High-fidelity Numerical Study on Air-tightness Detection System of Medicine Box

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Abstract. Planning an automatic detection system of the air tightness of medicine box is very necessary for growing demand for storage of pharmaceutical products. In this study, the high-fidelity CFD study is performed for the air tightness of the medicine box, using the LBM algorithm. The high-fidelity results indicate that after about 5.24 s, the stable value of the average static pressure of the ring cavity remains at about -9414 Pa. The slit flow in the early stage of micro-leakage is very complicated, especially for the initial stage. The location of the micro-leakage is concentrated in the directions of 1 o'clock, 4 o'clock, 7 o'clock and 11 o'clock along such edge of the end cap, therefore, the sealed end cover needs to be further improved. Additionally, the idea of this research work can provide a good basis and reference for the subsequent series of related airtightness studies.

1. Introduction
With the advent of China's aging era, the demand for pharmaceutical products has increased year by year. Among the many problems that arise, the storage of a large number of medical supplies is a very important link. Compared with the management system and storage environment, the airtight performance of the professional medicine box for direct packaging and storage of medicines becomes more important.[1] Therefore, planning a system for the automatic detection of the air tightness of medicine box is a very necessary work.

The key part of the system is related to the hydrodynamic behavior of the small leakage of the sealing gas and the change of the gas characteristic parameters. Since there are few existing studies in this area, and reference standards for gas sealing performance have not been established. The exploratory research in the early stage will be carried out here by means of Computational Fluid Dynamics (CFD), in order to reduce design costs and shorten the research period. The key detail structure of the air-tight medicine box is very important for the judgment of the sealing performance, especially for such as sealing gaskets. Consequently, the research work in this investigation will use CFD high-fidelity research based on Lattice Boltzmann Method (LBM). Additionally, the Wall-Adapting Local Eddy (WALE) viscosity model and the octree structure 3D scheme are also used in combination to adapt to complex geometric boundary conditions and improve the stability and accuracy of numerical computations.
2. Brief Description of Lattice-Boltzmann Method

The Lattice Boltzmann Method (LBM) is steadily becoming a relevant method for solving the fluid flow equations. Its direct connection to the kinetic theory of gases allows for a deeper understanding and more detailed modeling of physical phenomena. [3,4]

The common characteristic to the LBM models is that time-stepping model, based on a propagate-collide scheme, for such lattice discretization. The propagation step performed on a lattice enforces a constant timestep and a discrete set of velocities that ensure that such positions about particles motion is generally restricted to lattice coordinates. The set of velocities thus generates the lattice, in which the probability distribution functions for each lattice site are stored. [4]

For the continuum space with discrete velocities, the Boltzmann transport equation can be written as follows:

\[ \frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = \mathbf{\Omega}_i \]

Where \( \mathbf{\Omega}_i \) is the collision operator that computes a post-collision state that conserves mass and linear momentum. \( \mathbf{e}_i \) stands for velocity vectors, for which the discrete set of velocities has a common terminology refereed to the dimension. The number of velocity vectors \( D_nQ_m \), where \( n \) represents the dimension of a problem and \( m \) refers to the number of velocities direction.

For a two-dimensional model, the most common scheme is the D2Q9 model, involving 9 velocity vectors defined by:

\[
\mathbf{e}_i = \begin{cases} 
(0,0) & i = 0 \\
(1,0) & \text{or} \quad (0,1) & \text{or} \quad (-1,0) & \text{or} \quad (0,-1) & i = 1, 2, 3, 4 \\
(1,1) & \text{or} \quad (-1,1) & \text{or} \quad (-1,-1) & \text{or} \quad (1,-1) & i = 5, 6, 7, 8 
\end{cases}
\]

Where the above scheme is illustrated on Figure 1 below.

![Figure 1. D2Q9 Lattice model of velocities discretization](image)

For a three-dimensional model, the most scheme is the D3Q19 model, which involves 19 velocity vectors defined by:
Where the above scheme is illustrated on Figure 2 below.

![Diagram](image_url)

**Figure 2.** D3Q19 Lattice model of velocities discretization

Additionally, we can use the scheme D3Q27 for some more complicated flow situations, which can provide a higher number of velocity directions, and thus it will bring greater computational cost.

The \( f_i \) in equation (1) is Probability Distribution Functions (PDFs) for such discrete set of velocities in one lattice. If one were to assume that \( \Omega_i = 0 \), which means only a streaming operation would be performed. The discretized form on the lattice is as:

\[
\rho_{i} (r + e_i, t + dt) = f_i (r, t) + \Omega_i (f_1, \ldots, f_b) \quad (4)
\]

Where \( i = 1, \ldots, b \), in which \( b \) is the number of velocities direction of such applied lattice in CFD investigation. The stream-and-collide scheme of the LBM can be interpreted as a discrete approximation of the continuous Boltzmann equation.

As in the continuum Boltzmann equation, the macroscopic variables can be derived for the statistical moment of the PDFs:

\[
\rho = \sum_{i=1}^{b} f_i \quad (5)
\]

and

\[
\rho \vec{v} = \sum_{i=1}^{b} f_i \vec{e}_i \quad (6)
\]

Where such moment of zero-order corresponds to the macroscopic density, and the moments of first-order provide the momentum in the three directions. Additionally, the higher order quantities can be obtained using such further moments of the higher orders.
A Single-Relaxation Time (SRT) is based on the Bhatnagar-Gross-Krook (BGK) approximation, [5] which is used in the most common scheme:

$$\Omega_i^{BGK} = \frac{1}{\tau} (f_i^{eq} - f_i)$$  \hspace{1cm} (7)

Where $\tau$ is the relaxation time, and $f_i^{eq}$ is the local equilibrium function towards that the state is relaxed.

3. Brief Description of Working Principle and Program for Airtightness Testing

The automatic test system relies on positive pressure and holding pressure to realize such leak detection purpose. The double-layer sealing structure is used, and we use the compressed air as the working medium. By applying a certain degree of vacuum to the seal ring cavity and the seal outer cavity, relying on high-sensitivity flow sensors and pressure sensors, in conjunction with the measurement program, it can automatically determine whether the detection system seal is effective. The principle is shown in Figure 3.

**Figure 3.** Schematic diagram for the automatic test system of airtightness testing

The type of leakage mainly includes large leakage, small leakage and trace leakage, in which the leak rate is one of the very important parameters. The control flow of the automatic detection system is shown in Figure 4.

**Figure 4.** Control flow for such automatic detection system
By weighing the calculation accuracy and the amount of computation, this research work only conducts high-fidelity numerical calculations for the seal ring cavity and inside of the medicine box. The other parts are ignored for such sensors and the seal outer cavity, etc.

4. Numerical Computation Setup

4.1. Domain Division and Lattice Layout
The automatic detection system for air tightness of the medicine box, associating with the full-size integral high fidelity, is manifested in Figure 5 for the shape of the domain.

![Figure 5](image1)

**Figure 5.** The integral domain of medicine box air tightness test

Considering the improvement of computing efficiency, the resolved scale of overall situation is set to 0.032 m. At the same time, the adaptive refinement is adopted, in which the walls of the sealing cap and red marked sealing ring have a more refined scale of 0.004 m, relative to the overall size of the ring cavity of 0.54×0.46×0.44, approximately, in units of meters. Consequently, the square-lattice layout is displayed in Figure 6, with the number of transition levels 4.

![Figure 6](image2)

**Figure 6.** The square-lattice layout for integral domain of detection for air tightness
The white outline in Figure 6 is the solid area of the medicine box shell, which does not participate in numerical calculations. The numbers of corresponding lattice from Level 1 to Level 4 are 2482, 7748, 23166, and 121503, respectively.

4.2. Solution Settings
The turbulence model employs Wall-Adapting Local Eddy (WALE) model, which has good properties both near to and far from the wall and both for laminar and turbulent flows. This model recovers the asymptotic behavior of the turbulent boundary layer when this layer can be directly solved.

The initial pressure in the ring cavity is set to -0.095 MPa, and other domains maintain the ambient atmospheric pressure, by using the topological mapping function. The density of this standard air is 1.225 kg/m$^3$, and the corresponding dynamic viscosity is 1.789 Pa·s. Considering the influence of computing efficiency and grid independence, the transient iterative calculation timestep is used by $7 \times 10^{-5}$ s. The type of the walls for the ring cavity and sealing-cap components are all set to isothermal condition, avoiding internal energy transfer for being closer to the actual situation.

5. Numerical Results
The most critical parameter characteristics is the static pressure history variation for the air tightness detection system of medicine box. Using the Boolean operations defined by topological geometry, we can extract the corresponding calculation data, as shown in Figure 7.

![Figure 7. Ring cavity average static pressure history variation of air tightness detection system](image-url)

According to Figure 7, we can find that after about 5.24 s, the stable value of the average static pressure of the ring cavity remains at about -9414 Pa. This stable trend appears after about two seconds, and this earlier change feature can be roughly divided into two stages. The first is the initial stage of very rapid changes at the level of static pressure, and the second is a gradual and slowly changing stage like a parabola.

Through the above analysis, we can speculate that the slit flow in the early stage of micro leakage is very complicated, especially for the initial stage. The characteristics of subsequent hydrodynamic changes gradually tend to be stable and small.

In order to further visualize the early hydrodynamic characteristics for the slit flows, we give the corresponding velocity field distribution results, which is displayed in Figure 8.
According to Figure 8, the very obvious feature is presented for leakage location and morphology. Since the geometric model of the numerical calculation is based on the scanned file of the actual sample, the location and orientation of the micro-leakage obtained by the calculation have a good practical reference value. From the results for velocity field, the location of the micro-leakage is concentrated in the directions of 1 o'clock, 4 o'clock, 7 o'clock and 11 o'clock along such edge of the end cap. The maximum leak velocity value reached about the level of 7.65 m/s.

Therefore, the sealed end cover needs to be further improved at the above location to improve the overall airtightness of the medicine box.

6. Conclusion
In this investigation, the high-fidelity CFD study is performed for the automatic detection system for air tightness of the medicine box, using the LBM algorithm. Considering the complexity of the flow on the wall of the gap, the WALE model is also adopted.

The high-fidelity calculation results show that after about 5.24 s, the stable value of the average static pressure of the ring cavity remains at about -9414 Pa. The slit flow in the early stage of micro leakage is very complicated, especially for the initial stage.

Additionally, the location of the micro-leakage is concentrated in the directions of 1 o'clock, 4 o'clock, 7 o'clock and 11 o'clock along such edge of the end cap, therefore, the sealed end cover needs to be further improved for strengthening the airtight performance of this medicine box.

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