Optimization Analysis of the Structural Design of NNBI Cryosorption Pumps

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Abstract: Cryosorption pumps create a vacuum by adsorbing gas at low temperature through porous solid adsorbents. The transmission probability of gas molecules and heat loads of cryosorption pumps are important factors affecting its performance. Herein, Molflow software based on the Monte Carlo principle is used to analyze the effects of the structural design of cryosorption pumps on transmission probability. The influence of structural design on radiation heat transfer is analyzed by ANSYS Steady-State Thermal software. This provides a reference for the design of a cryosorption pump to validate the prototype of a neutral beam injector for the China Engineering Fusion Experimental Reactor (CFETR).

Keywords: cryosorption pump; Molflow software; gas molecule; Monte-Carlo; transmission probability

1. Introduction

Neutral beam injection (NBI) systems have been designed and developed internationally to provide the functions of auxiliary plasma heating and current drive in fusion devices [1]. With the advances in research on nuclear fusion, the high neutralization efficiency of negative neutral beam injection (NNBI) ensures it will play a role in future trends [2]. The cryo-vacuum system of NBI is part of a large, built-in system that requires development in terms of the following features: large gas load, long pumping periods, pumped gas containers, and high stability and reliability. Cryosorption pumps maintain the vacuum environment gradients in the chamber by pumping the hydrogen and helium generated in the process of neutral beam generation and transmission. According to the design index, the pumping time of NNBI cryosorption pumps reaches 3600 s. Therefore, it is necessary to develop cryosorption pumps that have a high pumping speed and a long, continuous pumping time.

The combination of a cryopanel and a radiation baffle is called a cryoarray; this is one of the main factors that determines the performance of cryosorption pumps. In the design of cryoarrays, various factors such as the pumping speed, heat load and costs are considered.

According to ITER NBI engineering design, the cryoarray is applied in the CFETR NNBI, as shown in Figure 1 [3,4]. The transmission probability and thermal loads are important factors that affect the performance of cryosorption pumps. Keeping the transmission probability as large as possible and appropriately reducing the thermal loads, so that the performance of the cryosorption pump is optimized as much as possible, can be achieved by optimizing the structure.

Several methods have been applied to calculate transmission probability and thermal loads, including theoretical and numerical methods [5–7]. Theoretical methods are applied to simple geometries, but not suitable for complex geometries. With the development of
technology, the numerical methods can improve the calculation accuracy and can be applied to complex geometries. Molflow software is a numerical analysis software based on the Monte-Carlo principle. In simulation, the quantitative gas molecules represent the actual number of gas molecules in a vacuum. Improvements in the software by the developers, Kersevan and Ady, have led to its wide application in the vacuum field. The software can effectively analyze the relationship between complex structures and transmission probability. ANSYS software is a mature finite element analysis software with a wide range of applications and it can effectively perform thermal analysis. Overall, the analysis results provide a reference for the structural design of the CFETR NNBI cryosorption pump.

\[
W = \frac{Q_1}{Q_2}
\]  

(1)

where $W$—transmission probability, $Q_1$—the number of hydrogen gas molecules touching the cryopanels per unit time, and $Q_2$—the number of all hydrogen gas molecules flying from the inlet per unit time.

Establishing a model for analyzing the transmission probability via Molflow software required several simplifications, which were mainly divided into two aspects: simplifying the structure of the cryosorption pump, and the law of gas molecule movement.

2.1. Structure of the Model

A cryosorption pump is composed of several sets of modules that have the same structure. Therefore, the analysis of the influence of the structure on transmission probability can be done by researching one single module of the pump. Here, the model design corresponds with that of the cryosorption pump of the ITER NBI. The model’s length width and height are 1 m, 2.7 m and 0.32 m, respectively. The cryosorption pump is composed of radiation baffles, cryopanels, a cooling piping system, shells, screws and fixing clips.

![Design structure of cryoarrays of CFETR NNBI.](image-url)

**Figure 1.** Design structure of cryoarrays of CFETR NNBI.

2. Analysis of Transmission Probability

The Molflow software was designed by Kersevan and Ady from CERN [8–10]. The software was originally applied for simulating synchrotron radiation or synchrotron light sources, but as the designers have continued to improve it, it has become widely used in the field of vacuum technology [11–13]. The transmission probability ($W$).

\[
W = \frac{Q_1}{Q_2}
\]  

(1)
The process of gas entering the pump is mainly divided into pre-cooling and adsorption. The bases, shell baffles and covers can be replaced by the plane of in the Molflow software, which can be omitted in solid works. Screws and fixing clips do not affect the pre-cooling and adsorption effect of the cryopump on the gas molecules; thus, these parts are omitted to reduce the cost of the simulation calculation. In addition, as the cooling piping cannot come into contact with the gas molecules, the cooling piping was simplified to the plane, as shown in Figure 2.

![Diagram of the cryosorption pump module.](image)

**Figure 2.** Diagram of the cryosorption pump module.

### 2.2. The Model of Gas Movement

According to actual conditions, the movement of gas molecule within the pump is complicated. Thus, to reduce the workload, on the premise that the accuracy of the simulation results would not be affected, the following simplifications were made with regard to the movement of gas molecules:

1. When gas molecules are incident from the intake surface, they follow Knudsen’s law, and the incident positions are evenly distributed.
2. In the steady state, the number of gas molecules incident from the intake surface per second is constant.
3. Diffuse reflection occurs when gas molecules collide with the wall, and the resulting reflection angles follows Knudsen’s law [14].
4. A limited number of test particles represent a larger number of physical molecules and the quantities derived from the test particles are scaled up to match the physical numbers.
5. The hydrogen molecular mean free path (20 °C, 10⁻² Pa) is about 0.5 m, and the representative physical length scale L of the shield space is about 0.22 m. Kn = λ/L > 1 [14]. Therefore, the status of gas molecules in the cryosorption pump is molecule flow, there is no mutual collisions between molecules, only the collisions between the molecules and the walls.
6. The gas molecules flying from the inlet that do not touch the cryopanels and are reflected back to the inlet will be absorbed by the inlet.
7. As long as the intake continues, the cryopanels will continue to absorb gas molecules and there is no maximum pumping capacity.

### 2.3. Physical Parameters and Boundary Conditions

The model was imported into Molflow. Firstly, the surrounding wall of the model was established. The front wall represents the intake surface, the upper and lower walls represent the cover plate, the rear wall represents the radiation shielding wall, and the left and right walls represent the elastic collision wall, as shown in Figure 3. The front wall represents the gas inlet, the green hits represent reflected gas molecules, the red hits represent gas molecules adsorbed by the cryopanels, and the blue hits represent created gas molecules in Figure 3.
and the temperature of the radiation baffle, surrounding wall, and gas inflow was set to 85, 80 and 300 K, respectively [3,4].

2.3.2. Sticking Coefficient

In order to calculate the transmission probability, it is necessary to ensure that gas molecules will be adsorbed after colliding with the cryopanels. Therefore, it is assumed that the sticking coefficient of H₂ on the 5 K cryopanels is 1. The sticking coefficient of the front wall was set to 1, which is convenient for recording the gas molecules that do not touch the cryopanels and are reflected back to the front wall.

2.3.3. Gas Inflow

The gas flow of each model was set to 0.5 Pa·m²/s.

2.3.4. Calculation Formula of Transmission Probability

The formula for calculating the transmission probability was edited by Molflow’s formula editor:

\[ W = 1 - \frac{A_x}{\text{SUMDES}} \]  

(2)

where \( W \)—transmission probability, \( A_x \)—gas molecules adsorbed on the front wall per unit time, \( X \)—facet number, and \( \text{SUMDES} \)—all the created gas molecules per unit time.

3. Results and Discussion

The transmission probability of the gas molecule was calculated via the Molflow software, which can calculate the ratio of the adsorbed gas molecule per unit time to gas inflow per unit time.

3.1. The Stages of the Cooling Structure

An increase in the stages of the cooling structure leads to an increase in the transmission probability and the space of the pump body. Thus, determining the stages of the cooling structure is important for the design of cryosorption pumps. Here, we established four models. The models were based on two-stage, three-stage, four-stage and five-stage cooling structures. The two-stage, four-stage and the five-stage cooling structures were based on the three-stage structure of the ITER NBI cryosorption pump with the third-stage cooling structure added to or reduced. The five models of transmission probability were analyzed by Molflow software. The transmission probability of these models is shown...
in Figure 4. The increase in the stages of the cooling structure makes the transmission probability larger, however, when the fourth and fifth stages were increased, the influence on transmission probability was small. The more stages in the cooling structure, the higher the costs. Therefore, the three-stage cooling structure is the best option.

![Graph](image)

**Figure 4.** The transmission probability W versus S.

### 3.2. Cryopanels’ Layout

To investigate the optimal cryopanel arrangement, four groups of models were established. In the first model, the three stages of cryopanels were all arranged parallel to the radiation shielding wall (A); in the second model, the third-stage cryopanels were perpendicular to the radiation shielding wall and the others were arranged in parallel (B); the first-stage cryopanels in the third model were arranged in parallel and the others are arranged vertically (C); the three stages of cryopanels in the fourth model (D), were arranged vertical to the radiation shielding wall. The Table 1 shows that the transmission probability were 0.29, 0.3, 0.311 and 0.324, respectively, as calculated by Molflow software.

| Group | W    | Standard Deviation |
|-------|------|--------------------|
| A     | 0.29 | 0.01               |
| B     | 0.3  | 0.005              |
| C     | 0.311| 0.004              |
| D     | 0.324| 0.008              |

It is clear that when the cryopanels were arranged vertically, the transmission probability was slightly higher than that of the parallel arrangement, but the difference in their probabilities was small. Taking into account the influence of the cryopanels’ layout on the size of the pump, the parallel and vertical layouts were adopted to appropriately adjust the size of the cryosorption pump, while ensuring that the heat radiation from the chamber cannot be directly radiated to the cryopanel. Therefore, the second or third model structure is the most feasible.

### 3.3. Optimization of the Structural Parameters

Figure 5 shows that the cross-sectional view of the cryosorption pump. In the figure, α refers to the angle of the third-stage radiation baffle, \( L_1 \) refers to the distance between the apexes of the third-stage radiation baffle, \( L_2 \) is the vertical distance between the vertex of the third-stage radiation baffle and the center of the second-stage cryopanel, \( L_3 \) is the vertical distance between the vertex of the second-stage radiation baffle and the center
of the first-stage cryopanel, and \( d_1 \) is the distance between the vertices of the first-stage radiation baffle. The distance between the vertices, \( h_1 \) is the vertical distance from the end of the side wall of the third radiation baffle to the apex of the first radiation baffle. The size of \( \alpha \) and \( L_1 \) affect the shape of the space between the cooling structures, and have a certain impact on the flow state of gas molecules at the inlet of the cryosorption pump. Also, the size of \( L_2 \) will affect the movement of gas molecules near the second-stage cryopanels and the size of \( L_3 \) will affect the movement of gas molecules near the third-stage cryopanels.

\[ \text{Figure 5. Cross-sectional view of the cryosorption pump.} \]

To examine the influence of the structural parameters \( (L_1, L_2, L_3, \text{ and } \alpha) \) on the transmission probability, we established the model of a pump with initial parameters, where \( \alpha = 82^\circ \), \( L_1 = 12 \text{ cm} \), \( L_2 = 3.8 \text{ cm} \), and \( L_3 = 4.5 \text{ cm} \). When the control variable method is used to study the influence of the parameters on the transmission probability (W), the other three parameters must be left unchanged.

The influence of \( \alpha \) at \( 10^\circ \text{–} 105^\circ \) on the transmission probability \( W \) was analyzed, as shown in Figure 6. Here, it can be seen that \( W \) generally decreased as \( \alpha \) increased.

\[ \text{Figure 6. The transmission probability } W \text{ versus } \alpha. \]
Meanwhile, Figure 7 shows the line graph of the gas molecules’ density distribution along the inlet direction when $\alpha$ is $20^\circ$ and $70^\circ$, with the abscissa representing the depth of gas molecules entering the pump body. The $W_{20^\circ} > W_{70^\circ}$, so the average gas molecule density of $70^\circ > 20^\circ$. It can be seen that when $L < 0.18$ m, the gas molecule density at $70^\circ > 20^\circ$. When $L > 0.3$ m, the density of gas molecules at $70^\circ < 20^\circ$. This indicates that more gas molecules flowed into the third-stage cryopanel as the $\alpha$ increased.

Figure 7. Gas molecules’ density distribution along the inlet direction when $\alpha = 70^\circ$ and $20^\circ$.

According to the actual situation, the influence of $L_1$ at 10, 12, 14, 16, 18 and 20 cm on the transmission probability was analyzed, as shown in Figure 8.

Figure 8. The transmission probability $W$ versus $L_1$.

Figure 8 shows that when $L_1 = 10–20$ cm, the transmission probability $W$ increased overall. Figure 9 shows the line graph of the gas molecule density distribution along the inlet direction when $L_1 = 10$ and 16 cm. Here, the density at 16 cm was slightly more than that at 10 cm, with a difference of only 0.003.
Figure 8. The transmission probability $W$ versus $L_1$. Figure 8 shows that when $L_1 = 10$–20 cm, the transmission probability $W$ increased overall.

Figure 9 shows the line graph of the gas molecule density distribution along the inlet direction when $L_1 = 10$ and 16 cm. Here, the density at 16 cm was slightly more than that at 10 cm, with a difference of only 0.003.

According to the actual situation, the adaptive range of $L_2$ is between 2.2–4 cm, thus, we analyzed the influence of $L_2$ at 2.4, 2.8, 3.2, 3.6 and 4 cm on the transmission probability, with the results shown in Figure 10.

Figure 10 shows that when $L_2 = 2.4$–4 cm, the transmission probability $W$ is almost unchanged, indicating that $L_2$ has little effect on the aspect ratio of the flow area between the cooling structures.

Figure 11 shows the line graph of the gas molecules’ density distribution along the inlet direction when $L_2 = 2.4$ cm and 4 cm. Here, the gas molecules’ density was almost the same for each $L_2$ value. $W_{4\text{cm}} < W_{2.8\text{cm}}$, but the gap is small, so Figure 11 shows that there is no obvious difference in the density of gas molecules.
Figure 12 shows that when $L_3 = 3.6$–5.2 cm, the range of $W$ was 0.321–0.323, that is, $L_3$ has little effect on the transmission probability $W$ because it has no obvious influence on the aspect ratio of the flow area between the cooling structures.

Figure 13 shows the line graph of the gas molecules’ density distribution along the inlet direction when $L_3 = 4$ cm and 5.2 cm, with the two cases found to be almost equal. $W_{4cm} \approx W_{5.2cm}$, but the gap is small, so Figure 13 shows that there is no obvious difference in the density of the gas molecules.
conduction, solid conduction and convection heat transfer. It is important to study the influence of the structural design on radiation heat because radiation heat is the largest heat source.

The ambient temperature in the cryosorption pump is basically stable, and the temperature of the components outside the pump can be set uniformly at 300 K [3]. We analyzed the influence of the structural parameters on the radiation heat transfer by using ANSYS Steady-State Thermal software, and the relationships among all of these elements were identified. A pump model was established with parameters referenced to ITER NBI ($\alpha = 82^\circ$, $L_1 = 12$ cm, $L_2 = 3.8$ cm, and $L_3 = 4.5$ cm) to study the influence of structural parameters on radiation heat.

When the control variable method was used to study the influence of the structural parameters on the radiation heat, the other three parameters were left unchanged.

### 4. Analysis of Radiation Heat Loads

The heat loads of cryosorption pumps mainly include radiation heat transfer, gas conduction, solid conduction and convection heat transfer. It is important to study the influence of the structural design on radiation heat because radiation heat is the largest heat source.

The above analysis indicates that the aspect ratio of the flow area between the cooling structures ($h_1 / L_1$) is the main influencing factor on the transmission probability $W$. By keeping $h_1$ unchanged, we can study the influence of $L_1$ on the transmission probability $W$. The decrease in $h_1 / L_1$ leads to a larger transmission probability. In terms of the influence on the transmission probability, $a$ has the same influence on the transmission probability as $h_1 / L_1$.

#### 4.1. Model Establishment and Physical Parameter Setting

The radiation baffles and radiation shields are made of aluminum alloy, and the cryopanel is made of copper.

Activated carbon was evenly distributed on both sides of the cryopanels and their emissivity $\varepsilon$ was set to 0.95. The radiation baffles’ internal surface and the outer surface of first-stage radiation baffles were polished with an emissivity at 0.15 because the radiation baffles’ internal surface directly faces the cryopanels and the first-stage radiation baffles directly face the chamber’s components. In order to reduce the reflected radiation from the chamber’s components to the cryopanels, the second-stage to third-stage of radiation baffles and the outer surface of the radiation shielding walls were blackened with an emissivity at 0.95. The temperature of the cryopanels was set to 4.5 K, the temperature of

![Figure 13](image)

**Figure 13.** Gas molecules’ density distribution along the inlet direction when $L_2 = 4$ and 5.2 cm.

The above analysis indicates that the aspect ratio of the flow area between the cooling structures ($h_1 / L_1$) is the main influencing factor on the transmission probability $W$. By keeping $h_1$ unchanged, we can study the influence of $L_1$ on the transmission probability $W$. The decrease in $h_1 / L_1$ leads to a larger transmission probability. In terms of the influence on the transmission probability, $a$ has the same influence on the transmission probability as $h_1 / L_1$.
radiation baffles was set to 85 K, and the temperature of the vacuum chamber was set to 300 K [3].

Due to hardware issues and computation costs, a six-sided grid is preferred for meshing. The structure of a hexahedral mesh is more stable than that of a tetrahedral mesh, and the node bundles of the unit will be much smaller, which reduces the calculating time. The element size of the upper covers, lower covers, radiation baffles, and cryopanels was set to 2 mm, according to the size of the component, the performance of the computer and the accuracy of the simulation result. The elements of the upper covers, lower covers, and the radiation baffles were set in the hexahedron form and given that the cryopanels and radiation baffles are extremely thin, these were set to a tetrahedron form and presented as a grid division diagram as shown in Figure 14, where there are 166,659 nodes and 46,488 units.

Figure 14. The meshing of the model.

4.2. Results and Discussion

A design requirement of $\alpha$ is to ensure that the third-stage cryopanels are not able to accept radiation from the chamber, meaning $\alpha$ has an adaptive range. $L_1$ has the most influence on $\alpha$, and is proportional to $\alpha$. When $L_1 = 10$ cm, $\alpha = 32^\circ$ and can resist the radiation from the chamber, as shown in Figure 15.

Figure 14. The meshing of the model.

Figure 15. The structure of the cryosorption pump’s module versus $\alpha = 32^\circ$. 
The influence of $\alpha = 40^\circ, 50^\circ, 60^\circ, 70^\circ, 75^\circ, 80^\circ, 85^\circ, 88^\circ, 90^\circ, 93^\circ, 96^\circ, 100^\circ, 105^\circ$ and $110^\circ$ on the absorbed radiation of the third-stage radiation baffle was analyzed, and the results are shown in Figure 15.

Figure 16 shows that when $\alpha$ continued to increase, the absorbed radiation of the three-stage radiation baffle exhibited an increasing trend, before ultimately stabilizing. Here, the third-stage radiation baffle showed the highest increase rate. $\alpha$ changes with the change in the angular coefficient of radiation heat from the vacuum chamber to the radiation baffles. In Figure 17, $W_2$ is a side wall of the third-level radiation baffle and $W_1$ is a heat emitting surface, and $\alpha$ increases with the increase of $\theta$.

According to the expression of the angle coefficient, it is known that as $\theta$ decreases with the increase of $X_{1,2}$. When more heat is emitted from the emitting surface to the side wall of $W_2$, the outer surfaces of the third-level radiation baffle receive more heat radiation. As Figure 15 shows, when $\alpha$ continues to increase, $L_1$ gradually decreases and the incident surface remains unchanged. Assuming that the radiation values of the chamber and components that radiate to the pump are constant, the absorbed radiation value of the shielding wall will decrease, while the value of the absorbed radiation of other radiation baffles will increase. Here, the third-stage radiation baffles showed the highest growth rate, while the second-stage radiation baffles had the lowest.

Figure 18 shows that when $\alpha$ continues to increase, the absorbed radiation of the first-stage cryopanels remains unchanged while the second-stage cryopanels continues to increase. The third-stage cryopanels’ radiation sources include the radiation from the inner
surface of the third-stage radiation baffles and the radiation wall, with the former being inverse to \( \alpha \), and the latter is proportional to it. As such, the third-stage cryopanels initially increased before decreasing and finally stabilizing, which indicates that the former had a more important influence on the absorbed radiation than the latter when \( \alpha = 40-85^\circ \), while the latter had a more important influence on the absorbed radiation than the former when \( \alpha = 85-100^\circ \). The two cases were almost equal when \( \alpha > 100^\circ \).

![Figure 18](image)

**Figure 18.** The absorbed radiation of three-stage cryopanels versus \( \alpha \).

The influence of \( L_1 = 10 \text{ cm}, 12 \text{ cm}, 14 \text{ cm}, 16 \text{ cm}, 18 \text{ cm} \) and \( 20 \text{ cm} \) on the absorbed radiation of the third-level radiation baffle was analyzed. As shown in Figure 4, when \( L_1 \) increases with the increase of \( d_1, d_2 \) and the radiation heat entering the inlet surface \( d_2 \). The geometric structure of the area is simplified as shown in Figure 19, and the expressions of the angle coefficients \( X_{d_2,d_1} \) can be calculated by:

\[
X_{d_2,d_1} = \frac{[W_{d_2} + W_{d_1}]^2 + 4}{{2W_{d_2}}} - \left[ (W_{d_1} - W_{d_2}) + 4 \right]^{\frac{1}{2}}
\]

(3)

\[
W_{d_2} = d_2/h_2, \quad W_{d_1} = d_1/h_2
\]

(4)

![Figure 19](image)

**Figure 19.** Simplification of the internal geometric structure of the cryosorption pumps.

Figure 19 shows that \( L_1 \) increases with the increase of \( X_{d_2,d_1} \), which leads to a gradual increase in the proportion of the chamber radiation transferring into the radiation shielding, whereas that transferring into the other radiation baffles gradually decreases. The absorbed radiation of the radiation baffles continued to increase with the increase in intake surface’s
radiation, as shown in Figure 20. Since the former has less influence on the radiation value of the radiation baffles, the absorbed radiation of the three-stage radiation baffles increases slowly.

![Figure 20. The absorbed radiation of three-stage cryopanels versus L1.](image)

Figure 20. The absorbed radiation of three-stage cryopanels versus $L_1$.

Figure 21 shows that the absorbed radiation of the first-stage and third-stage cryopanels remained unchanged with the increase in $L_1$.

![Figure 21. The absorbed radiation of three-stage cryopanels versus L1.](image)

Figure 21. The absorbed radiation of three-stage cryopanels versus $L_1$.

On analyzing the influence of $L_2 = 13.3–14.7$ cm and $L_3 = 11.1–12.1$ cm on the absorbed radiation of the cryopanels and radiation baffles, it became clear that the change in $L_2$ and $L_3$ had no influence here.

5. Conclusions

The structural design principles should be based on the principle of maximizing the transmission probability and then minimizing the radiant heat transfer. As the analysis demonstrated, the aspect ratio between cooling structures ($h_1/L_1$) is the main factor affecting both the transmission probability and radiation heat transfer. Keeping $h_1$ unchanged, we studied the influence of $L_1$ on the transmission probability. A decrease in $h_1/L_1$ leads to a larger transmission probability. Meanwhile, an increase in $h_1/L_1$ results in a larger $\alpha$. Keeping $h_1$ constant, we studied the influence of $L_1$ on the radiation heat transfer. The total radiation heat transfer of radiation baffles was larger but not obvious, but the total radiation heat transfer of cryopanels tends to remain stable when $h_1/L_1$ decreases, thus,
applying the maximum value in the appropriate range of $L_1$ is required. The change in $L_2$ had a small impact on both phenomena, and these can be adjusted according to the actual situation. From the above analysis, the structural design of the cryosorption pumps of CFETR NBI should be based on the principles of maintaining the aspect ratio ($h_1/L_1$) as small as possible, maintaining an $\alpha$ of not less than 40°, and attempting to minimize it.

**Author Contributions:** Author Contributions: Conceptualization, J.L.; data curation, J.L.; formal analysis, J.L., Y.T.; funding acquisition, C.H. and Y.X.; methodology, Y.X.; software, Y.X.; supervision, C.H.; validation, J.L.; writing—original draft, J.L.; writing—review & editing, Y.X. All authors have read and agreed to the published version of the manuscript.

**Funding:** This work was supported by the Comprehensive Research Facility for Fusion Technology Program of China under Contract No. 2018-000052-73-01-001228 and the National Key R&D Program of China under No. 2017YFE300101.

**Data Availability Statement:** The data that support the findings of this study are available from the corresponding author upon reasonable request. The data that supports the findings of this study are available within the article.

**Conflicts of Interest:** The authors declare no conflict of interest.

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