Numerical Simulation and Experiment of Gas Mass in pVTt Standard Container under Isothermal Boundary Condition

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Abstract

Focusing on a 36m^3 horizontal pVTt standard container, the intake process and homogeneous process of the gas in the container were numerically simulated in constant wall temperature and constant velocity as the inlet boundary condition. A new algorithm for calculating the average temperature in the standard pVTt container was proposed, whose name was mass temperature average. The simulation results showed that in the natural convection process after gas intake, the average mass temperature $\widetilde{T}$ of the gas in the container slowly decreased with time in parabolic shape and tended to wall temperature, while the average pressure drops sharply and quickly reached uniformity. Through numerical simulation and experimental verification, it was found that the gas mass in the container was linear with ln $\widetilde{T}$.

1. Introduction

The gas calibration facility to pVTt technique mostly uses a horizontal standard container. The container needs to be pumped and inflated when a sonic nozzle is calibrated on the facility. The temperature and pressure of the gas in the vessel are stable and uniform after the gas undergoes a long period of natural convection in the vessel.

Two methods are generally used to shorten the time when the temperature field in the standard container reaches a stable and uniform state: water bath or oil bath cooling[1-2].

For example, NMIJ from Japan uses the interlayer water bath constant temperature cooling method in pVTt container, which eliminates the seasonal influence and time-varying characteristics of environmental temperature gradient. The stabilization time is about 30 minutes, and the uncertainty of the facility is better than 0.05% (k=2) [3].This is also the method commonly used in China today.

The other one is to install a fan and air duct in the container [4] to force the gas in the container to convective movement. For example, a high-flow pVTt standard container in NIST is equipped with air ducts and agitator fans, while the gas reaches a stable state after being forced convection heat transfer for 45 minutes, and the uncertainty of the facility is 0.13% (k=2)[5-6].However, due to the heat of the fan itself and the influence of the ambient temperature, the gas stability effect in the actual measurement does not achieve the desired effect.

However, the methods above cannot completely avoid the influence of temperature inhomogeneity caused by intake and exhaust. So the scholars use numerical simulation technology to study the uncertainty characteristics of temperature field.

For example, Lihong Yang[7] of Shanghai Jiao Tong University used software FLUENT to numerically simulate the deflation process of empty containers and isothermal vessels, and obtained the velocity field distribution, temperature field distribution and their variation law during deflation. Ruiqin Bai et al [2] from Zhe Jiang institute of econometrics used software FLUENT to carry out unsteady simulation research on the temperature field characteristics of pVTt method facility under natural environment and constant temperature of water bath. They concluded that the stable time of constant temperature of water bath is shorter than that of natural environment, and they gave the idea of temperature measuring point layout. Xuening Zhao[8], from Shanghai University of Science and Technology, has carried out numerical simulation on the process of inlet and exhaust of pVTt standard container under two boundary conditions of adiabatic wall and constant temperature wall. The results show that under the condition of adiabatic wall, the stable time of gas temperature in the container is shorter.

Most of the literatures above only discussed the temperature field and pressure field in the pVTt container, but did not directly discuss the mass (or mass distribution) of the gas in the container.

In this paper, the numerical simulation model is optimized to explore the gas mass distribution law and internal relations in the container. Under the condition of constant wall temperature, the natural convection process of the air in a horizontal pVTt standard container with a volume of 36 m^3 was simulated, and the distribution cloud chart of the temperature and pressure of the air in the container was obtained. A new temperature averaging method, namely "mass average temperature $\tilde{T}$ ", is proposed, and the functions of $\tilde{T}$ ~t 、 p~t and $p/\tilde{T}$ ~Ln $\tilde{T}$ are obtained. The numerical simulation shows that $p/\tilde{T}$ is inversely proportional to Ln $\tilde{T}$. The 30 sets of experiments were carried out during the intake and natural convection processes of the facility. The experimental data were used to fit the trend curve, and the correctness of the inverse proportional linear relationship obtained via the numerical simulation was verified.

2. Working Principle

During the time interval $\triangle t$, the pVTt standard container of volume V is evacuated and inhaled, and when the process is completed and the temperature and pressure are both stable and uniform, the temperature T and the pressure p of the gas in the vessel are respectively measured. Regardless of the compression factor and the container temperature correction, the mass flow rate q_m of the gas flowing into the standard vessel can be calculated based on the ideal gas state equation.

$$q_m=\frac{\Delta m}{\Delta t}=\left(\frac{V}{R/M}\right)\left[\left(\frac{p}{T}\right)_2-\left(\frac{p}{T}\right)_1\right]\Big/\Delta t \tag{1}$$

Where R is the universal gas constant and M is the molecular weight of the gas, so $\left(\frac{V}{R/M}\right)$ is a constant. So, $(p/T)_2-(p/T)_1$ can qualitatively represent the mass of the gas in the container.

3. Governing Equation

By establishing the governing equation and solving the change of the air temperature T and the pressure p in the container over time after air intake, the internal relation between the gas mass in the container and the average temperature in the changing container were found. In theory, the average temperature of the gas in the vessel gradually approaches the wall temperature due to the boundary conditions of constant wall temperature.

Assuming that the air is a viscous compressible ideal gas, the continuity equation, the momentum equation and the energy equation are satisfied in the process of natural convection.

Continuity Equation

$$\frac{\partial\rho}{\partial t}+\nabla(\rho\vec{u})=0 \tag{2}$$

Where, ρ is the density of air (kg/m), t is time (s), $\vec{u}$ is the velocity of air (m/s).

N-S Equation

$$\rho\frac{D\vec{u}}{Dt}=\rho\vec{F}-\nabla p-\nabla\left(\frac{2}{3}\mu\nabla\bullet\vec{u}\right)+\mu\Delta\vec{u} \tag{3}$$

Where, μ is the aerodynamic viscosity coefficient (Pa.s), p for pressure(Pa).

Energy Equation

$$\rho c_v\frac{DT}{Dt}=-p\nabla\bullet\vec{u}+\nabla\bullet(k\nabla T)+\rho q \tag{4}$$

Where, c_v is the specific heat at constant volume J/(kg·K), T is the thermodynamic temperature in units (K), k is the thermal conductivity W/(m·K), q is the heat given by the heat source to the fluid per unit mass in unit time, $-p\nabla\bullet\vec{u}$ is the work done by the normal pressure p when the air volume is deformed relative to the line, and the item $\nabla\bullet(k\nabla T)+\rho q$ is the heat intake for other reasons such as heat radiation and heat conduction.

In the equations (2)~(4) above, there are six physical quantities(ρ, $\vec{u}$,T, p, etc.) unknown.. But there are only five equations. In order to make the system closed, we need to add an equation of state.

Ideal gas equation of state

$$pV=m\left(\frac{R}{M}\right)T \tag{5}$$

Where m is the air mass (kg), M is the average molar mass of air (kg/mol), R is the general ideal gas constant J/(mol·K) and V is the standard volume (m^3) of the vessel. At this point, all the equations are closed.

4. Mass average temperature

At present, in the calibration practice, n temperature sensors are arranged in the standard container, and the n temperature sensors are processed by arithmetic mean, which is

$$T = \frac{1}{n}\sum_{i=1}^{n} T_i$$

The obtained T is substituted into the formula (1) to calculate the gas mass. When the temperature of the gas in the vessel is uniform, the gas mass can be calculated with the arithmetic mean temperature to obtain a sufficiently accurate gas quality.

We believe that it is meaningless to perform arithmetic averaging of n temperature sensors when the temperature in the vessel has not reached uniformity. However, each temperature sensor can be used to calculate the mass of the gas in the vicinity of the temperature sensor. Assuming that the sensors are evenly distributed in the container, the gas mass in the 1/n region near each temperature sensor can be expressed as

$$m_i = \frac{p\left(V/n\right)}{\left(\frac{R}{M}\right)T_i} \tag{6}$$

Where p is the uniform and stable gas pressure. The total mass of the gas in the container is

$$m = \sum_{i=1}^{n} m_i = \frac{pV}{\left(\frac{R}{M}\right)}\left(\sum_{i=1}^{n}\frac{1}{T_i}\right)n^{-1} \tag{7}$$

Define

$$\tilde{T} = n\left(\sum_{i=1}^{n}\frac{1}{T_i}\right)^{-1} \tag{8}$$

The temperature expressed by the formula (8) is referred to as "mass average temperature".

According to the calculation, when the temperature unevenness deviation is 10K at 293K, the calculation of the gas mass in the container by the "mass average temperature" can improve the calculation accuracy by 0.03% compared to the arithmetic average temperature calculation method. The larger the deviation of temperature uniformity, the larger the deviation of gas mass calculated by arithmetic mean temperature. Unless otherwise stated herein, mean temperature means "mass average temperature ".

5. Modeling and boundary conditions

5.1 Modeling and grid generation

The physical model is a horizontal pVTt standard container with a diameter of about 2.2m and a total volume of about 36m^3. The inlet pipe has a diameter of 150mm and is located at the side of the horizontal tank, as shown in Figure 1.

Considering the advantages of fast generation of the structured mesh, the good mesh quality, and the easier convergence of calculations, structural meshing is used. Among them, the middle cylinder part is divided into hexahedral meshes, and the hemispheres on both sides are divided into tetrahedral meshes. In order to achieve better grid accuracy and a calculation speed, the left and right hemispheres, the air inlet, the inlet pipe and the cylinder connection part and the vicinity of the container are all encrypted.

The number of grids calculated by the container is about 3.5 million. The mesh quality parameter of more than 88% is greater than 0.85, the total mass parameter of the grid is greater than 0.6, the minimum angle is ≥45°, and the number of negative grids is 0. The container 3D model and its meshing are shown in Figure 1.

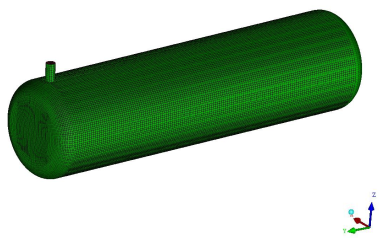

Figure 1: 36m^3 horizontal pVTt standard container model with grid division.

5.2 Control parameters and boundary conditions

In this paper, the pVTt standard container calibration process is simulated, that is, in the process of air inlet, after the calibration is completed and the valve is closed, in the process of natural convection of the gas in the container, the air temperature and the pressure in the container change over time, which belongs to unsteady, viscous compressible gas flow. The coupling, density-based and absolute velocity implicit transient solver is used in CFD calculation. The governing equations described in the third part of the paper are used, and the Realizable *k-ε* turbulence model is used. The medium is air and satisfies the ideal gas state equation. In addition, considering the influence of the gas mass force, a negative gravitational acceleration is added to the z-axis.

The wall surface of the container satisfies the condition of no slip boundary; the temperature of the wall surface of the vessel and the initial temperature of the container are both set to 297.3 K, which is consistent with the measured temperature; the initial pressure is 0.1 kPa, that is, the gas state after the end of the pumping and stabilization.

The inlet process was set as the boundary condition of the inlet with a constant flow rate, and the air flow rate was 0.284m^3/s, that is, the velocity of flow of the inlet air was 16.082m/s, which was also consistent with the actual flow rate of the sonic nozzle tested.

6. Numerical simulation and analysis

Due to space limitations, this article only describes the process of gas convection after the gas enters the container. Among them, the intake end time is taken as the initial state of the natural convection process.

From the ideal gas state equation, the gas temperature deviation is 0.5K at 20°C and the gas mass will produce a calculation error of 0.17%. When the pressure deviation is 10Pa, the gas mass will produce a calculation error of 0.02%. For the actual measurement practice, ignoring the sensor error, it is obvious that the temperature and pressure unevenness deviation should be as small as possible, for example, the temperature uniformity is controlled to be 0.1K and the pressure unevenness is controlled within 5 Pa.

In order to shorten the calculation time, when the average temperature difference in the container is less than 0.5k and the pressure difference is less than 10Pa, it is deemed that the average temperature and the pressure in the container have reached a uniform state, and the calculation is completed.

6.1 Intake Process

When the intake is about 1 minute, close the valve and the intake is over. When the valve closes, the temperature distribution cloud in the standard container is shown in Figure 2.

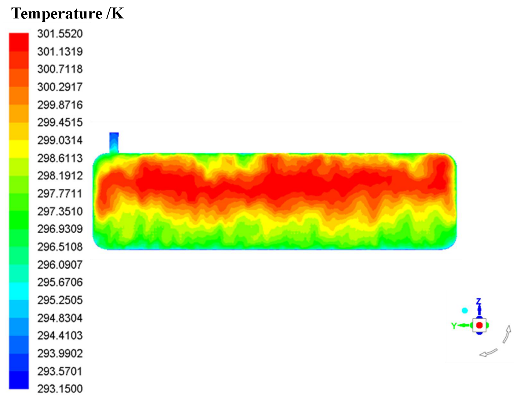

Figure 2: Cloud diagram of gas temperature distribution in the longitudinal section of the container at the end of inlet.

As can be seen from Figure 2, the temperature difference of the air in the container at the end of inlet is >8K.The temperature along the axial direction (x axis) of the container presents a zonal distribution, indicating that the temperature gradient in this direction is not obvious. And along the vertical direction of the container (that is, along the diameter of the container), there is a large temperature gradient. Because of the constant wall temperature, the gas temperature near the wall is low.

Due to the continuous filling of low-temperature air in the intake process, the inlet pipe temperature is relatively low. The gas temperature in the area where the inlet pipe is connected to the container is higher, which is due to the large flow rate of air filled and the violent movement of gas molecules. It can also be seen from Fig. 2 that the temperature in the hemisphere region at the left and right ends of the container is high due to insufficient heat exchange of the air; and because the density of the hot air is small, the temperature in the upper region of the container is also high.

6.2 Natural Convection Process

When the intake valve is closed, natural convection occurs in the air in the container. The numerical simulation shows that after about 10 minutes of convection heat transfer, the average temperature and the pressure of the air in the container are basically stable.

Figure 3 is the temperature distribution cloud diagram after the air in the container is basically uniform.

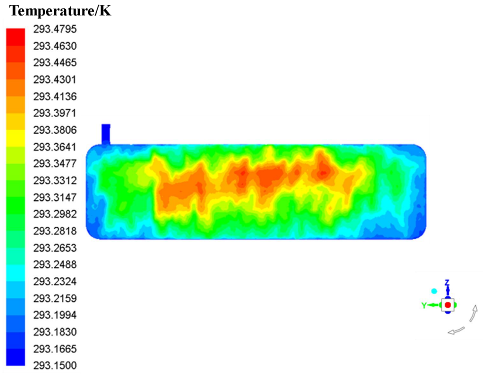

Figure 3: Temperature distribution cloud diagram after uniform air intake.

It can be seen that when the temperature field is in a stable state, it is symmetrically distributed along the axis of the container (x axis), and the maximum temperature difference in each region is < 0.3K. After the stability of convection heat transfer, the average temperature of the air in the container is close to the wall temperature. The isotherm is a circle along the axis of the container, and the temperature in the middle region is slightly higher than that in other regions.

Figure 4 is the pressure distribution cloud diagram after the air in the container is basically uniform.

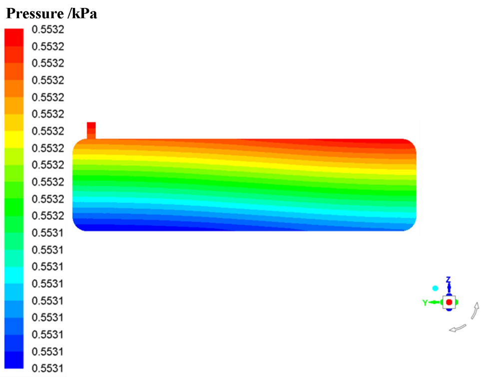

Figure 4: Cloud diagram of pressure distribution after uniform air intake.

It can be seen that when the pressure field is in a stable state, the pressure in the container presents a stratified and zonal uniform distribution.

7. Gas Mass Analysis and Experiment

The mass of gas in the vessel is calculated by determining the temperature and the pressure of the gas in the vessel. Figure 5 shows the comparison between the simulated and experimental results of the curve of the average temperature $\tilde{T}$ of air in the container with time t in the process of natural convection.

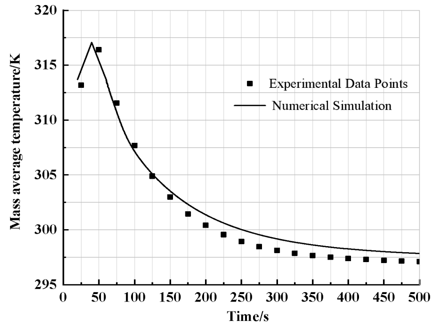

Figure 5: Curve of average temperature change of mass in homogeneous process.

According to the observation curve and the experimental results, the average temperature of the air in the container at the end of inlet is about 300.6K. At the beginning of natural convection, the mean temperature rises slightly and then decreases monotonously. At about 500s, the temperature field in the container is basically stable, and the average temperature tends to the wall temperature of 297.3K. This shows that the constant wall temperature condition can promote the natural convection of air in the container, effectively inhibit the fluctuation of the temperature field, and accelerate the temperature field to reach a uniform state.

Figure 6 is a graph showing the average pressure p of the air in the container during the natural convection process as a function of time t.

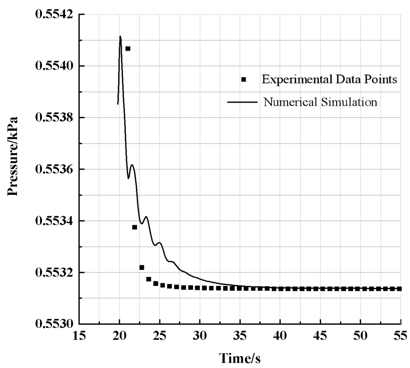

Figure 6: Curve of mean pressure change in uniform process.

It can be seen that in the early stage of natural convection, the average pressure fluctuation in the container fluctuates frequently and monotonously drops sharply, and then gets steadily and slowly.

The pressure field in the container is basically stable at about 35s and the average pressure at the time of stabilization tends to 0.5531 kPa.

The numerical simulation data in the uniform process is used to make a relationship between $p/\tilde{T}$ and Ln $\tilde{T}$, as shown in Figure 7.

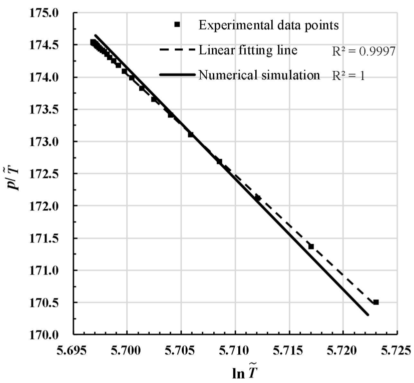

Figure 7: Numerical simulation results of the relationship between $p/\tilde{T}$ and Ln $\tilde{T}$ in a homogeneous process.

It can be seen that $p/\tilde{T}$ representing the mass of the gas is inversely proportional to Ln $\tilde{T}$ .The horizontal standard vessel was tested in a constant temperature environment. In the experiment, the temperature values of 40 temperature sensors and the average pressure at the recording time were recorded every 1 minute. Thirty experiments were carried out over a period of two months.

The relative error statistics of 30 groups of experimental data and simulated values are shown in Figure 8.

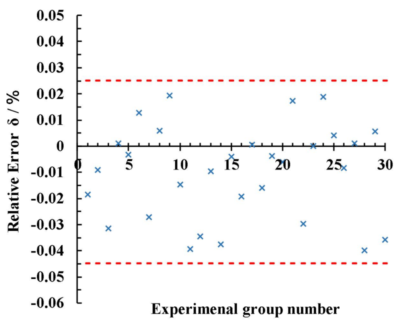

Figure 8: Relative error statistics of 30 groups of experiments.

By calculating the relative error between the theoretical linear equation and the experimental data, the absolute value of the average relative error is about $|\bar{\delta}|$ ≈ 0.0158%, of which the experimental data of 15 groups is $|\delta|$ < 0.0098%.

It can be seen from the Figure 8 that the error of the experimental data of a small group is >0.04%, which is due to the unstable water temperature of the container spacer during the experiment.

8. Conclusion

Under the condition of constant wall temperature, numerical simulation and experiment were carried out on the process of natural convection and air inlet of the 36m³ pVTt standard container, and the following conclusions were obtained：

(1) The algorithm of vessel mass average temperature is derived. The calculation precision of gas mass can be improved by using mass average algorithm compared with arithmetic average algorithm.

(2) In the process of natural convection, it is verified by numerical simulation and experimental data that $p/\tilde{T}$ and Ln $\tilde{T}$ satisfy the inverse proportional linear relationship, and the average relative error between the simulated theoretical value and the experimental results of the 30 groups is about 0.0158%.

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