CFD IN A BATCH REACTOR

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ABSTRACT
FLUENT software was used to simulate a batch reactor installed at a new resin plant in the Greek city of Komotini. Prior to being put into production, the batch reactor was operated with water, and experimental measurements were taken during the reactor cooling process. These measurements were subsequently used to validate the FLUENT model of the vessel. Then the reactor was simulated with the resin polymer material. The goal of this phase of the project is to calculate the cooling curves for varying cooling water flow rates and inlet temperatures. Since the cooling time may correspond to as much as half of the overall batch manufacturing time, the plant throughput can be significantly increased by selecting the optimal cooling scenario.

1. THEORETICAL BACKGROUND

Resin adhesives are typically manufactured in a batch process, which involves methylolation and polymerization. The polymerization process takes place in a mixing vessel under specific pH and temperature conditions. The pH levels are maintained with the controlled addition of an acid during the course of the batch process. Proper temperature levels are maintained by cooling coils that are immersed in the mixture. Control of the temperature throughout the process is necessary for two reasons. First, the resin product is cooled in order to halt the reaction at the end of the process. Second, if hot spots develop during polymerization, a condition known as thermal runaway can occur, in which the reaction continues out of control, resulting in regions of solidified product. When this "freezing" of the reactor occurs, the entire batch must be discarded.

2. EXPERIMENTAL BACKGROUND

The tank is constructed of stainless steel and it has a volume of $25m^3$. The mixing of the resin is achieved by two impellers, with three blades each. Also, three baffles are located every 120°. Two spiral stainless steel pipes of 3in diameter are located near the shell, covering the whole tank height and provide the cooling of the resin by means of water flow. Finally, around the vessel there is a heating jacket.

The experimental data were the following:

- The reactor was charged with 19 n of water.
- The rotational speed of the impellers was 100rpm.
- The flow of the cooling water was $27.5m^3/h$ in each coil.
- The temperature of the cooling water was 10÷17°C.
- The reactor was cooled down from 90.7 to 34.8°C in 1h.

3. RESULTS & DISCUSSION

For the simulation, GAMBIT1.3 preprocessor was used to create a 3D grid, composed by approximately 424000 volume cells. The simulation of the batch reactor was achieved using FLUENT5.4 CFD code.

In FLUENT, the multiple reference frames (MRF) model was used for the simulation of the impeller movement and the RNG k-ε turbulence model with standard wall functions for the simulation of turbulence. An isothermal flow-field was computed first, followed by a transient energy calculation to track the temperature drop during the vessel cooling process. Figs. 1 and 2 show the velocity vectors and the contours of velocity magnitude on two different slices through the reactor (a horizontal and a perpedicular one) taken from the steady state calculations.

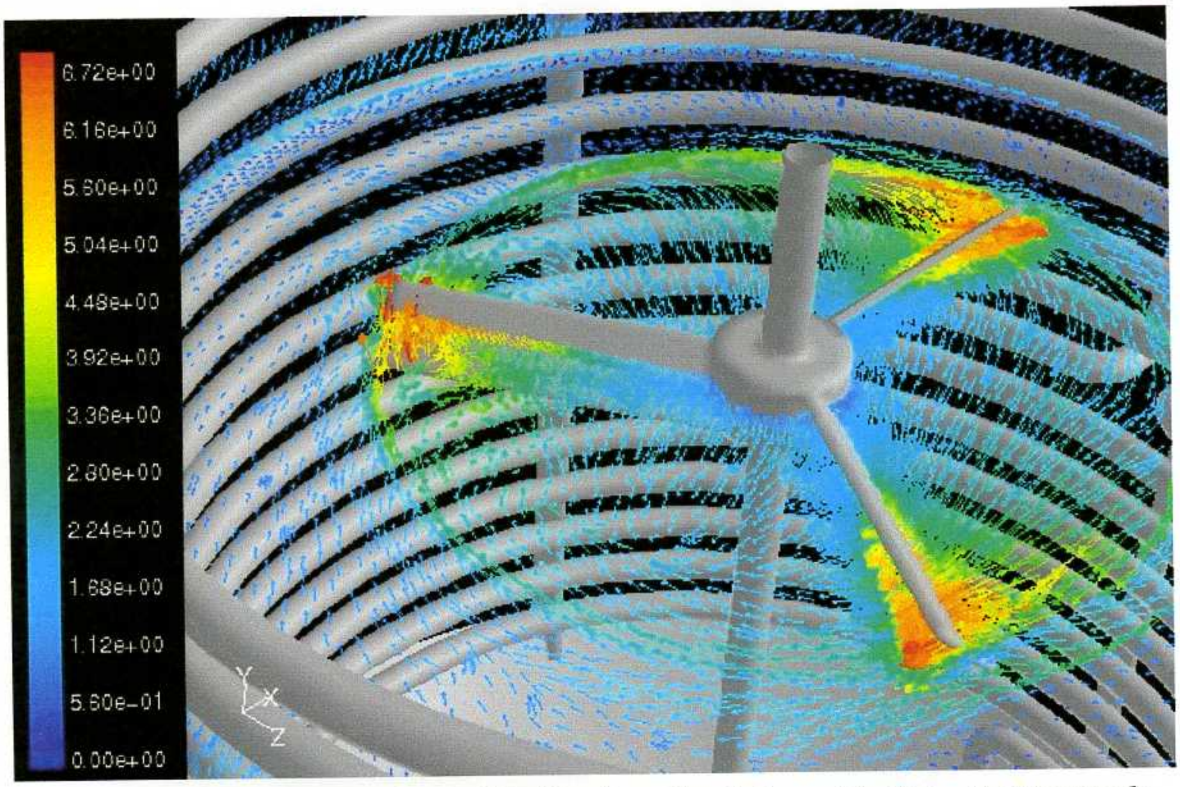

Figure 1: Velocity Vectors Around the Top Impeller Coloured by Velocity Magnitude.

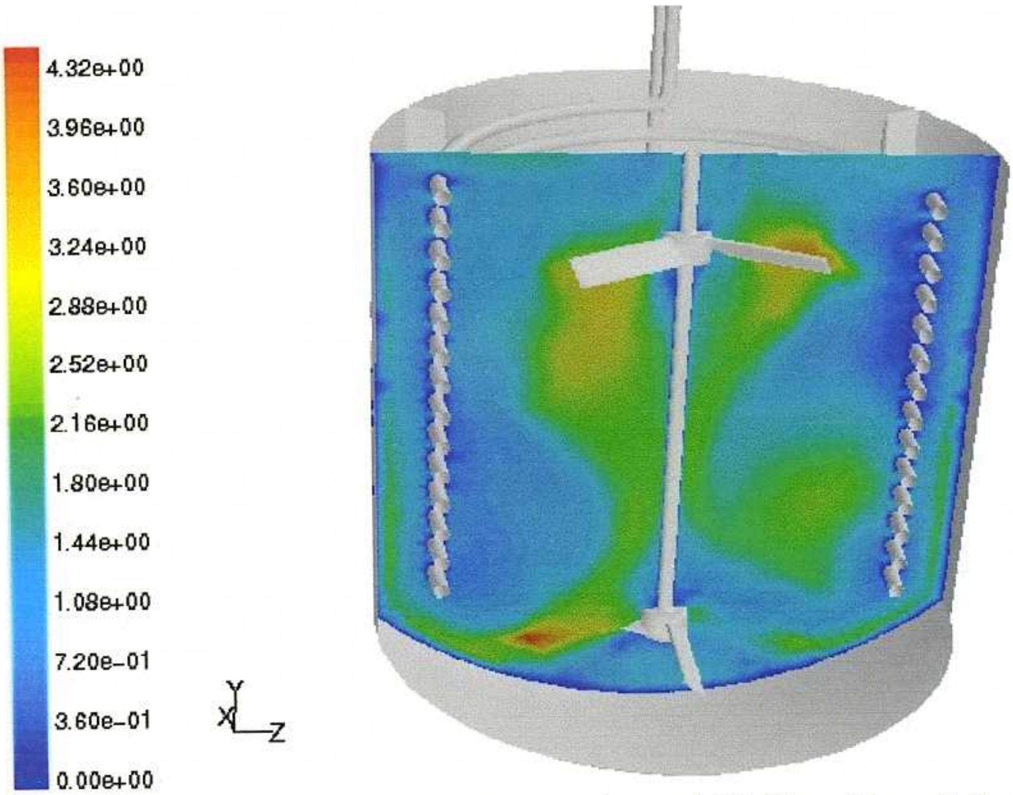

Figure 2: Contours of Velocity Magnitude on a Mid–Plane Through the Reactor.

Figs. 3 & 4 are taken from the unsteady calculations and show the contours of temperature in the two cooling coils and the contours of temperature on a mid–slice through the reactor.

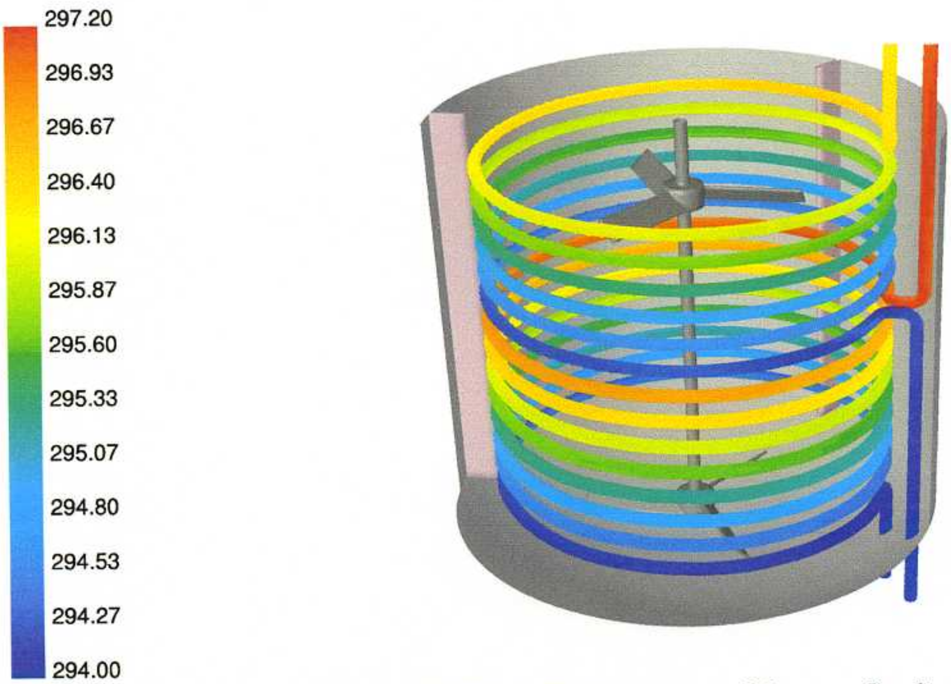

Figure 3: Contours of Surface Temperature of the two Cooling Coils after about 36min of Cooling.

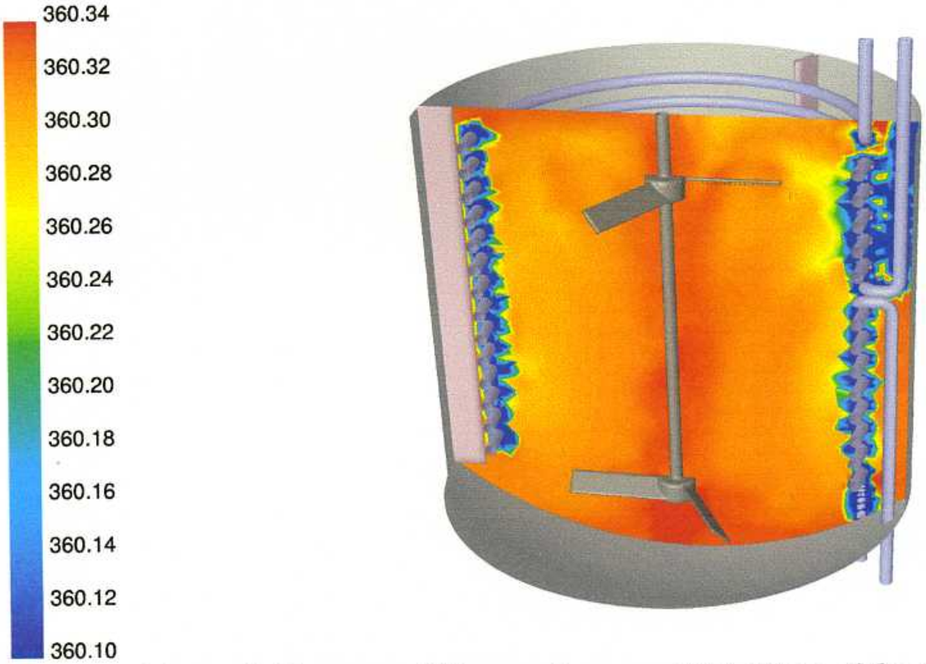

Figure 4: Contours of Temperature on a Mid–Plane of the reactor after about 11min of Cooling.

After a few mesh refinements, the predicted heat removal curve was found to match very good the experimental curve (Fig. 5).

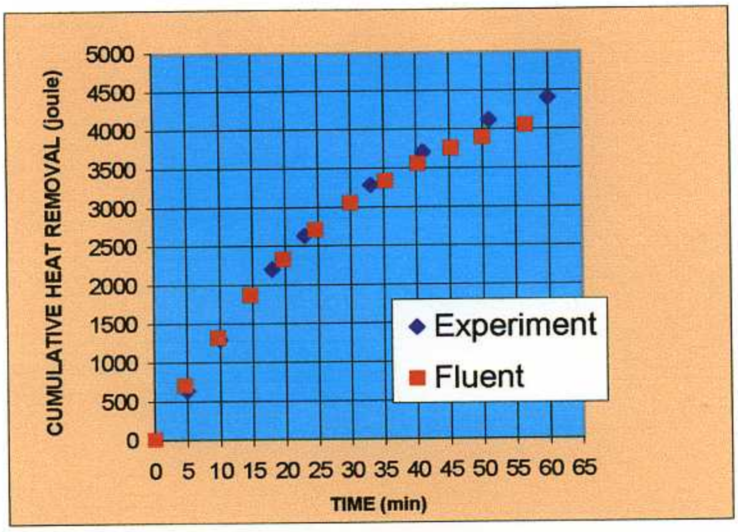

Figure 5: Measured and Predicted Cumulative Heat Removal from the Reactor.

After the validation of the model of the reactor had been achieved, FLUENT was used to predict the cooling profile of the resin. The rotational speed of the impellers, as well as the flow and the temperature of the cooling water were the same with those of the experiment. FLUENT prediction returned that the resin is cooled down from 363K to 351K in 50min under the above conditions. This is shown in Fig. 6.

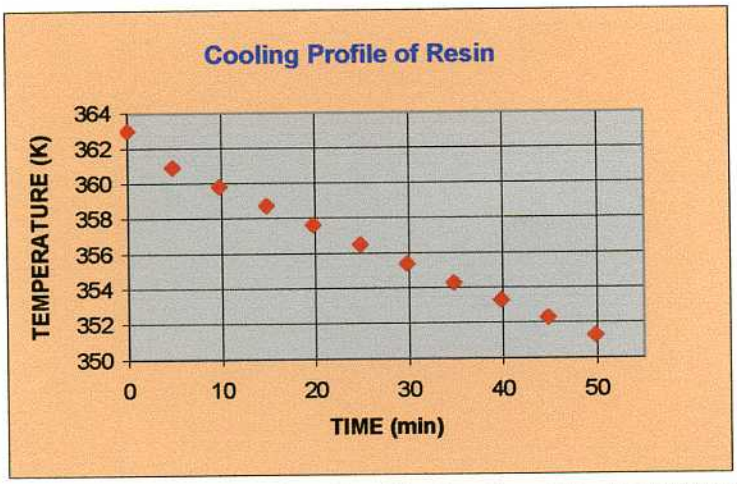

Figure 6: Resin Cooling Profile Predicted by FLUENT.

4. CONCLUSIONS

In this work, FLUENT software was used to simulate the flow field and the thermodynamic behavior in a batch reactor. In order to validate the FLUENT model of the vessel, a comparison was made between experimental data and FLUENT results. It was found that FLUENT leads to accurate predictions.

REFERENCES

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