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Simulation of PTFE Billet Sintering Using COMSOL

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Abstract: Sintering is an important step in the manufacturing of polytetrafluoroethylene (PTFE) billets. The heating and cooling rate of the billets in this process is very critical and affects the final properties of the billets. The sintering temperatures can be up to 375^{0}C depending on the process. Some of the PTFE billets can be as large as 0.4 m in diameter. The challenge in heating such large billets stems from the inherent low thermal conductivity of PTFE. A thermal gradient develops between the surface and the interior of the billet and if the heating rate is not appropriate this can cause cracking of the billets. The optimum heating rate will depend on the oven conditions (set-point temperature, oven temperature uniformity, load in the oven, airflow rate and air flow configuration) as well as the billet dimensions (diameter and thickness). Existing literature suggests determining maximum heating rate experimentally using recommended guidelines.

This paper uses COMSOL to aid in optimizing the temperature profile (ramps/soaks) required for a particular sintering process in a convection batch oven. In this study, COMSOL version 4.2 has been used in solving a sintering problem with the PTFE billet being a solid material of 0.3 m diameter. Results have been obtained that predict the temperature response of the center of the billet subjected to a certain ramp and soak profile. Also, further studies have been conducted in this paper to compare the billet response to temperature when the air flow over the billet is both horizontal and vertical. The results with horizontal air movement have also been obtained when the product is rotated at a constant speed. Both the horizontal and vertical air flow configurations have been compared with the ideal case of a constant temperature boundary condition where the surface of the billet is instantaneously brought to the hot air temperature.

Keywords: Sintering, PTFE, convection, temperature profile.

1. Introduction

PTFE is a thermoplastic polymer with some remarkable properties. It is insoluble in common solvents and is resistant to most acidic and caustic materials. It has a very high dielectric strength and the coefficient of friction between PTFE and many engineering materials is extremely low. It can be used in temperature applications up to 260^{0}C. Apart from its useful temperature range and chemical inertness, it cannot be cross-linked and exhibits some creep thereby making it a good sealing material. However, it has a high melt viscosity and therefore sintering is typically used in PTFE manufacturing. In this process, PTFE fine powder is compressed inside a steel mold which is then heated above melting temperature for a sufficient time to complete the sintering process. One application of PTFE is as thin film, skived from sintered cylindrical blocks.

Sintering allows the coalescence of the resin particles, which provides strength and void reduction. This process takes time as the PTFE molecules are less mobile. Therefore, the parts have to be held at the sintering temperature for a significant period of time to allow fusion, coalescence and void elimination. Typical heating cycles during the sintering of PTFE includes successive ramps and soaks (number of hold periods) from room temperature up to the sintering temperature in a convective batch oven environment. The low thermal conductivity of PTFE can cause a thermal gradient to develop between the surface and the interior of the billet. The heating process provides some stress relaxation but the thermal gradient can cause mechanical stresses in the billet and if the heating rate is not appropriate (faster than optimum) this can cause cracking of the billets. In the industry, a faster heating rate is favored but a balance is required between heating rate and obtaining a good quality part. This optimum heating rate will depend on the oven conditions (set-point temperature, oven temperature uniformity, load in the oven, airflow rate and air flow configuration) as well as the billet dimensions (diameter and thickness).

Sina Ebnesajjad[1] suggests determining maximum heating rate experimentally using the following guidelines: The maximum heating rate of small parts is 80-100^{0}C/hr. A typical heating rate is no more than 50^{0}C/hr up to 150^{0}C, 30^{0}C/hr up to 300^{0}C and 6 -10^{0}C/hr at higher temperatures. He suggests introducing number of hold periods to allow heating of the interior section of the part.

2. Problem Description and Analysis

As mentioned in the previous section, a problem of PTFE billet sintering is solved in this paper. The PTFE billet as shown in Figure 1 is a 0.3 m diameter solid with a length of 0.3 m.

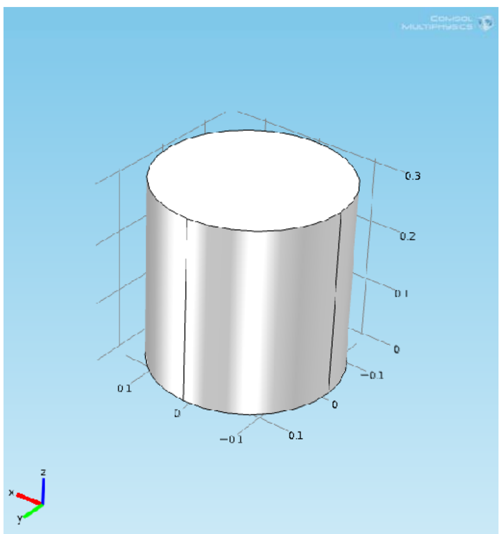

Figure 1. PTFE billet.

This PTFE billet is heated from an initial room temperature of 20^{0}C (T_i) in a convection oven environment up to a temperature of 370^{0}C. The convective heat transfer coefficient (h) is assumed to be 14 W/m^{2}K. The oven set-point follows the profile as shown in Figure 2. The heating part of the sintering cycle includes an initial ramp of 12^{0}C/hr to 260^{0}C, then a soak for 20 hrs, followed by a ramp of 10^{0}C/hr to 370^{0}C and the soak of 35 hrs at 370^{0}C. The soak at sintering temperature is critical to allow for void elimination and fusion of PTFE particles. The cooling cycle is critical at it controls the properties of the billet. The slower the cooling rate, the higher is the crystallinity of the billet. Also, the cooling rate should not be too fast to avoid large stresses that can fracture the billet. Sina Ebnesajjad[1] suggests the cooling rate for large billets to be between 8-15^{0}C/hr down to 250^{0}C and between 250^{0}C to 100^{0}C, it can be increased to 25^{0}C/ hr. The profile depicted in Figure 2 has a cooling rate of 10^{0}C/ hr up to 260^{0}C, a hold for 12 hrs followed by a cooling rate of 17^{0}C/ hr to 90^{0}C. In this study it is assumed that the air temperature (T_{ext}) in the oven exactly follows the set-point, which is unlikely to happen in practical cases.

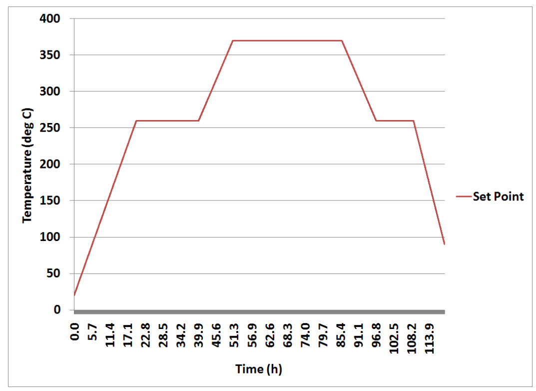

Figure 2. Oven Set Point (Air temperature) profile.

COMSOL Multiphysics[2] Heat Transfer Module has been used to solve the problem to determine how the center of the billet would respond to the air temperatures in the oven. The heat transfer problem is a 3-D transient one involving convection from the air to the surface of the billet and thereafter conduction heat transfer within the billet.

The governing heat transfer equation being

$$\rho C_p \, {}^{\partial T}\!/_{\partial t} + \nabla.(-k\nabla T) = 0 \qquad (1)$$

The boundary condition at all the surfaces being

$$-\boldsymbol{n}.(-k\nabla T) = h(T_{ext} - T) \qquad (2)$$

The initial condition of the billet being

$$T_i = 20°\mathrm{C} \qquad (3)$$

The properties of the billet (ρ, C_p, k) are assumed to be the same as that of a pure PTFE resin.

The air temperature (T_{ext}) is not always a constant and varies as per the profile shown in Figure 2. This problem has been solved in several steps, the solution for the first step being the initial condition for the second step and so on, and finally combining the solution of the seven steps. The temperatures at the core of the billet (center point) and at the surface are plotted as a function of time in Figure 3 and compared with the set point.

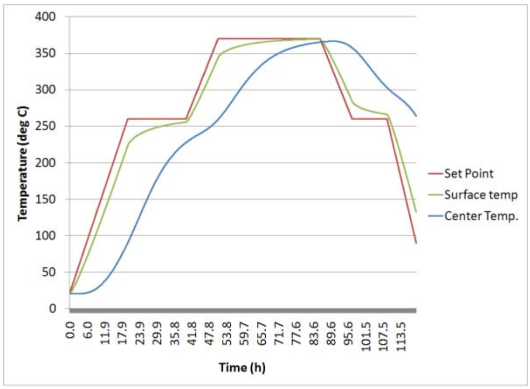

Figure 3. Surface & Center Temperature vs. Oven Set Point

It can be seen from the figure that the surface temperature more or less follows the set point on account of good convective heat transfer between the air and the billet. However, the core of the billet lags when compared to the surface temperature due to the low thermal conductivity of PTFE. This lag is extreme during the initial heating period of the billet as well as during the last cooling period. The set point profile can be improved either by decreasing the ramp up/down rates and or adding extra soak periods.

One such attempt at optimizing the profile is shown in Figure 4 where the Oven Set Point is modified for the cooling portion; the ramp down rates are one-half of those depicted in Figure 2 (5^0C/hr and 8.5^0C/hr) and the soak period (at 260^0C) between the two cool down ramps during the cool down is increased to 24 hrs. By performing this modification, the decrease in temperature difference between the surface and center during the cooling cycle is evident in Figure 4.

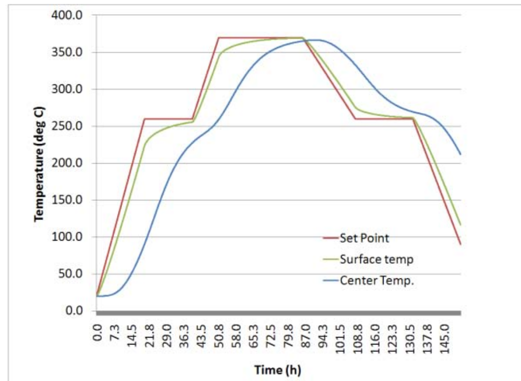

Figure 4. Surface & Center Temperature vs. Oven Set Point modified for the cooling portion.

The preceding problem did not consider the direction of air movement; as to whether the air flow is horizontal (perpendicular to the axis of the billet) or vertical. This aspect is looked into in the next subsection.

The same PTFE billet is now considered housed inside a square insulated box. The box is a 0.5 m cube. Two of its sides are open to allow air flow from one side to the other. In this sub-section, the PTFE billet is initially at 20^0C. The air is assumed to blow either vertically or horizontally across the billet at a constant speed of 4.0 m/s. The arrangement for a horizontal air-flow configuration is shown in Figure 5.

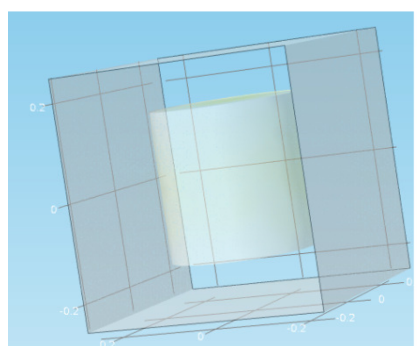

Figure 5. PTFE billet heated in a horizontal air-flow configuration.

The inlet air temperature is 370^0C. The core of the billet is analyzed to see how long it takes for the center to reach up to the air temperature for both air-flow configurations.

Before solving for the above two scenarios, the best possible heat transfer rate is analyzed by having the surface temperature of the billet instantaneously brought to a temperature of 370^{0}C from 20^{0}C (an infinite convective heat transfer coefficient). The entire billet is initially at 20^{0}C. COMSOL Heat Transfer Module is again used to solve the 3D transient problem. The convective boundary condition in Eqn. (2) is replaced by

$$T_{surface} = T_{ext} = 370°\text{C} \quad (4)$$

Next, the billet is assumed to be heated in a horizontal air-flow configuration as depicted in Figure 5. The conjugate heat transfer module under COMSOL Multiphysics is used to solve this problem. No slip boundary condition between the fluid (air) and the billet as well as between the fluid and the inside of the box is considered ($u_w = 0$). As before, the billet is initially at 20^{0}C and exposed to the air at 370^{0}C flowing at 4.0 m/s. The governing equations have been omitted for brevity. In the third part, the same exact problem is solved using the Conjugate Heat Transfer Module but with a vertical air-flow as shown in Figure 6.

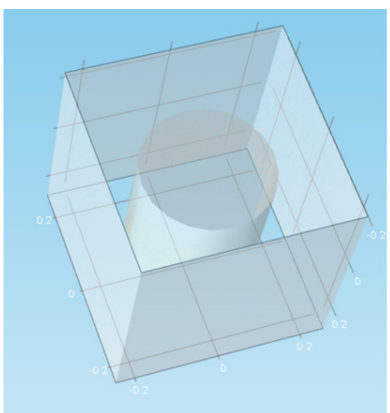

Figure 6. PTFE billet heated in a vertical air-flow configuration.

The temperature of the center of the billet with time is shown in Figure 7 for all the above three cases. It takes about 50 hrs for the billet to reach almost close to the air temperature (T_{ext}) in the case of the constant surface temperature. As is clear from Figure 7, the time it takes for the center of the billet to reach a certain temperature is much more for both horizontal as well as vertical air-flow when compared with constant surface temperature case. Also, the curves for the horizontal as well as the vertical air-flow configurations are almost identical.

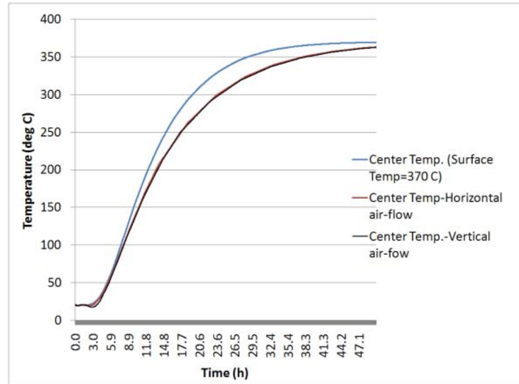

Figure 7. Comparison of the behavior of billet center temp with time for the three different cases: (a) constant surface temperature, (b) horizontal and (c) vertical air-flow.

The heating profile for the center of the billet could be further improved if the billet considered in Figure 5 is kept on a turn-table which is rotated at a constant speed with the air directed at it horizontally. The billet is considered to be rotated at a constant speed of 1 rpm. Again, Conjugate Heat transfer Module in COMSOL is used to analyze the rotating billet. The no slip-boundary condition still exists between the air-stream and the inside walls of the rectangular box. However, a sliding wall boundary condition is imposed on the surface of the billet.

$$u_{w,x} = \omega.y \quad (5)$$
$$u_{w,y} = -\omega.x \quad (6)$$
$$u_{w,z} = 0 \quad (7)$$

where
ω is the angular velocity and is defined as

$$\omega = {}^{2\pi N}\!/_{60} \quad (8)$$

N is the rotational speed in rpm.

The results for the temperature response of the center of the billet are compared for the three cases of constant surface temperature, stationary and rotating billet subjected to a horizontal air flow. These results are plotted in Figure 8. It is seen that the center temperature for the rotating billet has a response that is much closer to the ideal condition when the billet is instantaneously brought to the external air temperature. The center of the billet is heated at a much faster rate when the billet is rotated as opposed to it being kept stationary.

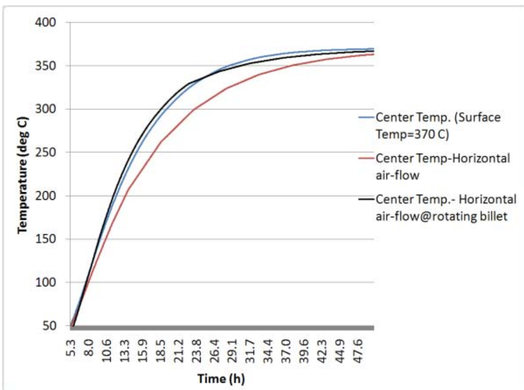

Figure 8. Comparison of the behavior of billet center temp with time for the three different cases: (a) constant surface temperature, (b) billet-stationary and (c) rotating billet.

3. Conclusions

This paper studied PTFE billet sintering for a few different cases. The response of the billet to a prescribed oven set-point was studied and was found that it provided opportunities to optimize oven profiles (set points) to obtain a better control of the process and the quality of the billet thus delivered. Next, the horizontal and vertical air-flow configurations were considered in the heating of the billet. It was also found that rotating the billet obtained the closest response to the ideal conditions.

As seen from the above study, a better understanding of the temperature profiles can be obtained through COMSOL without the need to perform numerous experiments using embedded thermocouples in the billet especially when the entire cycle is in the magnitude of several dozens of hours. Thus, simulations would provide quicker results. With the help of COMSOL this study has predicted how the core (center) of the billet responds to the temperature profiles in the oven. This is very useful information especially for thicker billets that have a tendency to crack during the heating cycle.

This particular study had a few assumptions such as only one billet was considered being heated (loading pattern not taken into account), the air-temperature perfectly matched the set-points of the oven and the oven had a perfect temperature uniformity.

Through further studies involving more realistic conditions, the use of COMSOL can aid in understanding the heat transfer in the billets and improve the efficiencies through optimization of the sintering process.

4. References

1. Ebnesajjad, Sina , “Non-Melt Processible Fluoroplastics”, Vol. 1, 2000.

2. COMSOL Multiphysics, version 4.2, Heat Transfer Module.