Autodesk® Moldflow Insight 2021

Reactive Microcellular and Chemical Foam Molding Simulation for 3D Meshes

Executive summary

This report describes the simulation of reactive microcellular injection molding and chemical foam molding processes for 3D meshes. It gives an introduction, and workflow. It then describes example cases.

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AUTODESK.

Introduction

In the Autodesk Moldflow 2021 release, the simulation of reactive microcellular injection molding and chemical foam molding are added for the 3D mesh type.

The Reactive Microcellular Injection Molding is a process where injection molding is done using a single-phase solution of polymer and supercritical fluid (SCF). Once this polymer solution is in the cavity and no longer pressurized, the supercritical fluid can come out of solution and form very small gas bubbles. This process is similar to the Thermoplastics Microcellular Injection Molding process. The only difference is that the molding material is a thermoset polymer.

In Chemical Foam Molding, typically, a small amount of resin is initially dispensed into the cavity. The remaining cavity volume is then filled by a foaming process occurring in this resin. The foaming gas is generated by a chemical reaction occurring in the resin during the molding process. The reaction process that generates this foaming gas is considered during the simulation. Polyurethane (PU) foam molding is the most common example of chemical foam molding.

Workflow

The new processes are “Reactive Microcellular Injection Molding” and “Chemical Foam Molding” as shown in Figure 1.

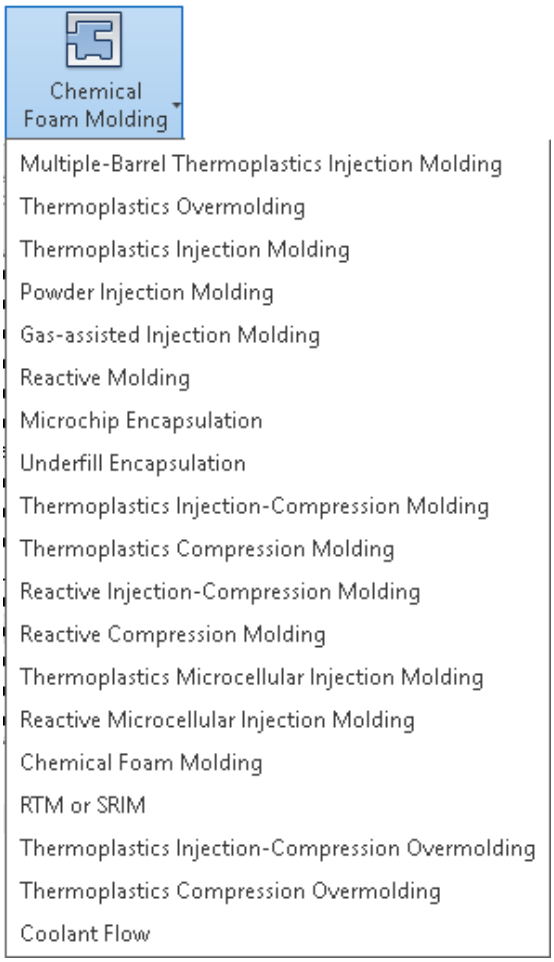


Figure 1: Selecting “Reactive Microcellular Injection Molding” or “Chemical Foam Molding” process.

There are several analysis sequences for reactive microcellular injection molding and chemical foam molding as shown in Figure 2.

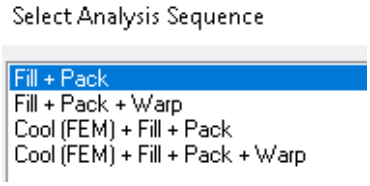
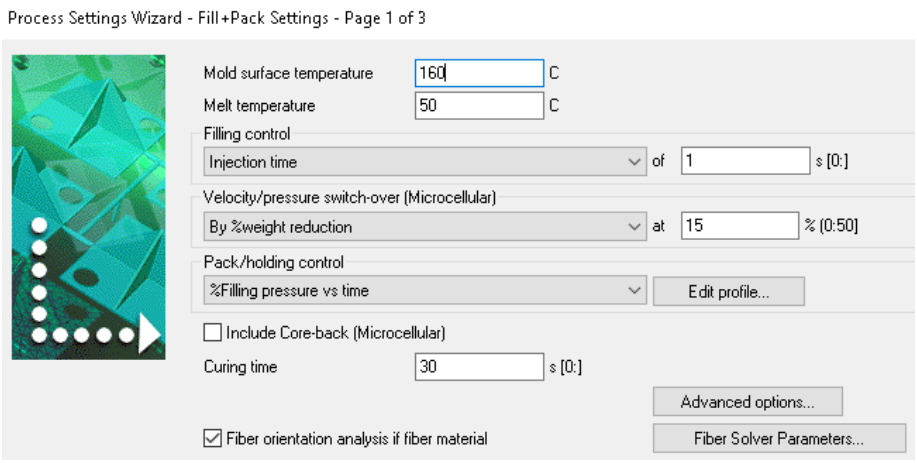
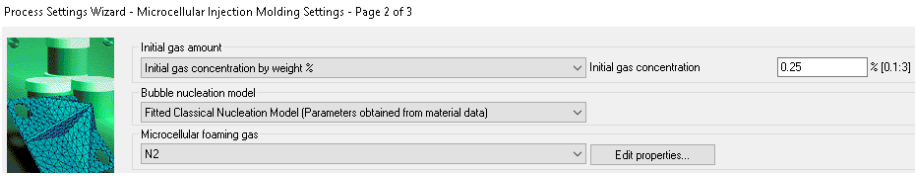


Figure 2: Selecting analysis sequence

For the “Reactive Microcellular Injection Molding” process, the process settings are similar to those for “Thermoplastics Microcellular Injection Molding” as shown in Figure 3. This process is used for the simulation of microcellular foaming for reactive materials with the foaming gas dissolved in the liquid polymer in the barrel at the start of injection.



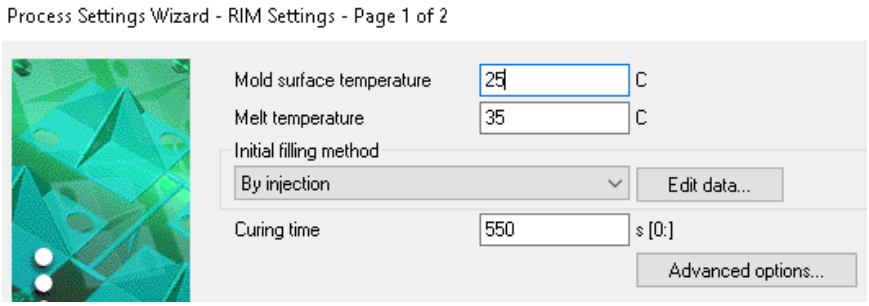
(a)



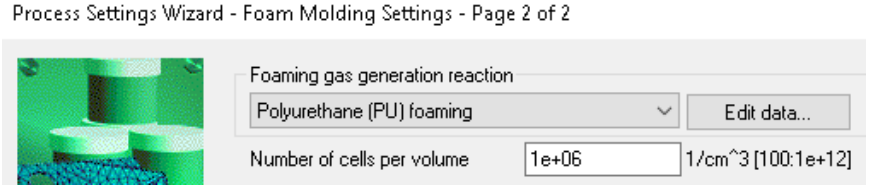
(b)

Figure 3: Process settings for regular reactive microcellular injection molding: (a) Fill + Pack settings and (b) Microcellular Injection Molding settings.

For the analysis sequences of Chemical Foam Molding (CFM), the process settings are shown in Figure 4. This is for the case where the foaming gas is generated in the cavity during molding by chemical reaction. For CFM, only a constant number of gas bubble cells per unit volume is supported (no bubble nucleation model is supported).



(a)

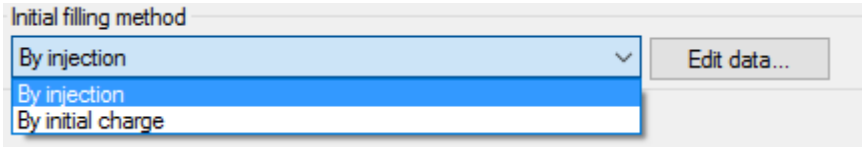


(b)

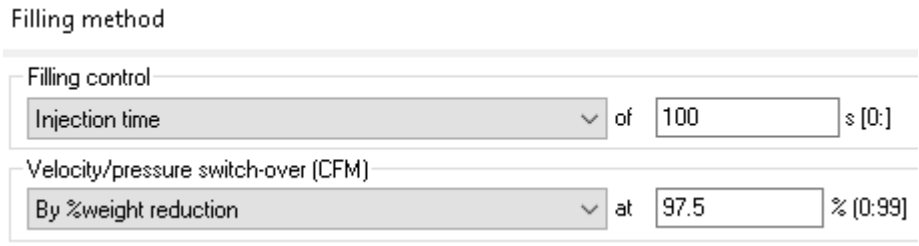
Figure 4: For CFM (Chemical Foam Molding) processes: (a) RIM settings and (b) Foam Molding settings.

For CFM analysis, the initial filling method can be selected as shown in Figure 5(a). This describes how the initial filling of the cavity will be done. The initial filling can be done by injection or by initial charge. When the initial filling is done by injection, process settings (such as filling control and V/P switch-over) can be assigned as shown in Figure 5(b). Typically, V/P switch-over will occur very early (at low filled volumes) for CFM cases.

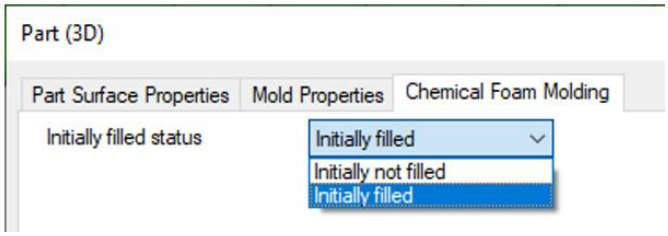
When the initial filling is done by initial charge, the initially filled region of the cavity can be specified by selecting the appropriate 3D elements, and selecting the “Initially filled” option for those elements as shown in Figure 5(c). In this case, any node can be assigned as an injection location.



(a)



(b)



(c)

Figure 5: Selecting the “initial filling method” for CFM cases: (a) Selection of initial filling method, (b) filling controls for initial filling “By injection” and (c) assigning the initially filled status for 3D elements.

For CFM, the “Foaming gas generation” method can be selected in the process settings as shown in Figure 6. It can be by “Polyurethane (PU) Foaming” or “General chemical foaming.

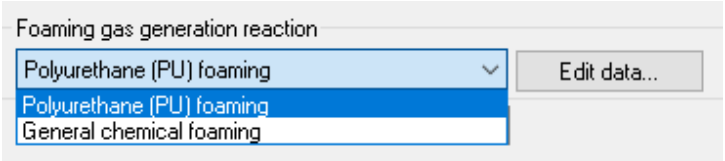
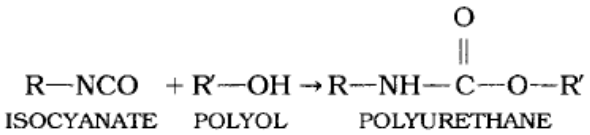


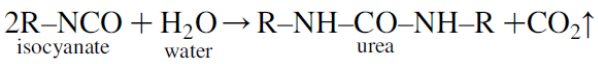
Figure 6: Foaming gas generation method.

The specific reaction for “PU foaming” is described below. This case involves 2 reactions. One is the gelling (curing) reaction as described by the following:



(1)

Another is the blowing reaction (which generates the foaming gas (CO_2)) as described by the following:



(2)

For “PU foaming” gas generation, PU foaming process condition data can be specified as in Figure 7. The data needed include “initial water concentration”, “initial Polyol concentration” and “initial Isocyanate concentration”. These are by weight %. The setup also requires the “initial dissolved CO2 concentration”. This is the amount of CO_2 gas that is dissolved in the melt before foaming.

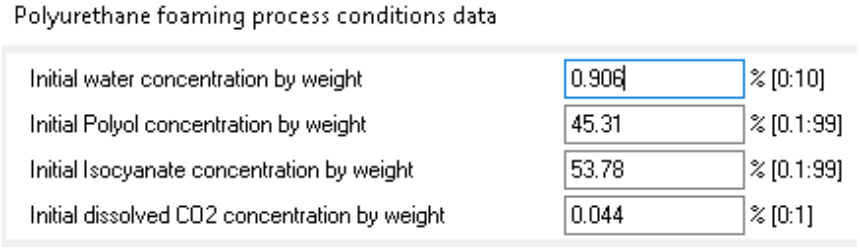


Figure 7: Process conditions data for PU foaming.

For PU foaming, the equivalent weight of Polyol and Isocyanate can be specified in the molding material data section as shown in Figure 8.

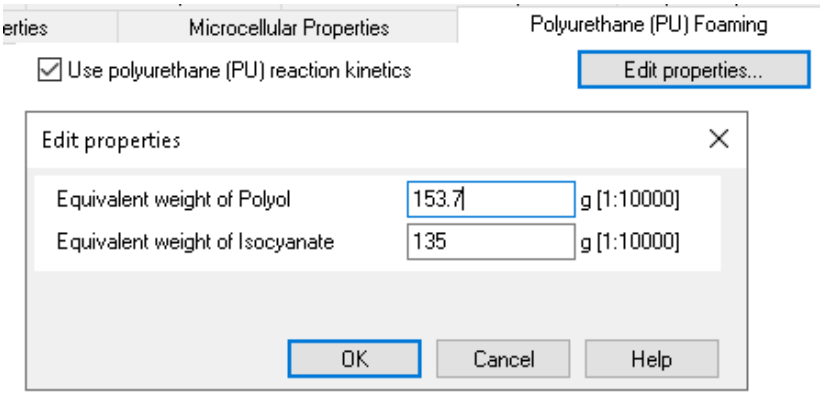


Figure 8: Equivalent weight of Polyol (OH) and Isocyanate (NCO) data in molding material properties data.

If the foaming gas generation reaction is something other than PU foaming, the “General chemical foaming” method can be selected. If “General chemical foaming” method is chosen, the required data are as shown in Figure 9. The required data include “foaming gas”, “initial concentration of chemical foaming agent” and “Foaming gas conversion % of chemical foaming agent by weight”.

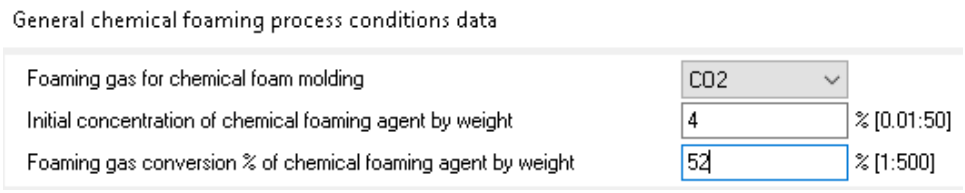
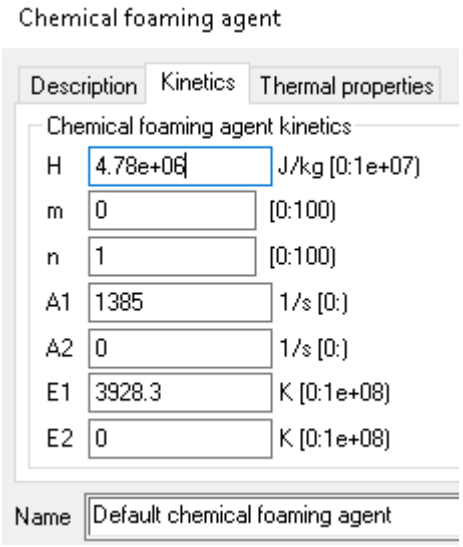
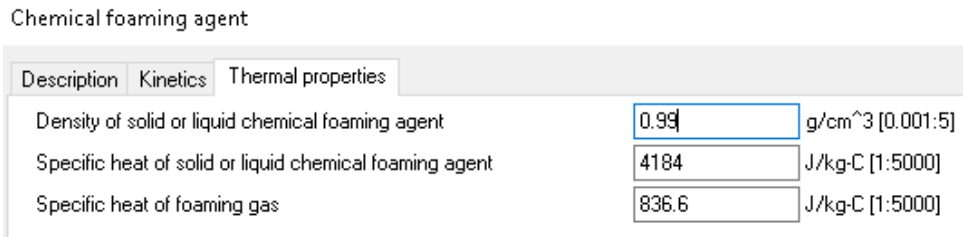


Figure 9: Process conditions data for “General chemical foaming” case.

The kinetics of the chemical foaming agent which generates the foaming gas can be specified as shown in Figure 10. For PU foaming, this is for the CO_2 gas generation reaction shown in equation (2). The kinetics equation for the chemical foaming agent is the same as that for thermoset curing kinetics (Kamal’s model). These data are found in the chemical foaming agent section of the advanced options. The density and specific heat data of the chemical foaming agent are also specified here.



(a)



(b)

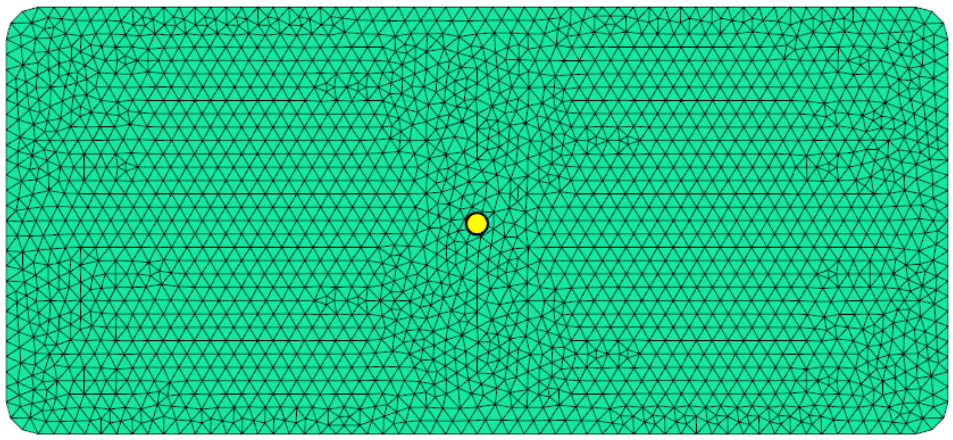
Figure 10: (a) Chemical foaming agent kinetics data and (b) thermal properties of chemical foaming agent.

Example Cases

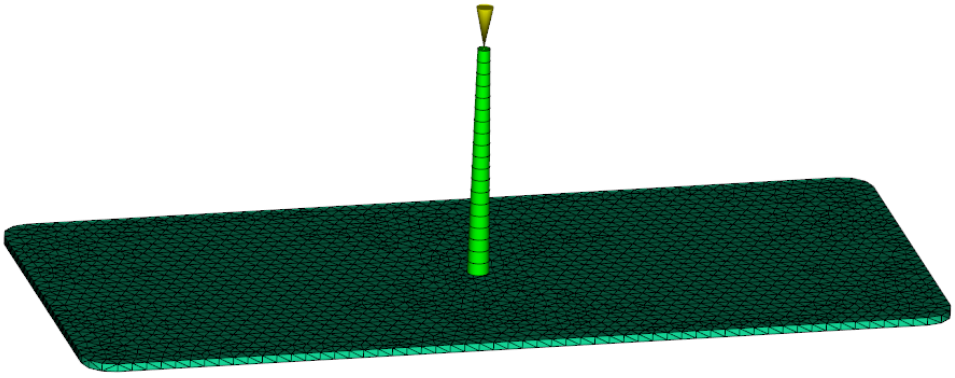
Some case studies will be presented below. One is for Reactive Microcellular Injection Molding. The second case study is for a Chemical Foam Molding (CFM) process with a cylindrical geometry, and the third case is for a CFM of a rectangular plate with varying cavity thicknesses.

Case Study 1

The mesh used in the first case study is shown in Figure 11. For this case, injection is via the beam elements in the center of the part. The material is an EMC (Epoxy Molding Compound). For the process conditions, the melt temperature is 50^{o}C, mold temperature is 160^{o}C. The injection time is 1 sec. The V/P switchover is set to target a 15% weight reduction. 0.25% by weight of N_2 gas is used as the foaming gas.



(a)



(b)

Figure 11: Mesh used in the case study of reactive microcellular injection molding.

A calculation result is shown in Figure 12. This shows the calculated bubble radius distribution at a cross section at the end of molding.

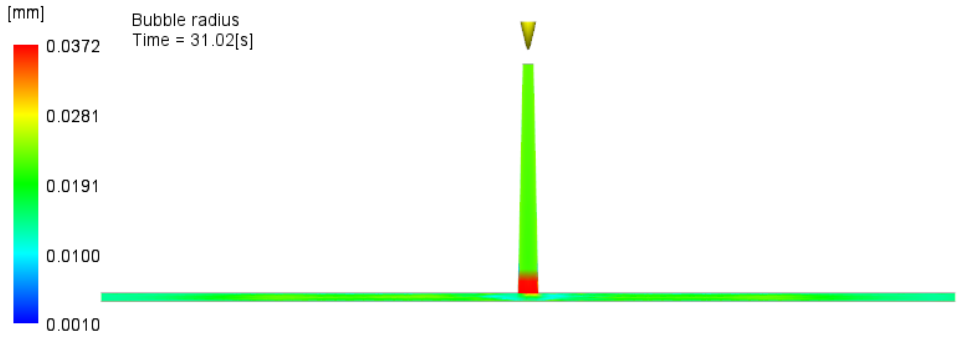


Figure 12: Bubble radius calculated at the end of molding (cross-sectional view).

Case Study 2

The second case study is a Chemical Foam Molding (PU foaming) process done for a cylindrical geometry as shown in Figure 13. The length of the cylinder is 1700 mm, and the diameter is 85 mm. The mold temperature is 25ºC, initial melt temperature is 35ºC. 2.5% of the cavity is filled initially by injection. The concentrations of water in Polyol were varied (0, 1, 2 and 3%). For the case of 2% water in Polyol, the initial water concentration is 0.906%, initial Polyol concentration is 45.31%, and the initial Isocyanate concentration is 53.78%. The equivalent weight of Polyol is 153.7, and the equivalent weight of Isocyanate is 135. The number of gas bubble cells was assumed to be 1.0×10^{12} /m^3.

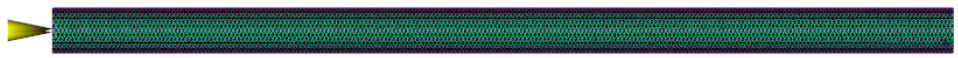


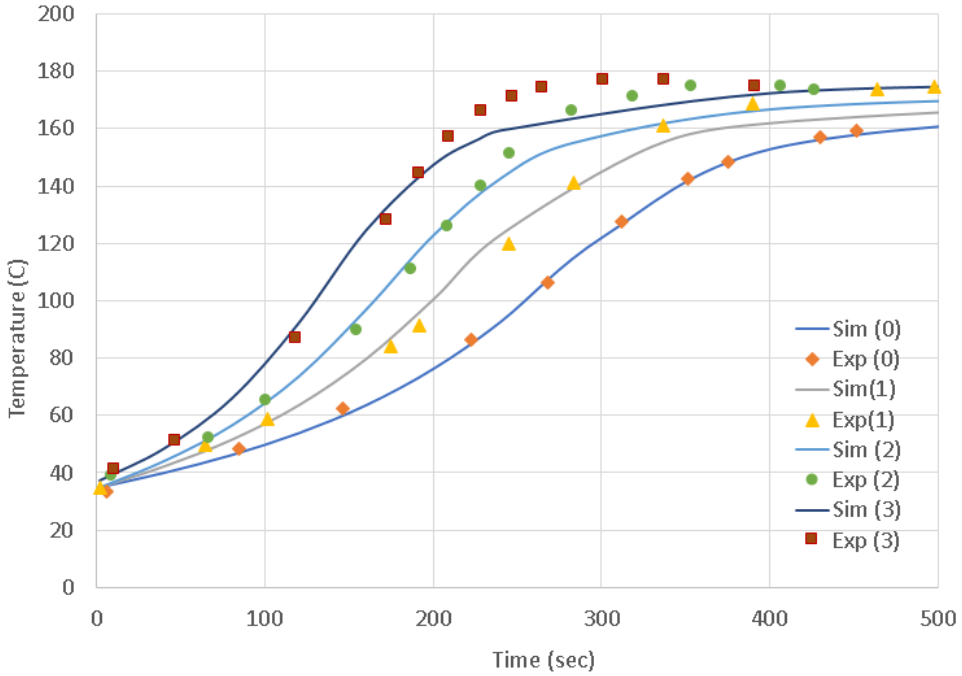
Figure 13: Mesh used in the second case study with 3D model.

The cavity will be filled by the expansion of the polyurethane due to foaming gas bubble nucleation and growth. The temperature will rise due to the heat generated from curing reaction and the blowing reaction. As the material expands, the density of the system will decrease. The temperature and the density distribution (cross-sectional view) near the end of molding are shown in Figure 14. The temperature change and density change over time from experiment and simulation are compared at the center of the cylinder near the injection location for various water concentration levels (Figure 15). The experimental data, material properties and process conditions data are obtained from Baser *et al* (1994). As can be seen, the simulation results match the experimental results reasonably well.

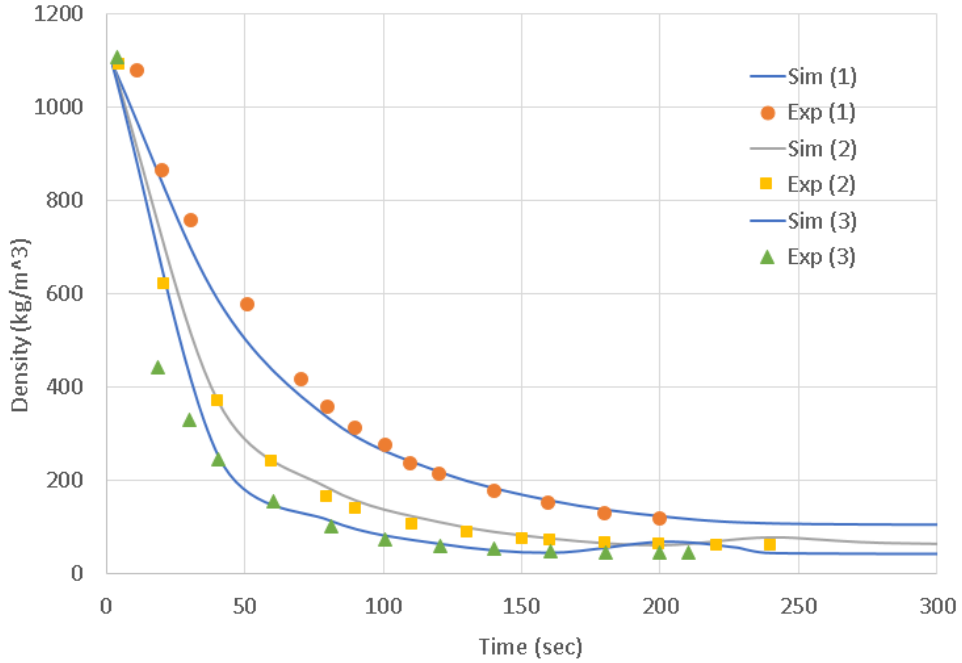
(a)

(b)

Figure 14: (a) Calculated temperature distribution (cross-section) at the end of molding, and (b) calculated density distribution (cross-section) at the end of molding.



(a)

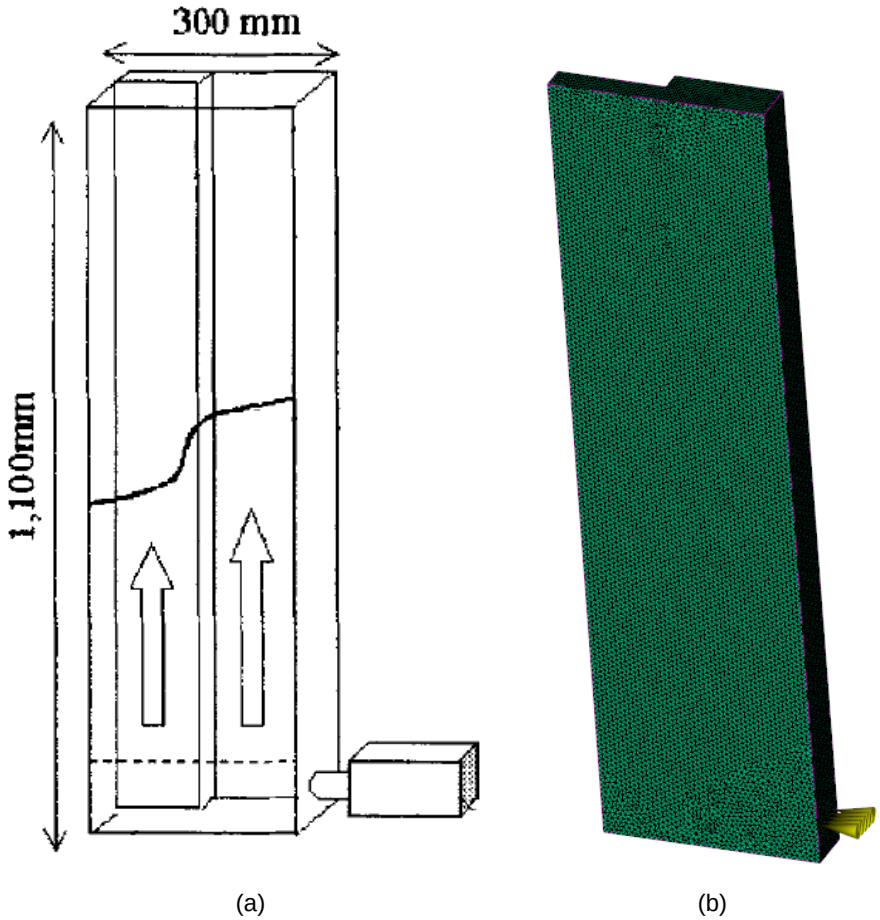


(b)

Figure 15: (a) Comparison of temperature history obtained from simulation ("Sim") and experiment ("Exp") for initial water concentration of 0, 1, 2 and 3%, and (b) comparison of density history obtained from simulation ("Sim") and experiment ("Exp") for initial water concentration of 1, 2 and 3%. The numbers in the legend represent "initial water concentration % in Polyol by weight".

Case Study 3

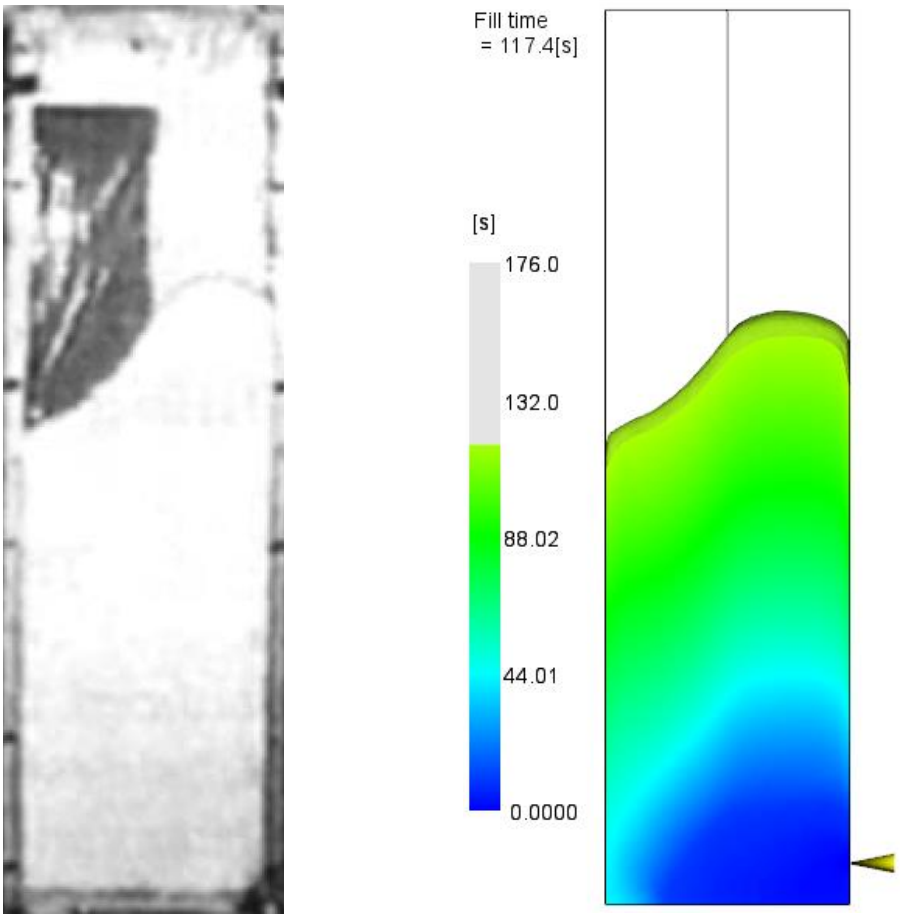
The third case study is a CFM (PU foaming) case in a rectangular geometry with varying cavity thicknesses as shown in Figure 16. This case is from Mitani *et al* (2003). The length of the plate is 1100 mm, and the width is 300 mm. The thickness is either 35 or 65 mm. The mold temperature is 30^{O}C, initial melt temperature is 30^{O}C. 9.1% of the cavity is filled initially by injection. The initial water concentration is 0.906%, initial Polyol concentration is 45.31%, and the initial Isocyanate concentration is 53.78%. The equivalent weight of Polyol is 153.7, and the equivalent weight of Isocyanate is 135. The paper by Mitani *et al* (2003) did not provide the viscosity value, so a reasonable value for the viscosity was used in the simulation (which is 100 times that of the default PU foaming material). The number of cells was assumed to be 1.0x10^{12} /m^{3}.



(a) (b)

Figure 16: (a) A schematic of the cavity used in the molding experiment and (b) the mesh used in the simulation.

The simulation result (fill pattern) is compared with experimental result in Figure 17 which shows good agreement.



(a) (b)

Figure 17: (a) The filling pattern obtained from experiment, and (b) the filling pattern obtained from simulation.

References

(1) Baser and Khakhar, “Modeling of the dynamics of water and R-11 blown polyurethane foam formation”, *Polymer Engineering and Science*, v. 34, 1994.

(2) Mitani and Hamada, “Prediction of flow patterns in the polyurethane foaming process by numerical simulation considering foam expansion”, *Polymer Engineering and Science*, v. 43, 2003.

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