A is pre-constant reaction (equals to 0.05).

Solution Method and Boundary Conditions

In this work, the finite volume method is used to discretize the governing equations by the SIMPLE algorithm. Discretization of energy, momentum and pressure equations is performed by first-order upwind, first-order upwind and standard methods, respectively. Convergence is considered when the residuals of the values reach 10^{-6}. A combined mesh of rectangular and triangular mesh was used in these simulations. Mesh dependency was considered, too. The effect of mesh number on the sulfur trioxide decomposition was investigated (as sample, Figure 3 shows for two systems, without baffles and with 20 baffles). Finally, the proper mesh, which had little effect on the results was selected for each system.

In the base model, a hot helium gas stream with a temperature of 1223.15 °K enters the helium channel. The reactants mixture with a temperature of 974.9 °K enters the reaction channel in the opposite direction. Boundary conditions at the entrance are based on specific mass flow rate and specific inlet temperature. The no-slip condition is established on the walls. The right, upper, and lower walls of the geometry are adiabatic. The left wall is considered a symmetrical boundary. The reaction takes place in the reaction channel and on the wall surface. The reaction takes place under a specific pressure (1.5 MPa). In this research,



a) b)

Figure 3. Mesh independency in system (a)without baffles, (b) with 20 baffles.

four parameters (Nusselt number, thermal performance coefficient, molar percentage of sulfur trioxide decomposition, and pressure drop) have been investigated for all models. The thermal performance coefficient is defined as Equation (18):

$$\eta = \frac{(\frac{Nu}{Nu_0})}{(\frac{f}{f_0})^{\frac{1}{3}}} \quad (18)$$

Nu_0 and f_0 are the Nusselt number and the friction coefficient in a channel without baffles, respectively. it is clear that the value of thermal performance coefficient equals to one for the model without baffles. Also, when the value of the thermal performance coefficient is greater than one, it means that system has better performance. Equation (19) is used to calculate the molar percentage of sulfur trioxide decomposition:

$$So_3\ Decomposition\% = [\frac{(So_3\ concentration)_{inlet} - (So_3\ concentration)_{outlet}}{(So_3\ concentration)_{inlet}}] * 100 \quad (19)$$

RESULTS AND DISCUSSION

Validation

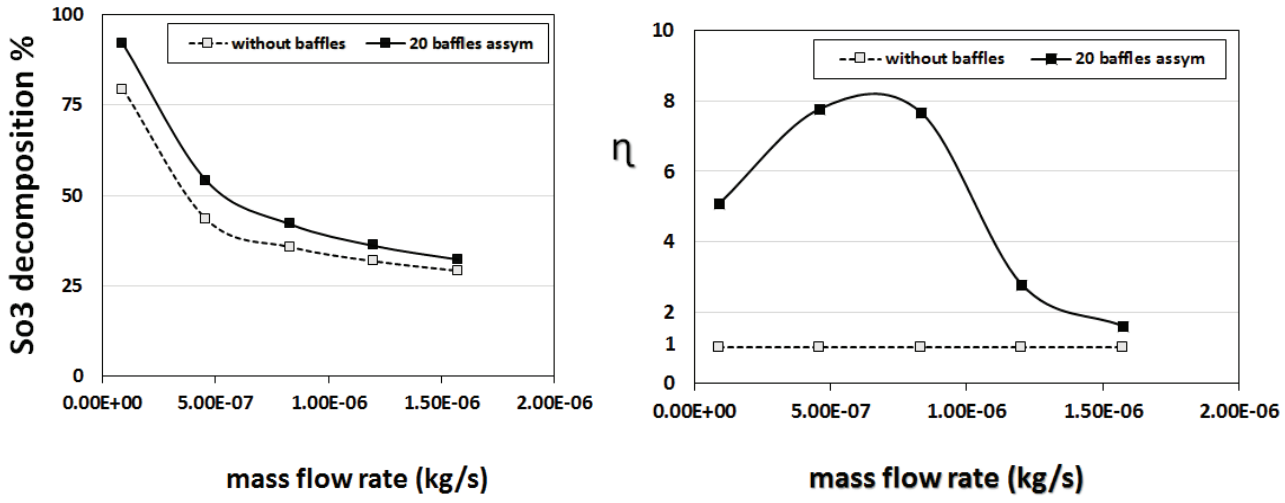
To validate the model, a study by Ponyavin [27] has been reviewed. In this work, rectangular channels with dimensions similar to Ponyavin's work has been used. A stream of hot helium gas enters the helium channel at 1223.15 °K and the reactants mixture enters the reaction channel at 974.9 °K in the opposite direction. The comparison of the results of Ponyavin's work and this simulation results show that the average error is 4%. The highest error equals to 7%, is observed at the flow rate 3.148 * 10^{-6} Kg/s. So, it can be said there is a good agreement between the results and the present model is acceptable.

Effect of the baffles

In this section, 20 rectangular baffles were used in the reaction channel asymmetrically on the upper and lower walls of the channel. Figures 4 shows the variations of molar decomposition of sulfur trioxide and the thermal performance coefficient versus inlet mass flow rate for this model and the model without baffles. The black line corresponding to the model with 20 baffles asymmetrically and the dash line represents the model without the baffles. Other operating conditions are the same as the base model. Results show SO_3 decomposition decreases with increasing the mass flow rate for both models. Also, the model with 20 baffles asymmetrically has higher decomposition rates than the model without baffles. By using these baffles in the flow path, the area of the reaction surface increases and, due to the superficial reaction of sulfur trioxide decomposition, its molar decomposition rate increases by about 12% compared to the model without baffles at the same flow rate.

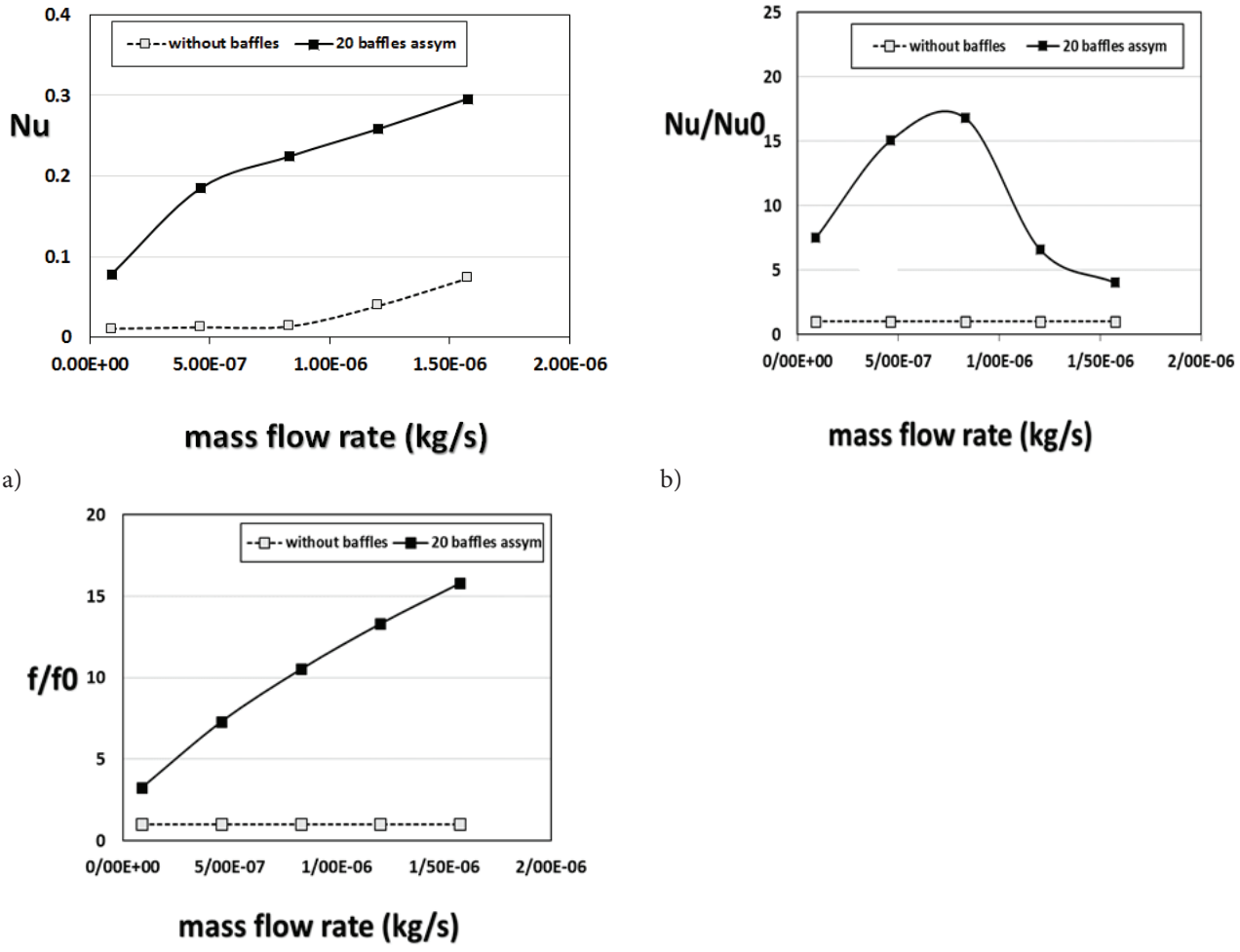
Moreover, from Figure 4 (b), it can be found that the value of the thermal performance coefficient of the model with 20 baffles asymmetrically is greater than one. So, it is desirable**.** With increasing the mass flow rate, initially the thermal performance coefficient increases, but with more mass flow rates, its value decreases. Corresponding to Equation (16), the thermal performance coefficient is related to the ratio of Nusselt number to friction factor (which can be calculated from pressure drop) for both models.

Figure 5 shows the variations of the ratio of Nusselt number and friction factor versus mass flow rates. As shown in Figure 5 (a), the Nusselt number in the model with 20 baffles asymmetrically is greater than the model without baffles. The Nusselt number has a direct relationship with the surface convection heat transfer coefficient. Due to the higher reaction surface of the model with 20 baffles asymmetrically, the surface convection heat transfer coefficient increases and, so, the Nusselt number increases for this model respect to the model without baffles. However,



a) b)

Figure 4. Comparison of (a) molar decomposition of sulfur trioxide and, (b) the thermal performance coefficient versus mass flow rates for the model with 20 asymmetric rectangular baffles and the model without baffles.



a) b)

c)

Figure 5. Comparison of (a) the Nusselt number, (b) Nu/Nu0 , (c) f/f0 versus mass flow rates for the model with 20 asymmetric rectangular baffles and the model without baffles.

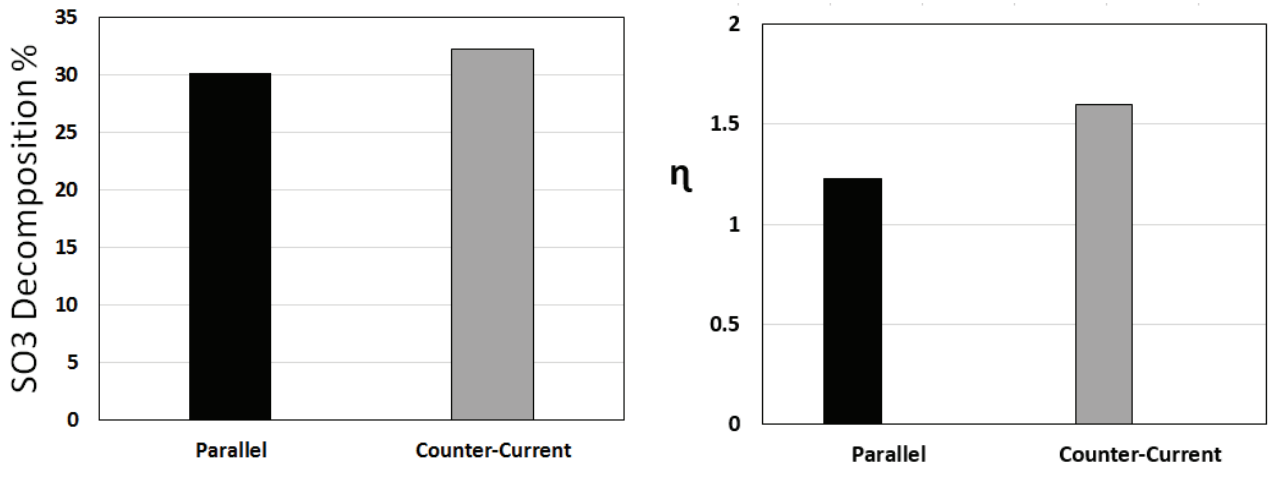
the ratio of the Nusselt number of these models is changed with increasing the mass flow rates, so, it can be found from Figure 5 (b), the ratio of the Nusselt number of these models (Nu/Nu0) initially increases and then decrease. Also, by adding the baffles, the friction factor increases due to increasing the pressure drop (Figure 5 (c)).

Effect of operating conditions

After the above consideration, it was found that the model with 20 asymmetric rectangular baffles had a better performance than the model without baffles. Therefore, this model was examined as the base model. In this base model, inlet flow rate equals to $1.574*10^{-6}$ (Kg/s) and mass fraction of sulfur trioxide and water equal to 0.8163 and 0.1837, respectively. The inlet temperatures of the reaction and helium channel are 974.9 K and 1223.15 K, respectively. The operating pressure is 1.5 MPa. In this section, the effect of the operating conditions such as the direction of inlet fluid flow, the inlet temperature of the helium channel and the type of reaction heat supply gas is investigated**.** In all sections, only that parameter is changed and other parameters will be constant (equals to their values at the base model).

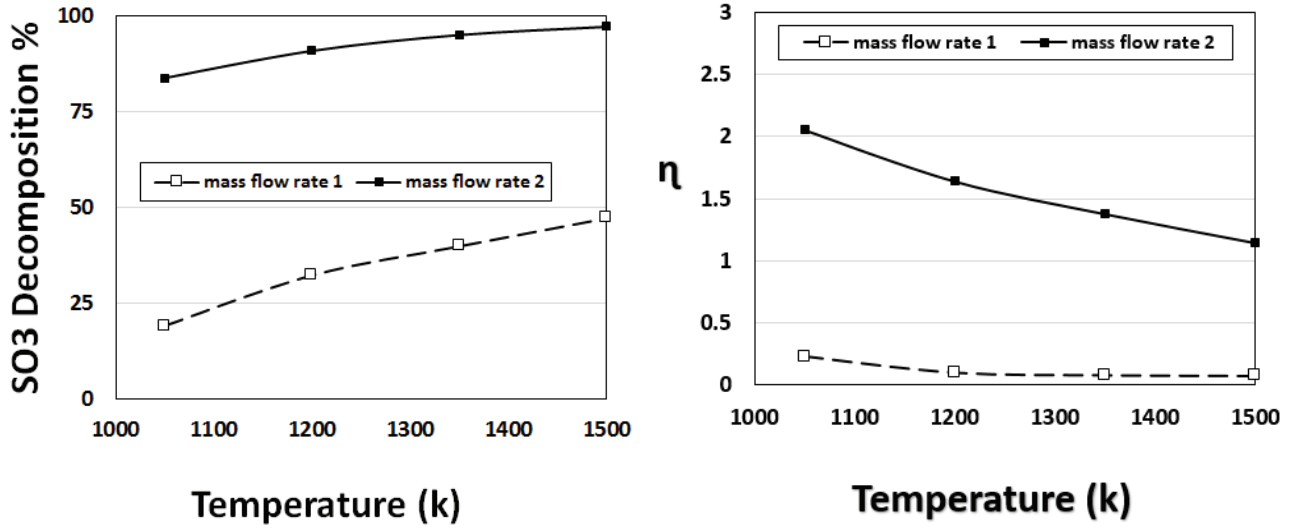
Figures 6 shows the variations of the molar decomposition of sulfur trioxide and thermal performance coefficient with different flow direction. When the inlet flow of reaction and helium channels enters from the same side of the microchannel heat exchanger, it was named as parallel. When inlet flow of reaction and helium channels enters in the opposite direction, it was named as counter-current flow. Other parameters are the same as the base model and only the direction of the inlet flow was changed. The black bar chart shows the parallel flow and the gray bar chart shows the counter-current flow. From Figure 6, it can be found that the molar sulfur trioxide decomposition, and the thermal performance coefficient with counter-current flow are higher than the parallel flow. It is consistence with the previous study [4]. In the model with counter-current flow, the molar sulfur trioxide decomposition is about 7% and the thermal performance coefficient is about 31% more than the parallel flow. For non-aligned motion, the surface convection heat transfer coefficient is a higher than in the aligned position. In fact, in the counter-current flow, the average temperature difference along each part of the channel is greater than the parallel flow. It therefore has a better thermal performance coefficient than other flows. Due to the direct relationship between the Nusselt number and the surface heat transfer coefficient, the higher value of the surface convection heat transfer coefficient leads to increasing the Nusselt number, which effects on the sulfur trioxide decomposition due to the superficiality of the decomposition reaction.

Figure 7 shows the variations of the molar sulfur trioxide decomposition and thermal performance coefficient versus the inlet temperature of the helium flow for two different mass flow rates (mass flow rate 1 > mass flow rate 2). Other parameters are similar to the base model. Results show that by increasing the inlet temperature of the helium flow by about 18% compared to the base model, the molar sulfur trioxide decomposition increases by about 32%. However, there is an about 21% reduction in the thermal performance coefficient. As the inlet temperature of the helium stream in the helium channel increases, the rate of heat transfer to the surface of the reaction channel increases. As a result, fluid contacts with the hot wall of the reaction channel, the molar sulfur trioxide decomposition increases. Also, as shown in Figure 7(b) the thermal performance coefficient decreases with increasing the inlet temperature of the helium flow.



a) b)

Figure 6. Comparison of (a) the molar decomposition of sulfur trioxide and (b) the thermal performance coefficient of parallel and counter-current flows in the model with 20 asymmetric rectangular baffles, P= 1.5 MPa, T_{mix} = 974.9 k, T_{he} = 1223.15 k, mass flow rate = $1.574*10^{-6}$ kg/s.



a) b)

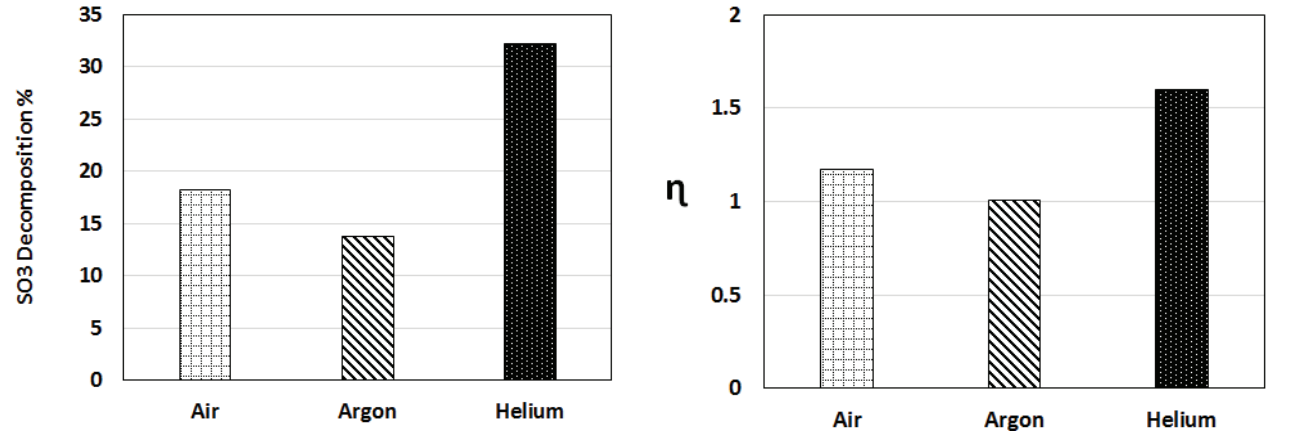
Figure 7. Variations of (a) molar dcomposition of sulfur trioxide, (b) the thermal performance coefficient in the model with 20 asymmetric baffles at different helium channel inlet temperatures, P = 1.5 MPa, Tmix = 974.9k, mass flow rate 1 = $1.574*10^{-6}$ kg/s, mass flow rate 2 = $9*10^{-8}$ kg/s.

With increasing the inlet temperature of the helium flow, the Nusselt number decreases. So, the thermal performance coefficient decreases.

In the base model, the gas used to supply the heat required for the reaction is helium hot gas. In this section, the effect of using hot argon and air gases is investigated and other condition are the same as the base model. Figure 8 shows the molar decomposition of sulfur trioxide and the thermal performance coefficient with these hot gases. From Figure 8, it can be found that the use of helium gas is much better than the other gases mentioned. Because the specific heat capacity of helium gas is more than two other gases, so, it can supply more heat than other mentioned gases. As a result, the sulfur trioxide decomposition increases.

Effect of Baffles shape

In this section, the effect of using different baffles shapes such as triangle, semi-ellipse, and trapezoid is investigated. These baffles have equal height and width. The geometric schematic view of these shapes of baffles is shown in Figure 9 (a-c). In this section, based on above considerations, the counter-current flow with inlet mass flow rate of $9*10^{-8}$ (Kg/s) and the inlet temperature of helium channel of 1350 ^{o}K is accounted. The reaction was done on the baffle walls.



a) b)

Figure 8. Variations of (a) the molar decomposition of sulfur trioxide, (b) the thermal performance coefficent in the model with 20 asymmetric baffles with different gases supplying the reaction heat, P = 1.5 MPa, $T_{in,gas}$ = 1223 15 k, T_{mix}= 974.9 k, mass flow rate = $1.574*10^{-6}$ kg/s.

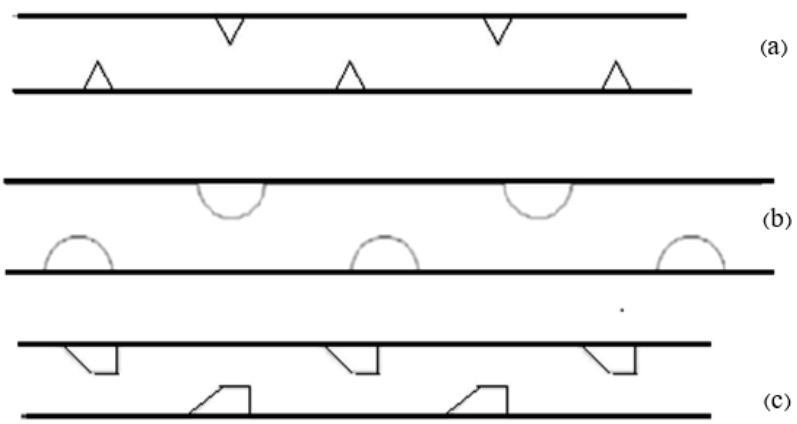


Figure 9. Geometric schematic view of (a) triangular, (b) semi-ellipse, (c) trapezoidal baffles.

Table 1. Reaction surface

Baffle shape	Area (mm²)
Rectangular baffles	24.8686
Triangular baffles	23.44102
Trapezoidal baffles	24.1548
Semi-ellipsoid baffles	19.7546

With changing the shape of the baffles, the reaction surface was changed. Table 1 lists the reaction surface for different shapes of baffles. Due to the superficiality of the reaction and its effect on the rate of molar decomposition, the reaction area of baffles can be affected.

Figure 10 shows the molar decomposition of sulfur trioxide for the models with different baffle shapes. Due to the proximity of the reaction surface of the geometry of the baffles used in the fluid flow path, different molar decompositions are observed. The molar sulfur trioxide decomposition for the model with rectangular baffles is slightly higher than other models. The molar of sulfur trioxide decomposition for the model with rectangular baffles is about 1.5% higher than the triangular model, about 0.3% higher than that of the trapezoidal model and about 8.5% higher than that of the semi-ellipse model. The critical point is the effect of the structure of these baffles on parameters such as pressure drop and Nusselt number. The type of curvature, the sharp edge of the baffles and the slope of the sides affect the amount of friction, pressure drop and Nusselt number.

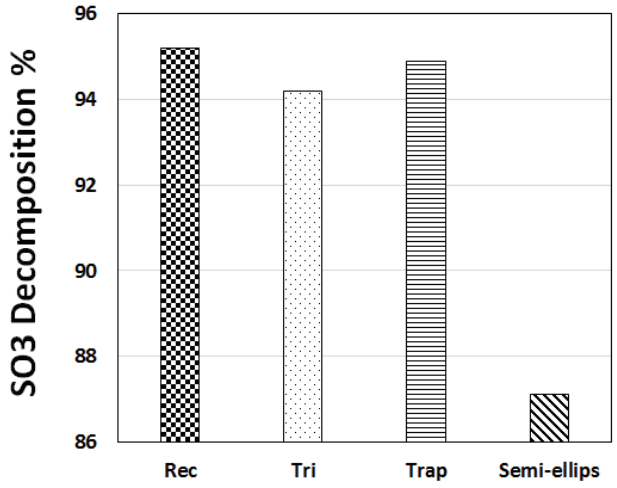


Figure 10. Comparison of the molar decomposition of sulfur trioxide in the model with 20 asymmetric baffles with different baffles shapes, mass flow rate = $9*10^{-8}$ Kg/s, P = 1.5MPa, T_{mix} = 974.9 k, T_{he}= 1350 k.

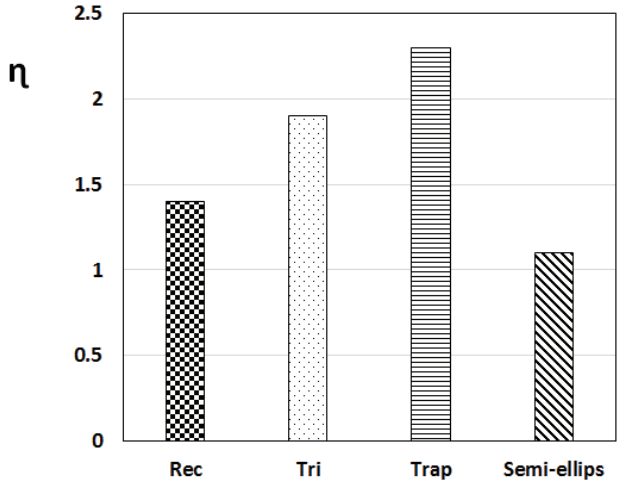


Figure 11. Comparison of thermal performance coefficents in the model with 20 asymmetric baffles with different baffles shapes, mass flow rate= $9*10^{-8}$ Kg/s, P = 1.5MPa, T_{mix} = 974.9 k, T_{he}= 1350 k.

Figure 11 shows the thermal performance coefficient of the models with different baffles. The lowest thermal efficiency is related to the semi-ellipse model. Due to the curvature of the semi-ellipse baffle heads, after each baffle, the low number of vortices formed reduces the rate of heat transfer from the surface of the channel to the fluid compared to other models. Also, the thermal performance coefficient of the trapezoidal model is higher than other models due to its better Nusselt number and lower pressure drop. The thermal performance coefficient of the model with triangular baffles is about 29% higher than the model with rectangular baffles, while, the model with trapezoidal baffles is about 41% higher than the model with rectangular baffles. In the model with semi-ellipse baffles, the thermal performance coefficient is about 25% lower than the model with rectangular baffles.

CONCLUSION

In this work, three-dimensional computational fluid dynamics analysis was performed on fluid flow, heat transfer and chemical reaction in a high temperature heat exchanger. Due to the superficiality of the decomposition reaction of sulfur trioxide, the surface area of the reaction was increased to improve its decomposition rate. This was done by adding rectangular baffles to the reaction channel. From this consideration, it can be found:

- With the addition of asymmetric rectangular baffles, about 30% was added to the reaction surface area compared to the no-baffle model.
- The molar decomposition of sulfur trioxide increases by about 12% compared to the no-baffle model.
- The conversion rate of sulfur trioxide in the system with counter-current flow was about 7% and the coefficient of thermal performance was about 31% higher than the parallel flow.
- By increasing the helium flow inlet temperature by about 18% compared to the base model, the sulfur trioxide conversion rate increases by about 32% but the coefficient of thermal performance decreases by about 21%.
- The use of argon and air gases instead of helium significantly reduces the conversion rate and thermal efficiency.
- In the model with 20 asymmetric triangular baffles, compared to the base model, the sulfur trioxide molar decomposition decreases by about 1.5%, but the coefficient of thermal performance increases by about 40%. While, in the system with 20 asymmetric semi-ellipse baffles, the molar decomposition of the system with semi-ellipse baffles reduces by about 7.5%. Also, its thermal performance coefficient is lower than the base model.

NOMENCLATURE

A	pre-exponential factor, s^{-1}
C	molar concentration, mol/m^3
Cp	specific heat at constant pressure, $J.kg^{-1}.K^{-1}$
D_{AB}	diffusion coefficient for species A in the B, $m^2.S^{-1}$
E_a	activation energy, J/kmol
f	friction factor
K	reaction rate, s^{-1}
k	thermal conductivity, $W.m^{-1}.K^{-1}$
m	mass flow rate, $kg.s^{-1}$
Mw	Molecular weight, kg/kgmol
Nu	Nusselt number
R_{rxn}	net rate of production of species i by chemical reaction, $kg.m^{-3}\ s^{-1}$
S_c	net rate of production of species A by chemical reaction, $kg.m^{-3}.s^{-1}$
S_h	heat of chemical reaction, $J.mol^{-1}$
T	static temperature, K
x_i	mole fraction of species i
Yi	mass fraction of species i

Greek symbol

η	thermal performance coefficient
μ	Viscosity, $kgm^{-1}s^{-1}$
ρ	density, $kg\ m^{-3}$
Φij	constant of ideal gas law

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AUTHORSHIP CONTRIBUTIONS

Authors equally contributed to this work.

DATA AVAILABILITY STATEMENT

The authors confirm that the data that supports the findings of this study are available within the article. Raw data that support the finding of this study are available from the corresponding author, upon reasonable request.

CONFLICT OF INTEREST

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

ETHICS

There are no ethical issues with the publication of this manuscript.

STATEMENT ON THE USE OF ARTIFICIAL INTELLIGENCE

Artificial intelligence was not used in the preparation of the article

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