Design of Quartz Chemical Delivery Parts for High Temperature Vacuum Chambers Based on Simulation Results

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1 Introduction

Many of today’s technologies and research techniques depend on process and methods in high and ultra-high vacuum. High temperature vacuum chambers require creative design and use of exotic materials in design to achieve quality performance. In order to obtain good performance, the temperature and gas delivery on the vacuum chamber surface must be uniformly distributed. In this work, a new funnel for high temperature vacuum chamber was successfully designed and tested using computer-based simulation techniques. The funnel was made of quartz crystal due to ability to absorb temperature, properties of low gas permeability and low temperature coefficient. In order to mitigate O-rings from high temperature failure and to reduce non-uniformity effect during temperature delivery, a new quartz funnel was developed. The simulation and experimental results show that uniformity distributions in temperature of vacuum chamber surface were obtained with new funnel design.

Keywords: High temperature Vacuum Chambers, computer simulation, quartz crystal to absorb temperature.

1 Introduction

Computer-based simulations program are extensively used across all fields of science to model real systems and their responses. As computing power becomes cheaper and commercially available software becomes more powerful, application of simulation models became widespread in science and engineering fields. Simulation and analysis programs are helpful to determine the optimum design parameters in the early stage of problem solving. The funnel is one of the most important parts of high vacuum chamber due to gas inflow region. In the literature, many funnel design studies have used computational modelling to optimize temperature delivery. Vacuum chamber designers should have the knowledge of the funnel thermal performance which will enable him to find efficient means to eliminate some of the problems and also to avoid the costly post construction additions and changes. High quality vacuum chambers are very important to the equipment’s performance under different vacuum condition during the process. Traditionally, vacuum chambers and their parts are made of variety of metals [1] but, high temperature vacuum chambers require use of exotic materials in design to achieve quality performance.
Table 1: Material properties of the fused quartz (SiO$_2$).

| Property                        | Value                                      |
|---------------------------------|--------------------------------------------|
| Quality Grade (Type 214)        | 2                                          |
| Apparent porosity (%)           | 0                                          |
| Density (g cm$^{-3}$)           | 2.2                                        |
| Melting point ($^\circ$C)       | 1715                                       |
| Thermal Conductivity (W m$^{-1}$ K$^{-1}$) | 1.46 @ 20$^\circ$C                      |
| Coefficient of thermal expansion ($\times10^{-6}$ K$^{-1}$) | 0.54 @ 20-1000$^\circ$C               |
| Coefficient of absorption (±max at 2800 nm), cm$^{-1}$ | 0.045                                     |

Hence, the funnel was made of quartz crystal due to properties of ability to absorb temperature and low temperature coefficient.

This paper describes a simple new high vacuum chamber funnel design using computational modeling of temperatures on and around the funnel. The aim of this paper was to achieve quality performance and obtain uniformly temperature distribution of vacuum chamber with design of a new quartz funnel including its temperature properties in the heater temperature range from 300 $^\circ$C to 650 $^\circ$C through simulation analysis.

2 Material Selection

Quartz crystal is an interesting and a remarkable material for design in diverse fields. The mechanical, physical and chemical properties of quartz crystal make it suitable for many uses. It is one of the common allotropes of silicon dioxide (SiO$_2$) and the most abundant mineral in Earth’s crust. Compared to other materials, it exhibits several unusual properties; including pressure, induced amorphization, low thermal expansion, ability to absorb temperature, high pressure and temperature phase transitions, frequency stability, anomalous elastic properties, soft mode behavior [2, 3]. Quartz in its various crystalline and amorphous forms finds several industrial applications including being a raw material. SiO$_2$ occurs naturally as sand or rock, and when melted, the resulting product is called fused quartz. Fused quartz is very pure, has a high chemical resistance, good thermal shock resistance and is very strong in compression.

Quartz crystal has a very low thermal expansion coefficient and can easily withstand quick changes in temperature. Also, it is very stable in varying temperatures, especially at atmospheric temperatures and pressures. The temperature coefficient is specified in units of parts per million over the operating temperature change. In this paper, in order to mitigate O-rings failure from high temperature and to reduce non-uniformity effect during temperature delivery, the funnel was made of fused quartz crystal (Type 214) due to ability to absorb temperature, properties of low gas permeability and low temperature coefficient. Material properties for the fused quartz (SiO$_2$) are given in Table 1 [4].

3 Design Rules for Vacuum Chamber

Vacuum chambers are commonly used in analytical applications and manufacturing process. The design of a vacuum chamber is critical to its ability to achieve and maintain contamination-free vacuum at high vacuum levels. The criteria are generally taken into consideration for the vacuum chamber and the design is realized within this framework. In order to achieve a significant leap in vacuum performance, the design requirements of a vacuum chamber must be clearly defined. Huntington designed an ultra-high vacuum, low-cost universal vacuum chamber suitable for a variety of research experiments including surface science. The chamber was made from stainless steel with a 14 inch nominal diameter [5]. Hauviller [6] designed an ultra-high vacuum and offered the methodology, methods and hints for designing vacuum chambers with his work. Owing to the high temperature vacuum chamber design requirements, its components should be designed according to the several boundary conditions [7-9]. Materials of vacuum parts, operating pressure and temperature, environmental conditions and minimum virtual leaks criteria are important in high vacuum design. To determine the ambient pressure and temperature are clearly the first step. The subsections are not necessarily exhaustive, but the list
of physical phenomena influencing the design of vacuum chambers is probably complete. Parts that will be inside the chamber should be made of low out gassing materials, and should be cleanable and bakeable to very high temperatures. Dimensional stability of the chamber is of fundamental importance for establishing base pressures and obtaining temperature integrity. Dimensional stability usually equates to chamber rigidity and there is a hierarchy of basic chamber shapes in terms of this rigidity. In the physical design of interior high vacuum chamber systems, high temperature gradient occurrence must be avoided or at least it must be minimized. High temperatures are sources of low temperature coefficient that are physically trapped within the vacuum chamber. Hence, the funnel was made of quartz crystal because of its low gas permeability [10-12].

The chamber must be designed to obtain good performance with uniformly distributed temperature and gas delivery on the vacuum chamber surface. Uniformity of temperature on funnel surfaces is important for efficient O-ring characteristics. Therefore, in vacuum chamber design, minimization of chamber parts and chamber surface with uniform temperature distribution are essential.

4 Design and Simulation Results of Vacuum Chamber

4.1 Design of New Vacuum Chamber

A description of a new vacuum chamber design for controlled studies of funnel is presented. The aim of new design is to mitigate O-rings from high temperature failure and overall improvement of the funnel design and its serviceability. The funnel was made of fussed quartz crystal due to properties of low gas permeability and absorption coefficient. Quartz funnel mounted on closed lid plate and heater blanket is used in order to control temperature distribution. Kalrez 7075 O-rings are also used between chamber bodies due to properties of improved thermal resistance that extends maximum service temperature to 327 °C (see Figure 1). For efficient heating a 2 kW heater was used. We simulated the temperature distribution on and around the quartz funnel when the heater is controlled at temperature range from 300 °C to 650 °C at 1 atm external pressure and room temperature. Axi-symmetric model is considered and 2D axi-symmetric thermal simulations are carried out. Gas flow effects are ignore due to low heat capacity of gas and low pressure limit effects of gas flow on temperature distribution.

4.2 Simulations Results of New Quartz Funnel Design

An example of vacuum chamber finite element (FE) modeling with new funnel design is investigated to show the accuracy of results from ANSYS. This section focuses on analysis of temperature distributions through the funnel when the heater is controlled at temperature range from 300 °C to 650 °C. The absent of O-ring has a direct impact on the uniformity of temperature into the vacuum chamber. An increase in the diameter of funnel causes a decrease in the temperature and hence enhances the uniformity of temperature generated into the vacuum cham-
The results obtained from the cross-section measurements showed that the shape of the funnel has maximal impact on the temperature uniformity.

As shown in Figure 2, the heater temperature was calibrated at 600 °C with the chamber body temperature of 1350 °C. Calibration was made at room temperature. Simulation condition for quartz funnel, thermal conductivity and coefficient of absorption are chosen as K=0.2 W/mK and 0.9, respectively.

To predict the temperature distribution by the simulation, the locations of 14 points on and around the funnel are shown in Figure 3. Also, a thermocouple number 8 which is not shown in the figure is placed on chamber body to estimate temperature of inner surface of wall of chamber body.

Through thermocouples measurements, Figure 4 shows the temperature distributions on and around the funnel in the range of 195-231 °C. In the case of modified funnel, the combining of the parts to one part significantly increases the temperature drop and makes the temperature uniformity higher than the previous case. The temperature values are very close to the value read from the Figure 4 in all points where the temperature drop equals approximately 35°C with respect to TC points.

After obtaining calibration results, temperatures of heater and chamber body are increased step by step to obtain temperature distribution by simulations and experiment for the new design. Experimental results are compared with FEM results at different vacuum condition (see Figure 5 and Figure 6).

As shown in both figures, results show good agreement between the experimental data and simulated temperatures. At higher temperatures, there is a difference between experimental and simulated temperatures. This is may be due to the change of radiation properties of the materials. For the first case, the temperature of chamber body was controlled by 135 °C with the heater temperature of 300 °C. The temperature distributions on and around the funnel were measured at the range of 140-230°C from TC of chamber through simulation. The temperature of inner wall surface of chamber body also was measured at 139 °C. The simulation and experimental results show that the temperature distribution near the heater is uniform within the manufacturing process region – at TC points 1-7.

For the second case, the temperature of chamber body was controlled by 150 °C with the heater temperature of 500 °C. The temperature distributions on and around the funnel were measured at the range of 163-405 °C from simulation results (see Figure 6). The temperature of inner surface of chamber body was also measured at 153 °C. The results generated with the FEM simulations show very good agreement.
with the experimental data, which can be used for the refinement of models and modelling parameters. Temperature results obtained from 14 points are changed accordingly based on the distance along the cross-section of funnel. Figure 5 and Figure 6 show the comparison of temperature uniformity among different TC points from both horizontal and vertical measurements. All the temperature intensity results align well on a single trend, which indicates that there is no distinguishable difference with the heater temperatures used. The temperature inside the chamber can be considered to have reached a fully developed temperature gradient beyond the simulation of TC points 1-7. On the other hand, a comparison of the vertical temperature fields does not change as the heater temperature decreases.

Temperatures of heater and chamber body are increased step by step to estimate temperature distribution on and around the funnel at higher temperature by FE simulations. When the temperature of chamber body was controlled at 180 °C with the heater temperature of 600 °C, temperature distribu-

**Figure 3:** Thermocouple position (TC) on and around the funnel.

**Figure 4:** Results of temperature distribution for calibration model.
In a subsequent study, the temperature of heater was controlled by 650 °C with the chamber body temperatures of 150 and 210 °C as seen from Figures 8 and 9, respectively. As seen from figure 8, when the temperature of chamber body was controlled at 150 °C, the temperature distributions thorough the funnel was measured between 181-538 °C. The temperature of inner surface of chamber body was also measured as 157 °C. On the other hand, as shown in Figure 9, temperature of chamber body increased to 216 °C and temperature delivery thorough the funnel was measured at the range of 239-546 °C at heater temperature of 650 °C. Temperature results obtained from 14 TC points are changed accordingly based on the distance along the cross-section of funnel. From the figures, it can be seen that the temperature measurements decreases with the distance from center of funnel. All the temperature intensity results align well on a single trend, which indicates that there is no distinguishable difference with the heater temperatures used.
Figure 7: Simulation results of temperature distributions (Heater 600 °C, Body 180 °C).

Figure 8: Simulation results of temperature distributions (Heater 650 °C, Body 150 °C).

Figure 9: Simulation results of temperature distributions (Heater 650 °C, Body 210 °C).
5 Conclusion

In this work, a new funnel, made of quartz crystal, for high temperature vacuum chamber was successfully designed and tested using computer-based simulation techniques. The results of this work show that the joint application of modern simulation methods such as process simulation is a powerful tool for the design and optimization of an innovative concept. Generally, these tools enable the simulation and analysis of numerous complex processes in the chemical engineering practice in an early stage of the project. The results of the analysis of temperature distributions as well as the results generated with the simulations mostly show uniformity distributions in temperature, which can be used for the refinement of models and modeling parameters. The work reported in this paper is a complete numerical investigation of parametric study of temperature distribution through the funnel of a chamber. On the base of obtained results, the new behavioral quartz model has been developed which appears to be more efficient than old design – with the new funnel design within the process region, uniform temperature distribution can be obtained on the vacuum chamber surface.

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