Finite Element Analysis of Reaction Vessel for Measuring the Solubility of Supercritical Carbon Dioxide

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Abstract. The thermal-structural coupling analysis of the pressure vessel are carried out by the finite element method to verify its safety, and the stress section are linearized. The results show that the analysis value of the temperature value of the vessel cavity are basically consistent with the change trend of the measured value, and the steady state error are only 2.7%; there is a large stress concentration at the opening of the upper window, and the maximum coupled stress value of the internal surface is 176.2 MPa. The maximum stress path is evaluated based on the analytical design standard JB4732-1995, and the structure satisfies the strength requirement.

Introduction

The reactor is an indispensable pressure equipment in the production process of reaction, heat transfer, mass transfer and separation [1]. In order to determine the solubility of supercritical CO2 in crude oil, a set of measuring devices was designed, which working normally under high temperature and high pressure conditions of 30 MPa and 150 °C. The reactor is subjected to the mechanical stress and the thermal stress during the working process [2]. There is a high concentrated stress in the opening or other discontinuous structure of the kettle body, which may cause cracks or even failure of the reactor [3,4]. There are three main types of hazards caused by reactor failure: 1) shock wave damages equipment and buildings, causing casualties; 2) debris injures people or penetrates equipment and construction; 3) medium overflow in the kettle causes poisoning, burning, and explosion [5].

In this paper, ANSYS Workbench was used to perform thermal-structural coupling analysis on the finite element model of the reactor, and obtained the temperature distribution and coupled thermal-stress distribution of the kettle, which provided a theoretical basis for ensuring the safety and reliability of the reactor.

Establishment of Finite Element Model

Three-dimensional model of the pressure vessel

The 3D model of the reaction vessel is shown in Figure 1(a), the main components of the reactor are: 1.ball stop valve, 2.fixed seat, 3.upper window, 4.upper window buckle, 5.upper window firmware, 6. kettle body, 7. front window firmware, 8. front Windows, 9. front window buckles.

(a) Three-dimensional Model (b) Finite Element Model of Meshing

Figure 1. Pressure Vessel Model.
Meshing

The mesh quality of the element model largely affects the accuracy of the analysis results. Automatic method was adopted for the reactor body and the window components; and the ball stop valve and the fixed seat adopted Hex Dominant method based on hexahedron. The meshed finite element model is shown in Figure 1(b). There are 79,590 elements and 136,863 nodes in the meshed model.

Material Parameters

Sapphire was selected as the window material of the vessel, and other components were made of 304 stainless steel. The material parameters of the finite element model are shown in Table 1.

| Material      | Density [Kg/m³] | Thermal Conductivity [W/(m°C)] | Specific heat capacity [J/(kg°C)] | Thermal expansion coefficient [10⁻⁶/°C] | Elastic Modulus [GPa] | Poisson’s ratio |
|---------------|-----------------|-------------------------------|----------------------------------|----------------------------------------|-----------------------|----------------|
| stainless steel | 7930            | 17.2                          | 502                              | 16.8                                   | 194                   | 0.285          |
| Sapphire      | 3980            | 25.12                         | 761                              | 5.8                                    | 435                   | 0.28           |

Load and Boundary Conditions

Temperature Load

In order to avoid excessive thermal stress caused by drastic changes in temperature, the heating holes were heated in stages: the initial temperature of the vessel was 25°C, the first stage was heated up to 60°C in 15min, held on 20min; the second stage was heated up to 100°C in 25min, held on 20min; the third stage was heated up to 150°C in 40min, held on 120min.

Convection Heat Transfer Coefficient

The heat conduction between the insulation layer and the reactor is regarded as heat conduction in the closed cylinders sandwich, which the gap δ between the external surface of the vessel and the internal surface of the insulation layer is uniform. The external surface temperature of the vessel is \( T_1 \) and the internal surface temperature of the insulation layer is \( T_2 \). The measured values of \( T_1 \) and \( T_2 \) were 150°C and 110°C when the temperature of the vessel was balanced. At this time, the temperature difference was \( \Delta T=40°C \). From the qualitative temperature \( T=(T_1+T_2)/2=130°C \), the air physical parameters are as follows: \( Pr=0.685, \nu=2.663\times10^{-5} m^2/s, \lambda=3.42\times10^{-2} W/(m°C) \).

The calculation formula of Grashov number is [6]:

\[
Gr = \frac{g\alpha_v\Delta T\delta^3}{\nu^2}
\]  
(1)

Where: \( g \) is gravity acceleration, 9.81m/s², \( \alpha_v \) is volume expansion coefficient, generally taking \( 1/(273+T) \).

According to \( Gr \) and \( GrPr \), it is found that the correlation of natural convection heat transfer criteria of air in the cylindrical sandwich of limited space is [6]:

\[
N_u = 0.11(Gr_Pr)^{0.29}
\]  
(2)

The formula for calculating convective heat transfer coefficient is [6]:

\[
h = \frac{N_u\lambda}{\delta}
\]  
(3)

Combined with (1)(2)(3), the convective heat transfer coefficient was calculated to be 2.54W/(m²•°C). Therefore, the convective heat transfer coefficients on the external surfaces of the vessel was set to 2.5 W/(m²•°C).

Pressure Load and Constraint Conditions

The temperature field distribution result of the pressure vessel obtained by the transient temperature analysis is introduced into the structural analysis module as a temperature load. A design stress of 30 MPa was applied to the wall surface of the vessel cavity; the cylindrical surface of the reactor holder was set as a fixed constraint. Finally, the coupled thermal stress of the vessel is solved.
Results and Analysis

Results and Analysis of Temperature

According to the analysis results, the temperature field distribution of the cross section along the axis of the reactor is shown in Figure 2 (a), and the temperature of the vessel body gradually decreases from front to back. The maximum temperature is 150 °C, located in the heating hole, and the minimum temperature is 140.7 °C, located at the end of the vessel cavity. The vessel is manually pressurized by a pressurized plunger. The maximum effective space in the cavity is the area shown in Figure 2(b). The temperature range of this zone is 147.3 °C~149.6 °C. During the experiment, the magnetic stirrer was set to ensure that the reaction medium was heated uniformly.

The temperature of the vessel cavity temperature measuring hole (shown in Figure 1) was displayed and recorded in real time by WEST/P6100 temperature controller, which measured by J-type temperature sensor. The measured temperature is compared with the temperature obtained by transient temperature analysis. As shown in Figure 3, the measured temperature reached its peak value at the end of three heating stages, respectively. At the temperature holding stage, the temperature decreased due to the hysteresis of the temperature control system. The maximum temperature difference between the simulated temperature and the measured temperature occurred at the end of the third stage of heating, which was 8.9°C. The steady measured temperature of the vessel chamber was 153.7°C, and the relative error was only 2.7% compared with the steady simulated temperature of 149.6°C. The simulated temperature of the vessel chamber was basically consistent with the measured temperature.

Results and Analysis of Thermal-Stress

Figure 4(a) shows the coupled thermal-stress distribution nephogram of the reaction vessel. The coupled thermal-stress decreased gradually from the internal surface to the external surface, and there was a large concentrated stress at the opening of the upper window. The stress dangerous section was along the axis. It was showed that the maximum coupled thermal-stress occurred at the opening of the upper window in Figure 4(b), which was 176.2 MPa, and the stress decreased gradually from the stress concentrated point to the adjacent area. According to the mechanical design manual, the ultimate stress $\sigma_t$ of 304 stainless steel is 137 MPa. Therefore, the strength of the stress concentrated area was checked by the analysis and design standard JB4732-1995 based on the elastic-plastic failure criterion[7].

![Temperature nephogram of vessel](image1)
![Temperature nephogram of maximum stress region](image2)

Figure 2. Temperature Field Distribution of the Vessel.

Strength Check

For performing stress analysis and strength check on the dangerous section in the coupling analysis result, two paths 1-1 and 2-2 through the wall thickness are set at the stress concentration point of the upper window opening (shown in Figure 4(b)). As shown in Figure 5, stress linearization is performed on the two paths to obtain local film stress $PL$, bending stress $Pb+Q$ and local film stress + bending stress $PL+Pb+Q$ along the path. The results show that the main stress along the two paths is the local film stress, and the bending stress caused by the deformation of the local discontinuous structure deteriorates the stress of the internal surface. This paper does not consider the fatigue damage caused by peak stress.
Table 2. Maximum Stress for Each Path (MPa).

| path | \( P_L \) | \( P_{L} + P_{b} + Q \) | region         |
|------|---------|----------------|----------------|
| 1-1  | 158.7   | 173.3          | Internal surface |
| 2-2  | 163.9   | 182.2          | External surface |

Table 2 shows the result of maximum stress of each path after linear treatment. The allowable stress of the material was selected as the reference strength limit \( S_m \) for stress analysis. According to the allowable limits of different kinds of stresses and combined stresses, the \( P_L=163.9 \text{MPa} < 1.5S_m=205\text{MPa} \) and the \( P_L+P_{b}+Q=182.2\text{MPa} < 3S_m=411\text{MPa} \) in the maximum stress path 2-2. Therefore, the reaction vessel is safe and reliable.

**Conclusion**

1. The simulated temperature of the vessel cavity was basically consistent with the measured temperature, and the stable temperature error was only 2.7%, which indicates that the temperature analysis was reasonable and effective.
2. There was a maximum stress value of 176.2 MPa at the opening of the upper window, which was much higher than the stress intensity away from the area, indicating that there was stress concentration at the opening of the upper window, and the dangerous section was a cross-section of the axis.
3. The stress linearization treatment of the maximum stress path 2-2 showed that the maximum PL value was 163.9 MPa, which was less than the allowable limit of 1.5 Sm; the maximum PL+Pb+Q value is 182.2 MPa, which was less than the allowable limit of 3 Sm. Therefore, the reactor structure meted the safety standards for analytical design.

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