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An investigation of sink mark formation in compression molding of polymeric composites

Ho, Chengter Ted, Ph.D.
The Ohio State University, 1993
AN INVESTIGATION OF SINK MARK FORMATION
IN COMPRESSION MOLDING OF POLYMERIC COMPOSITES

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the Graduate School
of
The Ohio State University

By

Chengter Ted Ho, B.S., M.S.

* * * * *

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To My Family
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4.3 Mold Filling Stage ............................................. 70
4.4 Resin Curing Stage ........................................... 83
4.5 Cooling and Sink Mark Formation ...................... 90
4.6 Concluding Remarks ......................................... 96

V. TECHNIQUES TO MINIMIZE SINK MARKS .......... 98

5.1 The Effects of Rib Number on Sink Mark .......... 98
5.2 Friction at the Bottom Mold Surface ............... 114
5.3 Back Pressure .................................................. 119
5.4 Effects of Molding Pressure on Sink Marks ....... 124
5.5 Concluding Remarks ......................................... 130

VI. SUMMARY AND RECOMMENDATIONS FOR FUTURE
    WORK ............................................................... 132

6.1 Summary ......................................................... 132
6.2 Recommendations for Future Work .................... 133

REFERENCES ............................................................ 135

APPENDICES

A. PROGRAMS AND EXAMPLES ............................... 140

A.1 Program RESIN for Calculating Resin Content .... 140
A.2 Example Input File for Program RESIN ............... 153
A.3 ABAQUS Program for Heat Transfer Including
    Curing ............................................................ 154
A.4 ABAQUS Program Used in Displacement Analysis ... 156
A.5 Pre-processing Program for ABAQUS Displacement
    Analysis .......................................................... 157

B. MOLDING OF BUMPER BEAMS ......................... 162

B.1 Introduction .................................................... 162
B.2 Molding Experiment .......................................... 165
B.3 Simulation of Mold Filling ................................... 168
B.4 Molding of Multi-Layered Charge ...................... 191
B.5 References ..................................................... 195
LIST OF TABLES

<table>
<thead>
<tr>
<th>TABLES</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1. Important molding variables [Meyer, 1987]</td>
<td>8</td>
</tr>
<tr>
<td>4.1. Thermal and chemical kinetic data for SMC used in this study [Lee, 1981]</td>
<td>67</td>
</tr>
<tr>
<td>4.2. Comparison of traced points in molding of plate with rib, (mold temp. = 130 °C, mold closing speed = 1 in / min.)</td>
<td>67</td>
</tr>
<tr>
<td>B.1. Composition of SMC used in bumper beam molding experiment</td>
<td>166</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURES</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1. Schematic of preparing sheet molding compound (SMC).</td>
<td>4</td>
</tr>
<tr>
<td>1.2. Schematic of a compression molding process.</td>
<td>5</td>
</tr>
<tr>
<td>1.3. Process illustration of SMC compression molding.</td>
<td>6</td>
</tr>
<tr>
<td>1.4. Sink mark on a panel with rib.</td>
<td>9</td>
</tr>
<tr>
<td>1.5. Two-piece panel.</td>
<td>10</td>
</tr>
<tr>
<td>2.1. Rib with protruding entrance [Smith and Suh, 1979].</td>
<td>14</td>
</tr>
<tr>
<td>2.2. Profilemeter readings from the surface of an SMC panel with rib.</td>
<td>16</td>
</tr>
<tr>
<td>2.3. Resin rich region exists over the rib in a cross section of an SMC panel with ribs. The flow pattern was &quot;bridging and looping&quot; [Kia, 1990].</td>
<td>16</td>
</tr>
<tr>
<td>2.4. A cross section of an SMC panel with ribs. The flow pattern was &quot;concurrent&quot; [Kia, 1990].</td>
<td>17</td>
</tr>
<tr>
<td>2.5. Parameter to assess the trend of concurrent flow [Xu, et al., 1992].</td>
<td>18</td>
</tr>
<tr>
<td>2.6. Parameter to assess the position of resin rich region [Xu, et al., 1992].</td>
<td>19</td>
</tr>
<tr>
<td>2.7. Back pressure to eliminate sink mark [Hirai and Yamabe, 1990].</td>
<td>26</td>
</tr>
<tr>
<td>3.1. Translation and rotation of a fiber during incremental deformation [Tszeng, 1992].</td>
<td>40</td>
</tr>
<tr>
<td>3.2. Assumed material properties as a function of conversion [Osswald, 1991].</td>
<td>46</td>
</tr>
</tbody>
</table>
3.3. Procedure of numerical simulation of molding process. ............ 49

4.1. Experimental set-up for measuring interfacial heat transfer coefficient. ................................................................. 58

4.2. Thermocouple locations of mold and charge, (a) top view, (b) side view. ............................................................... 59

4.3 Measured temperature history at the interface of first and second layers (T_m=63°C, T_i=23°C). .............................. 60

4.4 Boundary conditions in computation of temperature distribution at different IHTC. .................................................. 61

4.5 Measured temperature history (symbols) and theoretical calculation (lines) at the interface of first and second layers with no pressure on the charge (T_m=63°C, T_i=23°C). .............. 62

4.6 Measured temperature history (symbols) and theoretical calculation (lines) at the interface of first and second layers with a pressure of 2.5 psi on the charge (T_m=63°C, T_i=23°C). .......... 63

4.7. Schematic of mold setup showing the locations of two thermocouples before molding, [Fan, et al., 1988]. ............... 66

4.8. Comparison of temperature profiles between experimental data and simulation results in SMC molding at point no. 1 (mold temp.=130°C, mold closing speed=0.423 mm/sec., free resting period=10 sec.). ........................................ 68

4.9. Comparison of temperature profiles between experimental data and simulation results in SMC molding at point no. 2 (mold temp.=130°C, mold closing speed=0.423 mm/sec., free resting period=10 sec.). .................. 69

4.10. Initial finite element mesh of the charge and the mold. .......... 75

4.11. Calculated temperature after free resting for 10 seconds (mold temp. = 150°C, initial charge temp. = 25 °C). ............. 76

4.12. Calculated temperature at the time when folding occurs in the filling stage (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.). ......................... 77
4.13. Schematic of velocity distributions in simple upsetting. (a) isothermal without interface friction, (b) isothermal with interface friction, (c) non-isothermal without interface friction, (d) isothermal with interface friction. ............... 78

4.14. Preferential flow observed by Barone and Caulk [1985] (mold temp. = 150°C, mold closing speed = 1.75 mm/sec.). ......... 79

4.15. Calculated temperature at the end of filling stage (mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ............... 80

4.16. Calculated resin content distribution around the rib entrance area at the end of filling stage (mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ......................... 81

4.17. Cross section at the rib entrance shows the fiber rich area and resin rich area [Kia, 1991]. ................................. 82

4.18. Finite element mesh for resin curing and composite cooling. ...................................................... 84

4.19. Calculated temperature distribution at 20.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ......................... 85

4.20. Calculated fractional conversion distribution at 20.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ......................... 86

4.21. Calculated temperature distribution at 30.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ......................... 87

4.22. Calculated fractional conversion distribution at 30.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ......................... 88

4.23. Calculated temperature distribution at the end of curing stage (mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.) ......................... 89
4.24. Comparison of predicted top surface profiles of a plate with rib in two different amount of polymerization shrinkage, 1.5% and 0% (without resin/fiber separation). (a) full surface, (b) enlarged rib area (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.) .................................................... 93

4.25. Comparison of predicted top surface profile of a plate with or without resin/fiber separation (polymerization shrinkage = 1.5%,mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.) ........................................................................................ 94

4.26. Predicted top surface profile of a plate with rib in two different polymerization shrinkage, 1.5% and 0% (with resin/fiber separation, mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.). .................................................... 95

5.1. Geometry of two plates with one or two ribs. ................. 100

5.2. Initial finite element mesh and mold geometry in the simulation of molding a part with two ribs, (only a half cross section is analyzed). ..................................................... 101

5.3. Calculated temperature distribution after dwelling for 10 seconds, (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). ......... 103

5.4. Calculated temperature distribution after filling, (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). .................. 104

5.5. Calculated velocity distribution around the rib area at time = 10.6 seconds (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). ........ 105

5.6. Calculated velocity distribution around the rib area at time = 10.7 seconds (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). ...... 106

5.7. Calculated resin content distribution after filling (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). ................. 107

5.8. Calculated temperature distribution at time = 20.5 seconds (in the curing stage, mold temperature = 150 °C, mold
5.9. Calculated fractional conversion distribution at time = 20.5 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 110

5.10. Calculated temperature distribution at time = 31.1 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) .................................................................................................. 111

5.11. Calculated fractional conversion distribution at time = 31.1 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 111

5.12. Calculated temperature distribution at time = 40.8 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 112

5.13. Calculated fractional conversion distribution at time = 40.8 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 112

5.14. Calculated temperature distribution at time = 52.6 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 113

5.15. Predicted top surface profile of plate with two ribs (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 113

5.16. Calculated velocity plot of the charge with high friction at bottom mold surface (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ................................................................. 116

5.17. Calculated resin content distribution around the rib entrance with high friction at the bottom mold surface at the end of filling stage (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) ........ 117
5.18. Comparison of predicted top surface profiles under normal mold and mold with high friction at the bottom mold surface (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) .......................118

5.19. Back pressure during molding suggested by Hirai and Yamabe [1990] and approximation used in the simulation. . . . 121

5.20. Calculated resin content distribution at rib entrance at the end of the filling stage (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds) .................................................................122

5.21. Comparison of sink marks of back pressure molding and normal molding (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). ..... 123

5.22. Comparison of predicted top surface profiles under normal and low pressure during curing (polymerization shrinkage = 1.5 %, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). 126

5.23. Comparison of predicted top surface profiles with or without pressure release at 10 seconds after curing starts (polymerization shrinkage = 1.5 %, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). 127

5.24. Back pressure during curing. .................................128

5.25. Comparison of predicted top surface profiles with or without back pressure during curing (polymerization shrinkage = 1.5 %, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds). 129

5.26. Comparison of predicted sink mark depths of different techniques to minimize the sink mark formation, (normal molding = 1). ..........................131

B.1. FMVSS 215 impact pendulum device profile [Kowalski, 1982]. .................................................................166

B.2. Isometric view of bumper beam .................................166

B.3. Temperature histories of two molding samples ...............169

B.4. Central cross section of the bumper beam ....................172

xv
B.5. Schematic of initial SMC charge plies rest on the mold cavity. Two upper corners of the mold cavity contact with SMC charge. ................................. 173

B.6. Finite element mesh of the charge. ................................................. 174

B.7. Finite element mesh at time = 10.33 seconds. ................................. 177

B.8. Finite element mesh in the necking area at time = 10.33 seconds. .......................................................... 178

B.9. Finite element mesh in the folding area at time = 10.33 seconds. .......................................................... 178

B.10. Velocity distributions in simple upsetting. (a) isothermal without interface friction, (b) isothermal with interface friction, (c) non-isothermal without interface friction, (d) isothermal with interface friction. ................................. 179

B.11. Finite element mesh at time = 22.87 seconds. ................................. 181

B.12. Calculated temperature distribution of bumper beam after complete filling. .................................................... 182

B.13. Comparison of DSC data and computation data from curing model at three different temperatures, (a) 95 °C, (b) 105 °C, (c) 115 °C. ................................................................. 187

B.14. Calculated temperature distribution in the central cross section of the bumper beam at time = 71.9 seconds. .............. 188

B.15. Calculated fractional conversion distribution in the central cross section of the bumper beam at time = 71.9 seconds. ... 189

B.16. Calculated temperature distribution in the central cross section of the bumper beam at time = 109.8 seconds. .............. 190

B.17. Calculated fractional conversion distribution in the central cross section of the bumper beam at time = 109.8 seconds. ................................................................. 191

B.18. Comparison of temperature histories obtained from simulation with that obtained from molding experiment. .............. 192

B.19. Finite element meshes of two-layered charge used in filling simulation of molding of bumper beam. ...................... 196
B.20. Geometry and calculated temperature distribution of two-layered charge at step no. 355 (time: 7.06 sec.) ............... 197
CHAPTER I
INTRODUCTION

1.1 Applications of SMC

Sheet molding compound (SMC) is one of the most frequently used glass fiber reinforced polymers. Sheet molding compound is a sheet form of molding compound which is composed of a thermoset resin, fiber reinforcement and additives. These additives may include initiator (catalyst) for the resin, thickener, mold release agent, filler, shrinkage control agent (low profile agent) and others. A typical automotive grade SMC contains polyester resin, calcium carbonate filler and glass fiber.

The advantages of SMC over steel are corrosion resistance, good stiffness and strength-to-weight ratio, design flexibility, parts consolidation properties and relatively low cost (when used to replace several assembled metal parts with one SMC part). The most common applications of SMC in the automotive industry are exterior body panels and structural parts. For example, the SMC bumper system of 1992 Cadillac Seville consists of 126 parts compared with 249 parts previously [Reinforcement Digest, 1992]. The assembly time is reduced from 33.7 to 14.5 minutes. Plans to use SMC for the roofs, rear decks, and outer door panels of 1993 Chevrolet Camaro and Pontiac Firebird
have also been unveiled [Wood, 1990; Wood, 1989; Wigotsky, 1991].
Besides automotive industry, SMC has also been used in computer
enclosures, dishwashers, washing machines, clothes dryers, air
conditioners, refrigerators, bathtubs, and shower enclosures [Mallick,
1990; Modern Plastics, 1989].

1.2 Manufacturing of SMC

Manufacturing a part from SMC can be divided into two stages;
namely, charge preparation and molding. Figure 1.1 shows the process
of charge preparation. All the ingredients of molding compound except
the reinforcing fibers are mixed and metered onto a carrier film, such
as polyethylene. Glass fiber roving is chopped into specified length and
randomly dropped onto the moving layer of paste. A second layer of
resin paste on carrier film is then applied to the top of the chopped
fibers. The sandwich of resin paste and fibers then proceeds to a
compaction system to expel trapped air and impregnate the fibers with
resin. The SMC material is then rolled up and maintained at a
temperature ranging from 32° C to 38° C (90° F to 100° F). The
viscosity of the SMC increases over this period, so-called maturation.

Matured SMC is cut into pieces of pre-specified size for molding,
and the carrier films are removed. Several pieces of SMC may be plied
together to form the "charge," which is then placed in the mold (Figure
1.2). In most cases, the mold is heated to e.g., 150° C. This molding
process can be divided into three steps: (1) mold filling, (2) curing, and (3) ejection of parts and cool-down. The charge usually does not cover the entire surface of the mold in order to allow material flow during filling, which will expel the remaining trapped air. The filling stage is completed in 0.5 - 20 seconds [Meyer, 1987]. After filling, the charge remains in the hot mold for the polymerization to be completed (curing). At the end of the curing cycle, which usually takes 30 seconds to 2 minutes, the finish part is ejected from the mold and allowed to cool to ambient temperature. At each step, the process is governed by several phenomena, which are summarized in Figure 1.3.
Figure 1.1. Schematic of preparing sheet molding compound (SMC).
Figure 1.2. Schematic of a compression molding process.
Figure 1.3. Process illustration of SMC compression molding.
1.3 Issues in Manufacturing

Sheet molding compounds are complicated materials. There are more than 50 independent variables which have some effects on the final molded part [Meyer, 1987]. Among these 50+ independent variables, a list of the most important compression molding variables is shown in Table 1.1. Press slow close usually proceeds at a variable speed of 1-20 inches per minute. Mold pressure can be as high as 1200 psi or as low as 100 psi. Mold temperature depends on the particular resin-catalyst system in the compound. Most materials are formulated to be molded at approximately 150°C in order to obtain a reasonable cure cycle. The design of charge size, weight, shape, and placement is generally based on experience and trial and error. The charge weight is mostly based on the molded part weight. However, the charge size, shape, and placement must be tailored to be free from knit lines, which are formed at the joining of two divided flow fronts [Mallick, 1988].

Curing is a crucial stage in molding a part with thick cross section because it takes longer time to cure a thick part. To ensure complete cure, process engineers always let the part stay in the mold longer than it needs. Simulation of filling and curing not only will help to determine the minimal time to ensure complete cure, but also can be used to determine the charge shape and placement to ensure the mold cavity is completely filled.
Table 1.1 Important molding variables [Meyer, 1987].

1. Press Slow Close
2. Molding Pressure
3. Molding Temperature
4. Cure Cycle
5. Charge Size
6. Charge Weight
7. Charge Shape
8. Charge Placement

The term “sink mark” refers to a slight depression on the surface of parts directly over ribs and bosses, see Figure 1.4. A depression with long wave length (> 8 mm) would not be considered as sink mark [Hirai and Yamabe, 1990]. In many applications, a sink mark causes no problem because it does not affect the performance of the component. However, a sink mark becomes a cosmetic problem which prevents the automotive exterior body panels from being made of SMC. There are several techniques of design to mask sink marks. One of them is to place ribs behind styling lines. Another approach is to texturize the outer surface. However, most of the exterior body panels, such as hood, deck lids, and door panels, require a flat, unblemished exterior surface. Currently, two-piece panels (Figure 1.5) are being used to avoid the problems with sink marks. It is clear that one-piece panels with integrated ribs cost less than two-piece panels. Hence, it is
rewarding to investigate the mechanism of sink mark formation and the techniques to eliminate sink marks.

Figure 1.4. Sink mark on a panel with rib.
Figure 1.5. Two-piece panel.
CHAPTER II
LITERATURE REVIEW

This chapter gives a summary of the previous work and research on SMC manufacturing, particularly on the sink mark formation and elimination.

2.1 Experimental Investigation of Sink Mark Formation

Jutte [1973] identified two principal causes of sink marks, namely polymerization and thermal shrinkages. Polymerization of unsaturated polyester resins results in volume shrinkage which is called polymerization shrinkage. This can be minimized by proper use of low profile additives (LPA) [Jutte, 1973]. On the other hand, the thermal shrinkage results from cooling of the material. The thermal shrinkage can be described by the following equation:

\[ \Delta V = \alpha_t \cdot \Delta T \cdot V \]  \hspace{1cm} (2.1)

where

\[ \Delta V = \text{volume change}, \]
\[ \alpha_t = \text{thermal expansion coefficient}, \]
\[ \Delta T = \text{temperature differential and} \]
\[ V = \text{volume}. \]
This equation demonstrates that the thermal expansion coefficient as well as the temperature difference are the variables that can affect overall thermal shrinkage. Due to the presence of glass fiber and the variation of fiber content and orientation in rib area, the thermal expansion coefficient of the material is not homogeneous. Even for a material with homogeneous thermal expansion coefficient, a sink mark can still exist [Jutte, 1973]. Jutte [1973] has experimentally studied the effects of LPA, fiber length, fiber content, rib geometry and concluded that

1) Sink marks result from polymerization shrinkage can be minimized by proper use of LPA.

2) Short fiber length and high glass content can result in minimum sink.

3) For minimizing the sink mark in a given panel (thickness = 0.125 in), the recommended rib geometry is: minimum lead-in radius, usually 0.005-0.010 in, rib width in the range 0.125-0.375 in.

Boyd [1976] conducted more detailed tests to investigate the mechanism of sink mark formation. The three tests he conducted were (1) A SMC shrinkage test, (2) A paste shrinkage test, and (3) A sink resistance test. In order to minimize sink marks, he suggested:

1) Using a high reactivity polyester resin with optimum catalyst.
2) Using a low profile additive, a PMMA or PVA thermoplastic, depending on viscosity requirements and compatibility with polyester.

3) Using high filler loading.

4) Using lowest acceptable molding pressure.

5) Adjusting the mold temperatures to give optimum results with the specific compound.

6) Avoiding placing the charge directly above ribs and bosses.

Ampthor [1978] investigated the effects of the material and molding conditions on the sink mark of SMC parts in the similar way with Boyd [1976]. His conclusion is slightly different from that of Boyd [1976]. He investigated the role of resin on the sink mark problem. With an experimental resin with 30% less shrinkage than typical molding compound with LPA, the improvement on the sink depth was only 9%. The implication is that sink is a problem beyond polymerization shrinkage. For molding conditions, he had the same conclusion as Boyd [1976] on the effect of mold temperature. However, he reported that there was no significant improvement or consistent results in sink reduction when the parts were molded at different pressure, cure time, and cooling rate. He also conducted experiments on a patented concept [Pfaff, 1972], which utilized a charge comprising fibers of different length. He confirmed that long glass fiber over short glass fiber (2"-1/4"-1/4") showed unusually low sink. Ampthor [1978]
investigated the phenomenon of the "disruptive flow," which creates a triangular resin-rich area at the surface above the rib and its relation to the sink mark formation. They found that sink mark can be reduced by depressing the appearance of disruptive flow. The amount of disruptive flow and sink depended on the design of rib geometry. In investigation of flow around rib, Smith and Suh [1979] concentrated on the rib entry geometry. They suggested that the protruding entrance (see Figure 2.1) would result in non-detectable sink (less than 0.1 mil).

Figure 2.1. Rib with protruding entrance [Smith and Suh, 1979].
With the advancement of LPA, SMC can be formulated to have any degree of shrinkage, even negative (expansion). In some cases, the surface profile even protrudes from the rib area. As a consequence, Kia [1990] proposed a new term "rib readout" to describe the surface profile in rib area (see Figure 2.2). Similar to Ampthor [1978], he suggested that, because the dominant role of polymerization shrinkage had diminished, the contribution of other parameters had become more noticeable. He noticed that the magnitude of deformation over the ribs is dictated by the extent of glass-resin separation over the ribs. The glass-resin separation over the ribs is primarily determined by the flow pattern of the paste during the molding operation. He categorized the flow pattern into two types. One is "bridging and looping" and the other one is "concurrent flow." In the first type of filling pattern, the paste under compression primarily flows horizontally and bridges over the ribs. After the charge reaches the inside periphery of the mold, the molding pressure increases and forces the charge into the ribs, Figure 2.3 shows such an example. In the second type of filling pattern, the charge flows into the rib at the same time as it flows horizontally. Figure 2.4 is an example of the rib filled in such pattern. Experimentally, Kia [1990] found that there is more resin separation when the flow pattern is dominated by bridging and looping.
Figure 2.2. Profilemeter readings from the surface of an SMC panel with rib; (a) shows a "valley," (b) shows a "hill." [Kia, 1990]

Figure 2.3. Resin rich region exists over the rib in a cross section of an SMC panel with ribs. The flow pattern was "bridging and looping" [Kia, 1990].
Xu, et al. [1992] investigated the influences of friction on the flow pattern. They found that high friction on the mold surfaces will promote concurrent flow and less resin separation. Similar to the result of Kia [1990], concurrent flow will result in the formation of resin rich region hiding under the cosmetic surface. They suggested a measurement to assess the trend of concurrent flow, i.e.,

\[ D = \frac{T}{W} \]  \hspace{1cm} (2.2)

where \( T \) is the length in vertical (rib) direction and \( W \) is the length in horizontal (plate) direction of the charge, see Figure 2.5. Higher value of \( D \) means more concurrent flow. Another parameter,
R1 = h1/h2  \hspace{1cm} (2.3)

is also used to assess the position of resin rich region as shown in Figure 2.6. With the assessment of these two parameters, the experimental results showed that higher charge/mold interfacial friction will result in higher D and R1, which means that higher interfacial friction will promote concurrent flow and reduce sink.

Figure 2.5. Parameter to assess the trend of concurrent flow [Xu, et al., 1992].
2.2 Theoretical Studies of Compression Molding

A compression molding process includes filling, curing, and cooling. To date, most of the theoretical studies have focused on the mold filling of SMC parts.

Silva-Nieto, et al. [1980] proposed an incompressible isotropic model for the flow of sheet molding compound (SMC). They used finite difference technique to solve the governing equations of the SMC flow. Their model was based on the following assumptions:

1) The material is uniform, homogeneous, isotropic and incompressible.
2) The material has constant viscosity and the flow is Newtonian.

3) No fiber reorientation.

The main objective of their work was to obtain an optimum charge shape in order to mold a part free of weld-line. A tailored charge shape was proposed according to their model, which let the flow front meet near the mold edges simultaneously, resulting in parts free of weld-line.

Lee and Tucker [1987] and Lee, et al. [1984] used the finite element method to solve the mold flow equations of SMC compression molding. The assumptions of their model include:

1) The mold is thin and flat,
2) The material is incompressible and isotropic,
3) The viscosity depends on strain rate, temperature, and degree of cure,
4) The no-slip boundary condition applies at the mold surfaces.

The above assumptions are, in fact, the same as the generalized Hele-Shaw flow. Although the viscosity of the charge was assumed to be temperature dependent, the charge was assumed to be isothermal during molding. In simulation of molding, the element mesh was distorted significantly due to the no-slip boundary condition. They
applied the remeshing technique when the element shape was distorted up to a pre-determined degree.

Barone and Caulk [1988], based on the observations of their experiments on the compression molding of charges consisting of black and white SMC [Barone and Caulk, 1985], assumed that the mold flow of SMC is a two-dimensional membrane-like sheet. The sheet under compression extends uniformly through the cavity thickness with slip at the mold surface. They investigated three kinds of interface friction: (1) constant friction, (2) friction proportional to the relative velocity (hydrodynamic), and (3) friction proportional to the normal component of the stress vector (Coulomb). They assumed that the material resistance is negligible compared with the friction. By comparing with the experimental observation of the movement of flow-fronts, they concluded that the hydrodynamic model for the friction condition gives the best result.

The research group at OSU [Im, et al., 1987; Im, et al., 1988; Fan, et al., 1988a; Fan, et al., 1988b, Kim, et al., 1988; Kim, et al., 1989] proposed a power law constitutive equation with a yield stress to model the flow of silly-putty and SMC. The flow resistance of the molding material was measured by a squeeze flow rheometer. Based on the observation of the pressure curve they divided the compression molding into three stages. At the first stage, the compound is compacted and the air trapped in the compound is squeezed out. There is no outward flow and the pressure reading stays nearly zero in
this stage. In the second stage, the pressure starts to rise sharply with only a small reduction in charge thickness. The pressure increasing rate falls off at the beginning of the third stage. The pressure in this stage is referred to as the critical pressure. They used the ALPID (a FEM program for metal forming simulation) to simulate the non-isothermal flow of molding material. The calculated results compared well with the experimental data. Simulation of the molding of parts with substructure was not as successful as the one without substructure. The main reason for this discrepancy was explained as the presence of the anisotropy of the SMC charge. In addition, the abrupt change in molding pressure, due to the breakage of the bridge of fiber over the rib, is difficult to simulate using a continuum model.

2.3 Anisotropic Flow, Fiber Orientation and Fiber Content

In addition to anisotropy and the breakage of the fiber bridge over the structural rib, fiber reorientation and non-homogeneity in fiber content are also important issues in SMC manufacturing. Hirai [1986] proposed an anisotropic viscosity in simulating the filling of a T-shape mold. The viscosity used in his formulation was based on a modified isotropic plasticity theory. The flow rule was not derived directly from the anisotropic plasticity theory. By using an Eulerian description, he developed a progressive step-by-step analysis scheme to simulate the filling of a T-shape mold. It was found that the place on the top
surface of the substructure experiences tension force. These were the places where the sink mark might be present.

Hojo, et al. [1987], based on Hirai's anisotropic viscosity, proposed a method to calculate the distribution of fiber content in isothermally compression molded long-fiber-reinforced thermoplastic composites. The basic assumptions of their model were:

1) The material is a power law fluid and incompressible.
2) The velocity component in the thickness direction is negligible.
3) The fiber is in the shape of a sphere or a circular cylinder.

In their calculation, fibers are placed in the mold with constant spacing initially. The fiber content can be determined by determining the final position of each fiber after molding. Comparing with experimental results, their model predicted the fiber content reasonably well. They also concluded that the degree of non-homogeneity increases as the compression ratio increases or the closure speed decreases.

Kim, et al. [1992] modified the rigid-plastic FEM program, ALPID, based on Hill's theory of anisotropic plasticity theory. With the help from some experimental observations, they concluded that material anisotropy as well as friction in material/die interface played an important role in filling of substructure area. This study provided a new look at the sink mark problem. However, the results were
preliminary in that: (1) the anisotropic properties did not change according to the change of material principal axis; (2) only isothermal cases were discussed.

2.4 Techniques to Eliminate Sink Marks

Several techniques have been proposed to eliminate or reduce sink mark by investigation in the practices of SMC manufacturing.

a) Low Profile Additives (LPA)

The low profile additives (LPA) are typically thermoplastic materials which are mixed with the unsaturated polyester resin just prior to compounding. The main purpose of low profile additives is to compensate the polymerization shrinkage of the unsaturated polyester resin [Jutte, 1973; Ampthor, 1978; Kia, 1990]. As we mentioned earlier, although LPA can reduce the polymerization shrinkage, some other techniques must be used to minimize the sink mark.

b) Rib Geometry

Jutte [1973] recommended a minimum lead-in radius for the rib. Smith and Suh [1979] suggested a protruding entrance. In practice, minimum lead-in radius is the mostly used rib geometry. This is due to the difficulty of machining a mold with protruding edges.
c) Charge with Short and Long Fiber

A charge consisted of long glass fibers (2") over short fibers (1/4") was patented by Pfaff [1972]. However, this practice is not widely used in industries, partially due to the loss of mechanical properties by using short fibers.

d) Back pressure

Hirai and Yamabe [1990] suggested a back pressure to prevent the resin flow into the rib in the early stage of the filling, then a pressure release once the plate area has been filled. The major drawback of this method is the complexity of the mold set, in which the moving parts in the ribs must be tightly sealed to prevent resin from leaking, yet the parts must be able to move when the plate is filled.

e) Friction

Xu, et al., [1992] have observed that rough surface around the rib area may promote filling into the rib and reduce sink depth.

The effectiveness of these techniques will be examined by using the developed analysis method in a later part of this dissertation (Chapter 5).
Figure 2.7. Back pressure to eliminate sink mark [Hirai and Yamabe, 1990].
CHAPTER III
PROPOSED ANALYSIS METHOD

The manufacturing process to mold sheet molding compound (SMC) can be divided into three stages: filling, curing and cooling. In this chapter, the analysis method for modeling the transport phenomena in each of these stages is proposed and described in detail.

3.1 Mold Filling Stage

In the filling stage, a flat "charge" is placed into the mold cavity and the mold is closed to form the charge into the desired shape. A charge of SMC is a pre-weighted amount of material cut from a stack roll of SMC. In the actual manufacturing environment, the initial charge covers only 40-60% of the mold cavity surface. This is done to ensure adequate flow in order to expel the trapped air. Failure to expel the trapped air leads to a molded-in defect known as void formation. A major characteristic of the filling is large material deformation.

Many approaches used in numerically simulating the filling stage in SMC compression molding [Silva-Nieto, et al., 1980; Lee and Tucker, 1987; Barone and Caulk, 1988; Fan, et al., 1988b] have assumed that the material is macroscopically homogeneous. Barone and Caulk [1988] assumed that the SMC behaved as a two-dimensional membrane-link thin part. Although this membrane
assumption makes it possible to investigate SMC mold filling of parts with complex geometry, the approach is not suitable for the study of the formation of the sink mark defect due to part strengthening substructures. In this study, the finite element formulation used by Fan, et al. [1988b] was implemented to calculate SMC material velocity during mold filling. In this investigation, material flow is restricted to plane strain case. The restriction is dictated by the limitation of the FEM program. Nevertheless, this approach enables the investigation of the complex flow pattern into the part-strengthening substructure area.

Hojo, et al. [1987] proposed a fiber/resin separation model to calculate the individual velocities of the resin, the fiber, and the combined composite material. With these velocities, one can ultimately predict the resin content distribution in a flat plate sample. Implementation of this method on parts with a complex geometry and parts with part-strengthening substructure is more difficult.

The objective of this phase of the study is to apply the plane strain FEM formulation to calculate the velocity of the resin/fiber combined composite material. Additionally, a resin/fiber separation model, similar to the one by Hojo, et al. [1987], is incorporated to predict the resin distribution after completion of mold filling. The advantage of this technique combining plane strain flow with a resin/fiber separation model is the ability to predict the resin distribution in parts with a complex geometry. The drawback of this approach is that the simulation is restricted to cases of plane-strain.
In this study, the material is assumed to be isotropic and macroscopically homogeneous in calculating the velocity of the resin/fiber combined composite material. However, the SMC charge usually has long fibers (0.5 - 2 in) randomly distributed on the plane of the sheet. Due to this fiber arrangement, the SMC material shows anisotropic flow and bridge-and-looping in the filling stage. These characteristics are neglected in this study. Kim et al. [1992] has developed the anisotropic flow for the SMC material flow. It is possible to predict the resin distribution with anisotropic flow in the future. As for the bridge-and-looping, it still needs more extensive investigation until it can be understand how and when it happens.

3.1.1 Material Flow

In this investigation, the material is assumed to be rigid-plastic. Further, the material is assumed to follow the von Mises yielding criterion. This approach has been successfully implemented by Im et al. [1988]. The governing equations for the deformation of rigid-viscoplastic materials include equilibrium equations, strain rate and velocity relationship, and constitutive or material properties equations. Additionally, the incompressibility condition is assumed to apply during the plastic deformation. Finally, the energy equation is necessary during mold filling to accommodate the heat transfer from the mold to the workpiece as well as heat generated by plastic work and by chemical exotherm.
the mold to the workpiece as well as heat generated by plastic work and by chemical exotherm.

The rigid-plastic finite element formulation has been developed by Kobayashi and his co-workers [Kobayashi et al., 1989]. In fact, a commercial FEM package, DEFORM [1991], also based on this formulation. In this study, DEFORM will be used to calculate the flow of the composite material during the mold filling stage. A separate model to determine the resin/fiber distribution will be described in the next section. The rigid-plastic FEM is briefly described in the following. Detailed derivation of the equations can be found in [Kobayashi et al., 1989].

Consider a body occupying a volume V in a space at any instant. A traction $F$ is prescribed on a portion of the surface $S_F$, and a velocity $U$ is prescribed on the remainder of the surface $S_u$. The stresses, $\sigma_{ij}$, and the velocities, $u_i$, in the body must satisfy the following equations, repeated indices imply summation over the range of indices.

(a) Equilibrium equations:

\[ \sigma_{ij} = 0 \text{ in } V, \ i,j=1-3, \]  

(3.1)

where

$\sigma_{ij} = \text{stress component}$,
(b) Energy balance equation:

\[(\kappa_i T_i)_i - \rho c \dot{T} + \dot{r} = 0\]  \hspace{1cm} (3.2)

where

- \(T\) = temperature,
- \(\dot{T}\) = temperature rate,
- \(\kappa_i\) = thermal conductivity in the \(i\)-direction,
- \(\rho\) = density,
- \(c\) = specific heat at constant pressure, and
- \(\dot{r}\) = rate of heat generation per unit volume.

(c) Strain rate - velocity relationship:

\[\dot{\varepsilon}_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i})\]  \hspace{1cm} (3.3)

where

- \(\dot{\varepsilon}_{ij}\) = strain rate component,
- \(u_{ij}\) = velocity component.

(d) Incompressibility:

\[\dot{\varepsilon}_v = u_{i,i} = 0\]  \hspace{1cm} (3.4)

where

- \(\dot{\varepsilon}_v\) = volumetric strain rate,
Constitutive equations:

\[ \dot{\varepsilon}_y = \frac{3}{2} \frac{\dot{\varepsilon}}{\sigma} s_y \]  
(3.5)

where

\[ s_y = \text{deviatoric stress} \]

\[ = \sigma_y - \frac{1}{3} \delta_{yy} \sigma_{kk} \]  
(3.6)

\[ \bar{\sigma} = \text{effective stress} \]

\[ = \sqrt{\frac{3}{2}} \sigma_y \sigma_{yy} \]  
(3.7)

\[ \dot{\varepsilon} = \text{effective strain} \]

\[ = \sqrt{\frac{3}{2}} \dot{\varepsilon}_y \dot{\varepsilon}_y \]  
(3.8)

\[ \delta_{yy} = \text{Kronecker delta function.} \]

The rate of heat generation in the energy balance equation (3.2) includes the heat generation from plastic work and from chemical reaction. In plastic deformation, \( \bar{\sigma} = \sigma_y \) where \( \sigma_y \) is the flow stress. The flow stress \( \sigma_y \), in general, is a function of strain, strain rate and temperature. For the present case considering SMC, the flow stress is dependent on many other variables including fiber content and fractional conversion of the resin, i.e.,

\[ \sigma_y = \sigma_y(\bar{\varepsilon}, \dot{\varepsilon}, T, q_f, \alpha_c). \]  
(3.9)

where

\[ q_f = \text{fiber content} \]
\( \alpha_c = \) fractional conversion of the resin.

(f) Boundary conditions:

\[
F_j = F_j^* \quad \text{on } S_F, \quad (3.10)
\]

\[
u_i = U_i^* \quad \text{on } S_u, \quad (3.11)
\]

\[
T = T^* \quad \text{on } S_T, \quad (3.12)
\]

\[
q_n = q_n^* = \kappa_n \left( \frac{\partial T^*}{\partial n} \right) \quad \text{on } S_q. \quad (3.13)
\]

where the asterisks represent the quantity prescribed.

It should be noted that Equations (3.1-3.2) and the boundary conditions (3.10 - 3.13) define a complete set of boundary value problem. By using (3.3) and (3.5), the equilibrium equations can be solved for the dependent variables \( u_i \).

The equilibrium equation (3.1) and the energy balance equation (3.2) can be equivalently written in a weak form.

\[
\int_V \sigma_{ij} \delta u_i dV + \int_S (F^*_i - F_i) \delta u_i dS = 0 \quad (3.14)
\]

\[
\int_V \left[ (\kappa_i T_i)_i - \rho c \dot{T} + \frac{1}{2} \delta T dV + \int_S (q_n^* - q_n) \delta T dS = 0 \quad (3.15)
\]

The variations \( \delta u_i \) and \( \delta T \) satisfy the essential boundary conditions (3.11), but are arbitrary elsewhere. Through the standard FEM
discretization and manipulation, Equations (3.14) and (3.15) can be written in the following compact matrix forms:

\[
[K][U]=[P],
\tag{3.16}
\]

\[
\begin{bmatrix}
[K_i] + \frac{1}{\rho \Delta t}[C] + [Q] \\
\end{bmatrix} [T]_i = [r] + [q_1] + [q_2] + [C][\hat{r}],
\tag{3.17}
\]

where

\[
[K] = \left\{ \int [B]^T[D][B]dV \right\} + \left\{ \int [B]^T[M]^T k[M][B]dV \right\},
\tag{3.18}
\]

\[
[P] = \int [N]^T[F']dS,
\tag{3.19}
\]

\[
[K_i] = \int [\kappa_i][M]^T[M]dV,
\tag{3.20}
\]

\[
[C] = \int [\rho c][N]^T[N]dV,
\tag{3.21}
\]

\[
[Q] = \int_s \langle h, h_{ub} \rangle [N]^T[N]dS,
\tag{3.22}
\]

\[
[r] = \int [N]^TdV,
\tag{3.23}
\]

\[
[q_1] = \int_s \langle \sigma, \varepsilon, (T_e^4 - T_s^4), q_f \rangle [N]^T dS,
\tag{3.24}
\]

\[
[q_2] = \int_s \langle h, h_{ub} \rangle [N]^T T_e dV.
\tag{3.25}
\]
\[
\hat{T} = -\frac{1}{\beta \Delta t} T_{t+\Delta t} - \frac{1-\beta}{\beta} \hat{T}_{t-\Delta t}
\]

\(<A, B> = A \text{ or } B
\]

\(\beta\) = constant between 0 and 1,
\(t\) = time
\(\Delta t\) = time increment
\(h\) = environment convection heat transfer coefficient,
\(h_{\text{sub}}\) = heat transfer coefficient between mold and workpiece,
\(\sigma_r\) = the Stephen-Boltzman constant,
\(\varepsilon_r\) = emissivity,
\(T_e\) = environment temperature,
\(T_s\) = the surface temperature.

In this study, DEFORM was used to calculate the composite velocity with some add-on calculations described in subsequent sections.

3.1.2 Resin/Fiber Separation Model

Resin rich areas and fiber rich areas are commonly observed in the cross-section of a flat part with strengthening ribs. It is believed that the appearance of these resin rich or fiber rich areas plays a very important role in the formation of the sink mark surface defect [Ampthor, 1978; Kia, 1990]. Primarily, sink mark defects form because of greater shrinkage in resin rich area than in the bulk resin/fiber combined material. In the present study, a resin/fiber separation
model is incorporated into the FEM program to estimate the resin/fiber content variation. The resin/fiber separation model is based on the motion of individual fibers in a viscous resin flow.

The equation of motion for a single fiber in a resin matrix can be written as follows [Jeffrey, 1922]:

\[
\frac{m_r}{dt} = C_d \rho_m (v_m - v_f)^2 a_f + m_f g \frac{\rho_f - \rho_m \cos \Theta}{\rho_m} - f_r
\]

(3.26)

where

- \(m_f\) = mass of fiber,
- \(v_f\) = velocity of fiber,
- \(C_d\) = drag coefficient,
- \(\rho_m\) = density of resin,
- \(v_m\) = velocity of resin,
- \(a_f\) = cross-sectional area of fiber,
- \(\rho_f\) = density of fiber,
- \(g\) = gravitational constant,
- \(\Theta\) = angle between vertical direction and major axis of fiber,
- \(f_r\) = mutual restraint force due to frictional and interwound forces of fibers.

The inertial term, \(m_f \frac{dv_f}{dt}\), is negligible because the Reynolds number is very small [Hojo, et al., 1987]. The gravity and buoyancy
terms, \( m_f g \frac{\rho_f - \rho_m}{\rho_m} \cos \Theta \), can also be neglected. Therefore, Equation (3.26) can be simplified as

\[
C_d \rho_m (v_m - v_f)^2 a = f_r.
\]  

(3.27)

For a Newtonian fluid, the drag coefficient can be approximated as a function of the Reynolds number, \( R_{ef} \), and two parameters, \( k_1 \) and \( k_2 \), if the Reynolds number is small [Hojo, et al., 1988]. For a non-Newtonian fluid, the drag coefficient can be expressed as [Hojo, et al., 1987]

\[
C_d = j k_1 R_{ef}^{-k_2}
\]  

(3.28)

with

\[
R_{ef} = \frac{(v_m - v_f)d_f \rho_m}{\mu_m}
\]  

(3.29)

where

- \( j \) = correction factor,
- \( d_f \) = fiber diameter,
- \( k_1 \) = parameter,
- \( k_2 \) = parameter,
- \( \mu_m \) = viscosity of resin.

For spherical particle, the parameters \( k_1 \) and \( k_2 \) are 24.0 and 1.0, respectively [Hojo, et al., 1987]. Hence, the difference of fiber velocity
and matrix velocity can be found from Equations (3.27), (3.28) and (3.29) as

$$v_m - v_f = \frac{d f_r}{24 J a d \mu_m}.$$  

(3.30)

By assuming that the composite material velocity can be obtained from the rule of mixtures, i.e.

$$v_c = q_f v_f + (1 - q_f) v_m,$$  

(3.31)

the fiber and resin matrix velocities can each be determined from Equations (3.30) and (3.31) by providing the mutual restraint force $f_r$ and the composite material velocity $v_c$. As mention earlier, the composite material velocity is to be obtained by using the finite element program DEFORM. Presently, the mutual restraint force, $f_r$, can not be determined theoretically. Therefore, the mutual restraint force must be measured experimentally.

For a one-dimensional problem, the two unknown quantities, $v_f$ and $v_m$, can be determined by solving Equations (3.30) and (3.31). However, for a multi-dimensional problem, there are more unknown quantities than equations available and the problem is under-defined. For example a two-dimensional problem has four unknown variables, $(v_{fr}, v_{fy}, v_{mx} \text{ and } v_{my})$, but only three available equations: one in Equation (3.30) and two in Equation (3.31). Therefore, some additional
conditions must be provided to calculate the resin and fiber velocity in a multi-dimensional case.

A modified one-dimensional model was used in this study. In the model, it is assumed that there is no resin flow across the SMC charge plies. That means the resin flow is parallel to the current charge ply direction.

The algorithm in tracking the orientation of the ply is adopted from Tszeng [1992]. Figure 3.1 shows the translation and rotation of a fiber during incremental deformation. For an inextensible fiber, the relation for the new fiber angle $\phi''$ is

$$
\tan \phi'' = \frac{\Delta s \sin \phi - \Delta u_x \sin \phi \cos \phi + \Delta u_y \cos^2 \phi}{\Delta s \cos \phi + \Delta u_x \sin^2 \phi - \Delta u_y \sin \phi \cos \phi}
$$

(3.32)

where $\phi$ is the original orientation, $\Delta s$ is the fiber length and $\Delta u_x$ and $\Delta u_y$ are the components of the relative velocity between the two end points A and B (see Figure 3.1).

Tracking of the fiber content during the molding process is performed by assigning a certain number of regularly spaced points in the initial element mesh to represent the fiber in the charge. At each time step, the velocities of these fiber points are calculated by interpolating the fiber velocities at the nodal points. Positions of the fiber points can then be updated according to the fiber velocities. The new fiber content is calculated by counting the number of fiber points within each element.
Figure 3.1. Translation and rotation of a fiber during incremental deformation [Tszeng, 1992].
3.2 Resin Curing and Cooling Stage

3.2.1 Kinetic Model of Curing

After the charge has completely filled the cavity, the mold remains closed to allow the curing reaction (polymerization) to run to completion. The rate of conversion from monomer to polymer depends on the individual chemical compounds in the charge, as well as on the temperature and temperature history. The chemical reaction generates heat which contributes to an overall temperature rise in the part. A sudden temperature rise due to a high chemical reaction rate may cause scorching or charring problem. The chemical compound must be carefully formulated to ensure that the chemical reaction proceeds as quickly as possible, while avoiding scorching or charring problem.

The cure reaction of SMC is a free radical chain growth copolymerization between a styrene monomer and an unsaturated polyester molecule [Fan, et al. 1988b]. Kamal, et al. [1973] used an empirical equation to fit the reaction rate profiles of unsaturated polyester resins from differential scanning calorimetry (DSC) data. By definition, the empirical model fits the experimental data, however it does not consider the true reaction mechanism of free radical polymerization. Therefore, true empirical approach is of limited value outside the range of the DSC data. That is, extrapolation to reaction conditions beyond the scope of the DSC data is dangerous, at best. Therefore, a mechanistic approach is implemented in this work. The
kinetic model proposed by Stevenson [1980] and Lee [1981] is used in this study. There are several more complex models [Stevenson, 1986; Huang, et al., 1989] which are capable of accommodating more complex reaction systems and providing more detailed information. However, these models are also more difficult to define for a particular system and more difficult to implement. The kinetic model implemented for this study is adequate in predicting reaction kinetics insofar as the results are used in ultimately determine the formation of sink mark defect. The aforementioned kinetic model is briefly described in the following set of equations. A more detailed description can be found in the literature [Stevenson, 1980, 1986; Lee, 1981].

The SMC material cure reaction can be described as a combination of three steps: initiation, inhibition, and propagation. The useful curing reaction begins when the number of developed initiator radicals equals the effective number of inhibitor molecules initially present. That is, reaction begins as initiator moleculars are created. However, inhibiting moleculars consume or “kill” the initiates until no more inhibitors remain. At that point, the reaction can be effectively considered to begin converting monomers to the polymer. The governing equations for each of these three steps can be written as

Initiation:
\[
\frac{d[R^*]}{dt} = 2k_dI
\]  
(3.33)
where

\([R \cdot]\) = concentration of free radical

\(k_d = \text{rate constant of initiator decomposition}
\)

\(= A_d \exp(-E_d/RT)\)

\(I = \text{concentration of initiator.}\)

Inhibition:

\[ qZ_o = 2f_o \left(1 - \exp \left(\int_0^{t_z} k_d \, dt \right) \right) \]

\[ = 2f(I_o - I_r) \quad (3.34) \]

where

\(I_o = \text{initial concentration of initiator}\)

\(Z_o = \text{initial concentration of inhibitor}\)

\(I_r = \text{concentration of residual initiator after all the inhibitors}
\)

\(\text{having been consumed}\)

\(f = \text{initiator efficiency}\)

\(q = \text{inhibitor efficiency}\)

\(t_z = \text{induction time before propagation.}\)

Propagation:

\[ \frac{dM}{dt} = -k_p M[R \cdot] \quad (3.35) \]

or
\[
\frac{d\alpha_c}{dt} = 2f(t)k_p(1 - \alpha_c)\left[1 - \exp\left(\int_{t_0}^{t-\tau} k_d(t - t_\tau)\,dt\right)\right]
\]  \hspace{1cm} (3.36)

where

\[M = \text{monomer concentration}\]
\[k_p = \text{rate constant of monomer propagation}\]
\[= A_p \exp(-E_p/RT)\]
\[\alpha_c = \text{fractional conversion.}\]

The constants, \(k_d\) and \(k_p\), in this model are determined by using data from DSC [Lee, 1981].

The chemical reaction may start as soon as the charge has been placed on the lower mold surface. Since mold filling takes only a few seconds and the curing stage takes 40 - 80 seconds, it is justifiable to neglect the chemical reaction during the mold filling stage [Kia, 1991]. Although the chemical reaction is assumed not to start until the mold cavity is completely filled, the heat transfer from the mold to the workpiece or flowing charge in the mold filling stage still influences the curing stage by changing the initial temperature of the curing stage.

The kinetic model is implemented as a heat generation routine in ABAQUS [1989], see Appendix A. The temperature distribution at the end of the mold filling stage is extracted from the DEFORM data base and used as the input initial temperature conditions in ABAQUS.
3.2.2 Physical Properties and Shrinkage during Curing and Cooling

The physical and mechanical properties of the polymer composite product are functions of resin content, molding and curing temperatures, and fractional conversion of monomer to polymer or extent of reaction. Thus, the physical and mechanical properties continuously vary during the manufacturing process. In the time stepping calculation, the heat transfer including chemical reaction is computed first in each step. Subsequently, the temperature and curing results are extracted and used in the deformation analysis. The mechanical properties used in stress analysis are based on a linear interpolation as shown in Figure 3.2. The material is assumed to behave as a fluid (Poisson's ratio = 0.499) for a fractional conversion below a certain level (5% in this study). At the end of curing (fractional conversion ≥ 80%), the material is regarded as having its final mechanical properties (Poisson's ratio = 0.34). In the curing process, the Poisson's ratio is assumed to vary linearly between 0.499 and 0.34, i.e. Osswald [1991].

The shrinkage due to the temperature change can be converted into stresses through the coefficient of thermal expansion in the ABAQUS program. However, the polymerization shrinkage needs to be processed outside the main program. The calculation of the stresses during the curing process is divided into several steps with small temperature increments at the nodes for each step. The polymerization shrinkage is then converted for an equivalent temperature change and added into the temperature increment at the corresponding step. The
relation between the amount of shrinkage and the fractional conversion is assumed to be linear. That is, the fractional amount of total polymerization shrinkage at each step corresponds to the fractional increment of the reaction conversion.

![Figure 3.2](image)  

**Figure 3.2.** Assumed material properties as a function of conversion [Osswald, 1991].
3.3 Procedure for Simulation of the Molding Process

The procedure for simulation of the molding process is shown in a block diagram (Figure 3.3). The simulation begins with the initial charge of SMC material pre-located in the central region of the mold cavity. The charge is compressed to take the shape of mold cavity. DEFORM is used for determining the composite material flow during the filling stage. After the mold is completely filled, the nodal velocities and the nodal temperatures at each time step are extracted from the DEFORM data base. These velocity and temperature histories are read to the fiber/resin separation model to calculate the resin/fiber content distribution.

After calculation of the resin content, the distribution of temperature and stress data at the end of mold filling are transferred from the DEFORM program to the ABAQUS as the initial conditions for the curing stage. The resin content from the fiber/resin separation model is also transferred to the ABAQUS input file. The heat transfer analysis, including polymerization reaction, is carried out first. The temperature and fractional conversion histories are extracted from the ABAQUS data base. The entire curing process is divided into several steps. The step size is determined by the maximum temperature increment in the ABAQUS input file. The ABAQUS program will reduce the time increment if the temperature increment at any node exceeds the pre-determined amount. The polymerization shrinkage is incorporated into the temperature data.
The cooling stage is an extension of the curing stage. The temperature drops from the final curing temperature to room temperature. The added modules used in the calculation are listed in Appendix A.
Figure 3.3. Procedure of numerical simulation of molding process.
3.4 Concluding Remarks

The numerical procedure to predict the formation of the sink mark defect was described in this chapter. The molding process was divided into three stages, namely mold filling, resin curing, and composite cooling. Based on the work of Fan et al. [1988b], in the filling stage the material was assumed to be isotropic and rigid-viscoplastic, for the calculation of the composite material velocity. A resin/fiber model based on Jeffrey's fiber suspension model was developed to predict the resin content distribution. In contrast to the model proposed by Hojo et al. [1987], the resin/fiber separation model was implemented with finite element program which extended the capability of the model to deal with complex geometry and flow.

The material in the curing stage was assumed to be elastic-plastic. The kinetic model based on that of Stevenson [1980] and Lee [1981] was programmed as a heat generation subroutine in a commercial FEM program, ABAQUS. A computational scheme was developed to account for the polymerization shrinkage during the solidification. The cooling stage was finally analyzed by the ABAQUS program.

Among the framework of the proposed procedure for simulation of the molding process, there are some limitations and future work which should be addressed.

1. The phenomenon of resin/fiber separation does not affect the composite material flow during mold filling. The flow stress is a function of resin/fiber content. However, this is not
implemented in this study due to the limitation of the FEM package selected. It is necessary to implement the flow stress as a function of resin content in the future development.

2. Determination of the mutual restraint force, $f_r$, is not established. The mutual restraint force should be a function of fiber content, fiber length (aspect ratio), orientation, and sizing (surface treatment) of the fiber. It may also change as the fiber configuration changes during mold filling. All of these issues need an in-depth investigation of interaction between fibers.

3. The anisotropic fiber configuration in the SMC material is neglected. The assumption of isotropic material properties needs to be removed to accommodate the anisotropic flow properties due to the special fiber distribution pattern of the SMC material. The bridging-and-looping flow mechanism during the filling of the rib area is an important factor in the formation of the resin rich area [Kia, 1991]. It is a challenge for the future work to be able to model this flow mechanism.

4. The calculations of heat transfer and displacement are uncoupled. It is assumed that the displacement of the SMC material during curing does not affect the heat transfer characteristics. In fact, the SMC material would lose contact locally with the mold surface near peak exotherm due to the polymerization shrinkage. The boundary conditions in heat transfer should be adjusted accordingly. For future
development, it would require a new numerical scheme to calculate the heat transfer at a smaller time step and to calculate the displacement only at necessary steps.
CHAPTER IV
THEORETICAL PREDICTION OF SINK MARK FORMATION

A better understanding of sink mark formation and the techniques to minimize the sink mark are highly demanded, primarily due to the economic advantages of integrating strengthening support ribs into flat plates. There are several experimental studies [Jutte, 1973; Ampthor, 1978; Dziewałkoski, et al., 1992] which investigate the formation of the sink mark defect. Unfortunately, all of these studies involve very costly experiments. A theoretical modeling approach would be very advantageous in exploring the techniques to minimize the sink mark problem. This chapter describes how the modeling technique has been employed to calculate the formation of sink marks. The interfacial heat transfer in the molding process will be described first, followed by the verification of the filling and the curing models. Subsequently, the calculation of the sink mark formation will be discussed in detail for the three stages of mold filling, resin curing, and SMC composite cooling.

4.1 Interfacial Heat Transfer

The heat transfer coefficient between the mold surface and the charge (or workpiece) surface in non-isothermal forming processes,
such as compression molding of SMC or hot forging of metal pieces, plays an essential role in the successful transfer of heat from the mold to the workpiece. It has been reported that in the forging of metals, the interfacial heat transfer coefficient (IHTC) changes with different lubricants and with the molding pressure [Burte, et al., 1989]. In the compression molding of SMC, the pressure difference between the mold surface and the charge can vary from near zero at the free resting state up to 1500 psi during molding [Meyer, 1986]. The flow stresses in an SMC charge are more sensitive to temperature variations than those in a metal workpiece. Therefore it is expected that the IHTC will change more rapidly in compression molding of SMC than in the non-isothermal forming of metal pieces. Hence, a better knowledge of the IHTC is critical for correctly modeling the entire molding process.

The following results illustrate how the temperature history at a single point in the charge is experimentally measured for different clamping pressures. Additionally, the temperature is theoretically calculated by varying the IHTC. By directly comparing these two sets of data, the best IHTC can then be determined.

A molding set-up (Figure 4.1), previously designed for resin transfer molding (RTM), was instrumented with thermocouples at different positions. A data acquisition system was used to collect the temperature data. The information was used to study the variation of heat transfer coefficient as a function of the interfacial pressure. Figure 4.2 illustrates the geometry of the mold and the locations of the thermocouples. The mold was heated to a steady state temperature
using Omega temperature controllers. The temperature of the mold, measured by T/C #3 shown in Figure 4.1, dropped 2 °C in 2 minutes with no loading on the charge and dropped 4 °C in two minutes with 2.5 psi pressure applied to the charge.

The experimental data are shown in Figure 4.3. The results illustrate that a higher molding pressure promotes more efficient heat transfer from the mold or tool to the SMC charge. The reason for this is that a higher molding pressure increases the contact area of the hot tool on the deformable SMC charge. Increasing the contact area effectively increases the IHTC by reducing the interfacial voids trapped between the tool and the workpiece.

Theoretical calculation of the temperature history was performed by solving a 1-D heat transfer problem. The 2-D heat transfer module in DEFORM was used to perform the numerical calculation with the proper boundary conditions as shown in Figure 4.4. The boundary conditions for the cross-sectional surfaces were set in the program as insulated surfaces. This ensures that heat transfers only in the thickness direction. The IHTC between individual charge layers was assumed to be the same as the IHTC between the mold surface and the SMC charge. It was further assumed that the temperature at the base of the mold was constant. Heat transfer from the top surface of the SMC charge was assumed to occur by free convection to the environment.

The calculated temperature at the interface of the first ply and the second ply was taken as the average temperature of two contact points
at the interface. The measured temperature for the case when no pressure was applied is plotted along with the calculated temperature histories for three different IHTC in Figure 4.5. According to Figure 4.5, a value of 0.05 W/m²·°C is appropriate for the IHTC in the initial dwelling period when no pressure is applied. In the computation of the IHTC at higher molding pressures, the charge pattern described in Figure 4.4 was modified by adding a steel top plate to account for the dead weight used in the experiment. The IHTC between the SMC charge and the steel plate was assumed to be the same as with the other interfaces. The free convection boundary was then moved to the top surface of the steel plate. The measured data and the calculated data for the high interface pressure case are illustrated in Figure 4.6. From Figure 4.6 it can be seen that the measured temperature rises more rapidly than the theoretical curves. This discrepancy is believed to be due in part to the assumption of 1-D heat transfer in the theoretical calculation. The charge in the experiment has a limited cross-section and therefore the thermal inertia is much smaller in the experiment than in the theoretical calculation. Another factor contributing to the discrepancy may be that the surface texture is not only a function of pressure, but it is also a function of temperature. As the temperature rises, the material becomes soft. Therefore, the voids at the interface may diminish more easily at higher temperatures which effectively increases the IHTC. The complex interfacial phenomena require an investigation far beyond the scope of this study. For this work, the IHTC was assumed to maintain the value of 0.05
W/m$^2$-°C during the initial dwelling period of the molding of the SMC charge and to have a value of 0.5 W/m$^2$-°C during compression period, per Fan, et al. [1988b]. These values yield a satisfactory result at a verification described later.
Figure 4.1. Experimental set-up for measuring interfacial heat transfer coefficient.
thermocouples
#1 & #3
51 mm (2 in)
thermocouple #2
51 mm (2 in)
band heaters
dead weight
(steel plate)
thermocouple #1
6.3 mm (.25 in)
4.8 mm (3/16 in)
thermocouple #2
2.1 mm (0.083 in)
4.8 mm (3/16 in)
thermocouple #3
19 mm (3/4 in)

Figure 4.2. Thermocouple locations of mold and charge, (a) top view, (b) side view.
Figure 4.3 Measured temperature history at the interface of first and second layers ($T_m=63^\circ C$, $T_j=23^\circ C$).
Figure 4.4 Boundary conditions in computation of temperature distribution at different IHTC.
Figure 4.5  Measured temperature history (symbols) and theoretical calculation (lines) at the interface of first and second layers with no pressure on the charge ($T_m=63^\circ C$, $T_i=23^\circ C$).
Figure 4.6 Measured temperature history (symbols) and theoretical calculation (lines) at the interface of first and second layers with a pressure of 2.5 psi on the charge ($T_m=63^\circ C$, $T_f=23^\circ C$).
4.2 Verification of Mold Filling and Resin Curing Simulation

The proposed simulation technique was verified by comparing the simulation results with experimental results reported by Fan et al. [1988b]. The test part was 178 mm (7 in) wide and 4.1 mm (0.2 in) thick with a 6.35 mm (0.25 in) thick by 17.8 mm (0.7 in) deep strengthening support rib. The dimensions of the mold and the charge are shown in Figure 4.7. Two thermocouples were buried in the charge to measure the temperature during compression molding. These thermocouples were also used as tracking points for the flow front progression during mold filling. The mold was closed at a speed of 25.4 mm/ min. (1 in/min.). The mold temperature was set at 130 °C (266 °F).

The material properties used in the simulation are listed in Table 4.1. The kinetic model used for the chemical reaction was adopted from Stevenson's [1980] work as described in Chapter 3. The flow stress was assumed to be the same as in Fan's work [Fan et al., 1988b],

\[
\bar{\sigma} = \sigma_0 + \kappa \dot{\varepsilon}^{0.155} \tag{4.3}
\]

where

\[
\sigma_0 = 0.0532 \times 10^{3010.0(1 / T - 1 / 295)} \tag{4.4}
\]

\[
\kappa = 2.4574 \times 10^{880(1 / T - 1 / 295)} \tag{4.5}
\]

The dwelling time was assumed to be 10 seconds. In this period, a low IHTC of 0.05 W/m²°C was used between the charge and the lower
mold surface. As the mold filling stage began, the IHTC was given a value ten times higher, or 0.5 w/m²-°C which is the same value used by Fan et al. [1988b]. The flow front progression measured at the tracking points in the molding experiment is compared to the simulated flow front in Table 4.2. Simulation agrees reasonably well with the experimental data. As can be expected, the prediction of filling the rib (point No. 1) does not agree with the data as well as the simulation in the plate area. Discrepancy may arise from the assumption of a single-layered charge or from the assumption of isotropic properties. The temperature curves at points No. 1 and No. 2 are shown in Figures 4.8 and 4.9, respectively. The temperature prediction at point No. 2 is very close to the experimental measurement. At point No. 1, the simulation has a higher peak exotherm temperature than in the actual molding. However, the overall temperature prediction agrees reasonably well with the experiment at both points. In a previous study by Fan [Fan, et al., 1988b], the time to reach the peak exotherm occurred at nearly the same point as in the current simulation. Similarities in the curing model and the molding parameters account for the agreement. The most prominent difference in these two computations are the temperatures at the peak exotherm. This study took advantage of the automatic time step increment adjustment in ABAQUS which resulted in a smaller overshoot compared to the experimental peak height. Based on this point alone, the current study shows an improvement over the previous work.
Figure 4.7. Schematic of mold setup showing the locations of two thermocouples before molding, [Fan, et al., 1988b].
Table 4.1. Thermal and chemical kinetic data for SMC used in this study [Lee, 1981].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ (g / ml)</td>
<td>1.89</td>
</tr>
<tr>
<td>$C_p$ (N·m / kg·°C)</td>
<td>1.083</td>
</tr>
<tr>
<td>$k$ (N·m / m·s·°C)</td>
<td>0.3864</td>
</tr>
<tr>
<td>$h$ (N·m / m²·s·°C)</td>
<td>0.5</td>
</tr>
<tr>
<td>$h_{\text{free resting}}$ (N / m·s·°C)</td>
<td>0.05</td>
</tr>
<tr>
<td>$H_R$ (N·m / m³)</td>
<td>80</td>
</tr>
<tr>
<td>$A_d$ (app. unit)</td>
<td>$5.7242 \times 10^9$</td>
</tr>
<tr>
<td>$E_d$ (N·m / kg·mole)</td>
<td>16054</td>
</tr>
<tr>
<td>$A_R$ (app. unit)</td>
<td>$1.33 \times 10^9$</td>
</tr>
<tr>
<td>$E_R$ (N·m / kg·mole)</td>
<td>8410</td>
</tr>
<tr>
<td>$2f_{l_0}$ (mole / g·SMC)</td>
<td>$7.32 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 4.2. Comparison of traced points in molding of plate with rib, (mold temp. = 130 °C, mold closing speed = 1 in / min.).

<table>
<thead>
<tr>
<th>Point No.</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original Coor.</td>
<td>(0.0, 2.08)</td>
<td>(31.75, 2.08)</td>
</tr>
<tr>
<td>Molding Exp.</td>
<td>(0.0, -9.48)</td>
<td>(46.0, 1.04)</td>
</tr>
<tr>
<td>[Fan et al., 1988b]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Simulation</td>
<td>(0.0, -12.29)</td>
<td>(46.5, 1.04)</td>
</tr>
</tbody>
</table>

unit: mm
Figure 4.8. Comparison of temperature profiles between experimental data and simulation results in SMC molding at point no. 1 (mold temp.=130°C, mold closing speed=0.423 mm/sec., free resting period=10 sec.).
Figure 4.9. Comparison of temperature profiles between experimental data and simulation results in SMC molding at point no. 2 (mold temp. = 130°C, mold closing speed = 0.423 mm/sec., free resting period = 10 sec.).
4.3 Mold Filling Stage

The first stage in SMC compression molding is the mold filling stage. As described in a previous section (Section 3.3), the general purpose computer code DEFORM was utilized to determine the material flow. Additionally, a resin-fiber separation model was incorporated with the DEFORM calculations. The initial FEM mesh for the SMC charge and the mold geometry is shown in Figure 4.10. The charge rested on the bottom mold surface for 10 seconds (i.e. dwell time) before the upper mold came in contact with the workpiece. The mold temperature was set at 150 °C and the initial charge temperature was 25 °C. The mold closing speed was 8.47 mm/sec. (20 in/min.). The initial resin content in the charge was 79 % by volume (70 % wt.).

The calculated temperature distribution at the end of the free resting period or after the dwell time expired is shown in Figure 4.11. Due to the heating from mold surfaces, the SMC material closer to the tool was softer than the material farther inside the charge. As a consequence, the charge tended to fold at the free front, as shown in Figure 4.12. This is related to the spatial variation of flow stress described as follows. In compression molding of SMC, the mold is preheated to a high temperature in order to promote the chemical reaction (curing) within the SMC charge. The charge material in direct contact with the mold surface has a higher temperature than material farther inside the charge. Hence, the outer edge of the charge contacting the mold surface has a lower flow stress than the overall charge. The spatial variation of flow stress creates a different flow
pattern compared with the isothermal case. Figure 4.13 schematically illustrates four different flow patterns in a simple upsetting of a material whose flow stress was assumed to be a function of temperature only. When there is no friction, the velocity distribution is uniform in the isothermal case as shown in Figure 4.13a. The friction at the interface resists the flow in the vicinity of the interface. Therefore, the material at interface has a lower velocity as shown in Figure 4.13b. In the non-isothermal cases (Figure 4.13c), the material at the interface has a higher velocity due to the lower flow stress caused by the higher temperature. Although the friction decreases the velocity at the interface, the velocity at the interface is still higher than that in the center area, as shown in Figure 4.13d. In a sense, the molten SMC material at the interface serves to lubricate the workpiece. This preferential flow has been reported by Barone and Caulk [1985] as shown in Figure 4.14. The colored charge clearly shows preferential flow at the mold and workpiece interface. This preferential flow will cause folding when the flow front reaches the side wall and flows back on itself.

When the charge folds at a wall, no convergent solution can be achieved in the simulation. Continuation after folding was accomplished by slightly altering the charge geometry in the folding area and artificially filling the small cavity formed by the folded charge, see Figure 4.12. Subsequently, a new mesh was used. This procedure actually assumes that the contact surfaces become an internal material. Retention of the field variables (strains and temperatures),
was accomplished by interpolating the values in a program outside DEFORM. After artificially filling the fold's air pocket and creating the new mesh, the field variables were retrieved from the external interpolation program by the DEFORM code.

The calculated temperature distribution at the end of mold filling is shown in Figure 4.15. These results indicate that only a thin layer of the charge has been heated to a moderately high temperature (60 °C) during the entire mold filling period. At this temperature, the chemical reaction rate is very low, which justifies neglecting the contribution of chemical reaction in the mold filling stage.

To characterize the mutual restraint force described in Section 3.1, flat panels with 432 mm (17 in) width × 560 mm (22 in) length in molded in a member company of the Engineering Research Center. The SMC material used in the molding is formulated to have half amount of the filler (calcium carbonate) than regular molding material for reducing viscosity. The charge was 406 mm (16 in) width × 168 mm (6.6 in) length. It was place a one end of the mold cavity in order to have longer flow path to generate resin/fiber separation. The molded panels were cut into small piece at different positions to measure the resin content. The resin content was calculated by the weight difference before and after the piece being put in a oven to burn off all the resin. The measured resin contents at different positions showed no resin/fiber separation within measurement error. The implication of this molding experiment is that a special molding material with very low viscosity needs to be formulated. Current commercial molding
compound is formulated with very high viscosity to ensure no resin/fiber separation even at some extreme conditions. A possible way to reduce viscosity is to reduce the thickening agent. The purposes of thickening agent is to increase the viscosity for material handling. Therefore, reducing thickening agent would reduce compound viscosity.

For using in the numerical simulation, a estimated value of 0.5 which does not show resin/fiber separation in a simple flat panel, but shows resin/fiber separation in the molding of panels with integrated ribs was applied in this study. Therefore, the utility of this study is restricted to a qualitative investigation of the sink mark formation. Figure 4.16 illustrates the prediction of the resin content distribution in the vicinity of the rib entry after the completion of mold filling. Note that the initial resin content was assumed to be 0.79 (79% resin paste with 21% fiber). In this study, a region with resin content larger than 0.94 is regarded as resin rich area and a fiber rich area has a resin content smaller than 0.64. Figure 4.16 shows a fiber rich area on the inside edge of the rib entry, which is similar to the experimental observation by Kia [1991] (Figure 4.17). According to Figure 4.16, a resin rich area indeed appears directly on top of the rib entrance, which is also apparent in Figure 4.17. Note also that the simulation predicts a fiber rich area adjacent to the resin rich area. This juxtaposition of fiber and resin rich areas has not been experimentally observed. One reason for the discrepancy in the simulated results may arise from the assumption of a homogeneous and isotropic material
instead of the strata or layered structure of anisotropic material which truly describes the SMC charge. Additionally, some of the flow mechanisms observed experimentally, such as bridging-and-looping when the SMC ply bridges the rib prior to splitting and folding into the gap (much like shuffling a deck of cards,) cannot be presently simulated.
Figure 4.10. Initial finite element mesh of the charge and the mold.
Figure 4.11. Calculated temperature after free resting for 10 seconds (mold temp. = 150°C, initial charge temp. = 25°C).
Figure 4.12. Calculated temperature at the time when folding occurs in the filling stage (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25°C, free resting period=10 sec.).
Figure 4.13. Schematic of velocity distributions in simple upsetting. (a) isothermal without interface friction, (b) isothermal with interface friction, (c) non-isothermal without interface friction, (d) isothermal with interface friction.
Figure 4.14. Preferential flow observed by Barone and Caulk [1985] (mold temp. = 150°C, mold closing speed = 1.75 mm/sec.).
Figure 4.15. Calculated temperature at the end of filling stage (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.).
Figure 4.16. Calculated resin content distribution around the rib entrance area at the end of filling stage (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.).
Figure 4.17. Cross section at the rib entrance shows the fiber rich area and resin rich area [Kia, 1991].
4.4 Resin Curing Stage

Resin curing is assumed to begin immediately upon completion of filling the mold cavity. As shown in Figure 3.4, ABAQUS is the major computational tool in determining the temperature and fractional conversion of the monomer to the polymer during the resin curing stage. The initial conditions for the curing analysis were transferred from the mold filling analysis performed by the DEFORM code. A new mesh for resin curing and composite cooling is shown in Figure 4.18. The chemical reaction involved in polymerizing the original SMC charge is called an exothermic reaction because the cure reaction generates internal heat. This reaction exotherm is much like the heat generated as concrete or plaster solidifies. As a consequence of generating internal reaction heat, the composite temperature often peaks higher than the mold temperature. Thus, the mold acts as a heat source during mold filling and the initiation of the reaction. However, as the cure reaction proceeds, the mold participates as a heat sink. The mold temperature is designed such that curing can be completed as quickly as possible, yet no part of the charge is over-heated which could cause charring in the composite.

The calculated temperature and fractional conversion distributions are shown in Figures 4.19 through 4.23. The temperature is higher at the edge of the sections due to the higher surface to volume ratio which promotes heat conduction in the thickness direction. Hence, the curing reaction begins from the ends of the plate and the rib (see Figure 4.20). Due to the thickness difference,
the curing in the flat plate is completed earlier than the polymerization in the rib (see Figure 4.22). The rib entrance is the region at which curing finally ceases. Figure 4.23 corresponds to the moment when the curing reaction has completely finished. At that time step, the rib entrance area had a temperature higher than the mold temperature, indicative of the reaction exotherm.

Figure 4.18. Finite element mesh for resin curing and composite cooling.
Figure 4.19. Calculated temperature distribution at 20.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25°C, free resting period=10 sec.).
Figure 4.20. Calculated fractional conversion distribution at 20.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25°C, free resting period = 10 sec.).
Figure 4.21. Calculated temperature distribution at 30.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.).
Figure 4.22. Calculated fractional conversion distribution at 30.75 seconds after molding starts (in the curing stage, mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.).
Figure 4.23. Calculated temperature distribution at the end of curing stage (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25°C, free resting period=10 sec.).
4.5 Composite Cooling and Sink Mark Formation

After curing is completed, the SMC polymer composite part is ejected from the mold cavity. There are no constraints on the molded part except part weight. The stress and temperature distributions from the curing analysis were used as the initial conditions for the cooling analysis. ABAQUS was used to determine temperature, as well as shrinkage and deformation. To differentiate the contributions from several factors on the formation of the sink mark, calculations were first conducted for a part without considering the resin/fiber separation. Investigation of uniformly distributed fiber without polymerization shrinkage provided the net effects of non-homogeneous solidification (curing). Next, a small amount of polymerization shrinkage, 1.5%, was considered to investigate the effects of shrinkage due to polymerization. Once again referring to a similar process, this shrinkage is much like the shrinkage of poured concrete as it dries and cures. The center of the top surface was selected as a reference point with no displacement. Several top surface were compared based on this reference point.

In the case without polymerization shrinkage, the profile of the top surface shown in Figure 4.24 was rather straight, indicating a minimum deformation in this entire region except for the rib area. That is, the deformation was concentrated in the rib area where the cure reaction stopped last. As the polymerization shrinkage became more dominant, the area affected by the last cured zone spread out farther. The middle section had nearly no deformation because the
curing at this section was quite uniform, as seen in Figure 4.24. The effects of differential solidification at the edge of the plate existed only when polymerization shrinkage had occurred.

The effect of resin/fiber separation on sink mark formation is shown in Figure 4.25. Figure 4.25 illustrates that the surface profile of the part simulated using the resin/fiber separation model exhibited a valley and a hill. In contrast, the profile when the resin/fiber separation model was not considered exhibited a single smooth hill. Even with no polymerization shrinkage the resin rich area still caused a sink mark, as shown in Figure 4.26.

The depth of the sink mark was only around 2 μm. The sink depth of panels with different geometries and molding conditions measured by Jutte [1973] ranged from 1.8 μm (0.05 mil) to 30 μm (1.2 mil). In this study, the polymerization shrinkage accounted for only 1.5% due to the difficulty in the elastic-plastic displacement analysis. In addition, the prediction of resin distribution did not agree well with experimental observation. Hence, the results of this study cannot provide detailed quantitative predictions for sink mark formation under a variety of processing conditions. However, the advantage of this work is the ability to provide qualitative information about the formation of sink mark defects in SMC polymer composite products with strengthening support ribs. The upshot of these results is that the resin rich area formed over the rib plays a major role in the formation of the sink mark defect. These results corroborate the work by Kia [1990] which also indicates the direct cause and effect
relationship of resin rich region to sink mark formation. Further experimentation is recommended for future researchers to collect data to confirm the validity of the numerical simulations for the wide ranging levels of complexity and eloquence (i.e. simple upsetting to inclusion of a complex resin/fiber separation model). It is also suggested that a molding technique which minimizes resin/fiber separation would be the best strategy for eliminating the formation sink marks. The subsequent chapter discusses several techniques proposed to minimize the formation of sink marks.
Figure 4.24. Comparison of predicted top surface profiles of a plate with rib in two different amount of polymerization shrinkage, 1.5% and 0% (without resin/fiber separation). (a) full surface, (b) enlarged rib area (mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.).
Figure 4.25. Comparison of predicted top surface profile of a plate with or without resin/fiber separation (polymerization shrinkage = 1.5%, mold temp. = 150°C, mold closing speed = 8.47 mm/sec., initial charge temp. = 25 °C, free resting period = 10 sec.).
Figure 4.26. Predicted top surface profile of a plate with rib in two different polymerization shrinkage, 1.5% and 0% (with resin/fiber separation, mold temp. = 150°C, mold closing speed=8.47 mm/sec., initial charge temp. = 25 °C, free resting period=10 sec.).
4.6 Concluding Remarks

The interface heat transfer coefficient between the SMC charge and the mold surface at the free resting or dwell period was characterized by comparing experimental data with numerical calculations. This interface heat transfer coefficient was used in the heat transfer simulation before the upper mold came in contact with the SMC charge. The mold filling and resin curing models were verified by repeating the same cases from a previous study [Fan, et al. 1988b]. The temperature histories obtained from the simulation agreed well with the experimental data.

The simulation of the mold filling pattern and the resin distribution were the first step in predicting the sink mark formation. Similar to the experimental observation by Kia [1991], the calculated resin distribution showed a fiber rich area on the inside edge of the rib entry and a resin rich area appeared on top of the rib entrance. However, there was also a fiber rich area adjacent to the resin rich area predicted by the simulation that has not been experimentally observed. The discrepancy in the simulated results may arise from the assumption of a homogeneous and isotropic material and from neglecting some of the flow mechanisms observed experimentally, such as bridging-and-looping.

With a small amount of polymerization shrinkage added in the calculation, the numerical simulation in this study confirmed that the resin rich area was a critical factor in the sink mark formation. The information provided by numerical calculation can provide quality
information about sink mark formation. Further works on the flow mechanism in the filling stage and displacement analysis in the curing stage are needed to provide the quantity information about the sink mark formation.
CHAPTER V
TECHNIQUES TO MINIMIZE SINK MARKS

There have been several techniques proposed in the literature to minimize the formation of sink marks while molding parts with substructures [Amptor, 1978; Dziewatkoski, 1992; Hirai and Yamabe, 1987; Smith and Suh, 1979; Xu, et al., 1992]. In this chapter, several techniques will be investigated by using the numerical procedure described in Chapter 3 as a tool to discover the mechanisms behind these techniques. Furthermore, the best technique to minimize sink mark formation will be selected based on the findings of this work.

5.1 The Effects of Rib on Sink Mark Formation

It has been proposed that the use of relatively thin parallel ribs in place of a single thicker rib would result in a reduction in the sink mark depth. However, Jutte's [1973] work disputes that proposal wherein two thin ribs (1.5 mm (0.06 in) thick × 25.4 mm (1.00 in) deep) with the same section stiffness as a single thick rib (2.5 mm (0.1 in) thick × 32 mm (1.25 in) deep) resulted in a greater sink depth. Jutte recommended that the rib thickness be 3.2-9.5 mm (0.125-0.375 in).
inches) in order to minimize the formation of sink marks. It may be possible that such a thin rib pair contributed to the deeper sink mark in the two-ribbed part.

In this study, flat plates with two strengthening ribs (6.4 mm (0.25 in) thick \times 9.7 mm (0.38 in) deep) having the same thickness and section stiffness as a single rib (6.4 mm (0.25 in) thick \times 12.7 mm (0.5 in) deep), see Figure 5.1, were compared. The rib thickness was within the recommended thickness range which would exclude the influence of the rib thickness. This could be used to compare the influence of rib depth and material flow in multiple ribs. The material properties and molding conditions were the same as those used in the simulation of a single rib molding. Because of symmetry, only one half of the mold was needed for the calculation. The initial finite element mesh and mold geometry are shown in Figure 5.2.
Figure 5.1. Geometry of two plates with one or two ribs.
Figure 5.2. Initial finite element mesh and mold geometry in the simulation of molding a part with two ribs, (only a half cross section is analyzed).
The calculated temperature distribution after dwelling for 10 seconds is shown in Figure 5.3. This figure indicates that the temperature rise in the contact area was moderate. The folding phenomena discussed in Section 4.4 are also happened at the end of the panel and end of the rib as shown by the numerical simulation. The calculated temperature distribution corresponding to the moment the cavity was completely filled is shown in Figure 5.4. The non-symmetric pattern in the rib area suggested that the material flow into the ribs was not the same as the pattern which described flow into a single rib. A closer examination of this result is illustrated in Figure 5.5. This figure shows the velocity distribution at the time step immediately before the plate area was completely filled. The velocity at the side wall B was higher than the velocity at the side wall A. After the plate was completely filled, all the material flowed into the rib area so that the velocity pointed inward. The velocity at the side wall A was higher when the velocity was primarily inward, as illustrated in Figure 5.6. These velocity patterns generate different resin distributions compared with the distributions found for molding a plate having a single rib. The calculated resin content distribution after filling is shown in Figure 5.7. A resin rich area was found on the inside half of the rib. The resin content variation on the top surface over the rib was smaller than the variation in the plate having a single rib (see Figure 4.16 for comparison).
Figure 5.3. Calculated temperature distribution after dwelling for 10 seconds, (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.4. Calculated temperature distribution after filling, (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.5. Calculated velocity distribution around the rib area at time = 10.6 seconds (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.6. Calculated velocity distribution around the rib area at time = 10.7 seconds (mold temperature = 150 °C, mold closing speed = 8.47 mm/sec., free resting period = 10 seconds).
Figure 5.7. Calculated resin content distribution after filling (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figures 5.8 - 5.14 illustrate the results from the curing simulation. Figure 5.8 indicates that the temperature began to rise due to the heat conduction from the mold walls around 20.5 seconds after molding started. The chemical reaction also began from the outer edge of the plate and rib, as shown in Figure 5.9. In contrast to the case of curing the plate having a single rib, curing also began for the present situation at the center of the web area. Figure 5.10 illustrates that the temperature in the center of the web area exceeded the boundary condition mold wall temperatures because of the heat generated by the reaction exotherm. At the same time step, however, curing at the rib entrance had not yet begun, see Figure 5.11. Figure 5.12 illustrates that the web area had cooled to a lower temperature at time = 40.8 seconds. The only remaining area left to be cured was the center of the rib, as shown in Figure 5.13. The center of the rib experienced a high temperature after the part was completely cured, as shown in Figure 5.14. The results of simulation follow the general trend in curing SMC compression molded parts with strengthening ribs. Generally, curing began at the outer edge. The center of the web between the ribs and the rib entrance area were the last locations to finish curing.

The predicted profile of the top surface is shown in Figure 5.15. The depth of the sink mark was measured by the same method Jutte [1973] used. This method is shown in Figure 5.15. Briefly, a straight line was drawn to connect the two peaks surrounding the sink mark. The sink depth was measured from this line to the lowest point of the
valley. The sink depth in the present case (two ribs 0.38 mm deep) was 0.0007 mm. In comparison, the sink depth in the case of a part with a single rib (0.5 mm deep) was larger at 0.0013 mm. As discussed previously, the resin content distribution was a major factor in the sink mark formation. This conclusion was drawn from the simulation results. The smaller sink mark in the plate with multiple support ribs may result from a smoother resin distribution over the rib locations. Another contributing factor affecting the sink mark is the depth of the rib itself. The rib depth in a multiple-ribbed plate was smaller than the one in a single-ribbed plate. The shorter rib in the multiple rib case led to a larger portion of the rib being filled by the concurrent flow and produced a smaller resin rich area, which corroborates the results by Kia [1991].
Figure 5.8. Calculated temperature distribution at time = 20.5 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).

Figure 5.9. Calculated fractional conversion distribution at time = 20.5 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.10. Calculated temperature distribution at time = 31.1 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).

Figure 5.11. Calculated fractional conversion distribution at time = 31.1 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.12. Calculated temperature distribution at time = 40.8 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).

Figure 5.13. Calculated fractional conversion distribution at time = 40.8 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.14. Calculated temperature distribution at time = 52.6 seconds (in the curing stage, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).

Figure 5.15. Predicted top surface profile of plate with two ribs (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
5.2 Friction at the Bottom Mold Surface

Xu, et al. [1992] indicated that the friction at the bottom surface of the mold promoted resin flow into the rib. As suggested by Kia [1990], this concurrent flow may minimize the sink mark depth. The experiments carried out by Xu, et al. employed a “saw tooth” type surface to increase the friction at the bottom mold surface adjacent to the rib entrance on either side. The approximation model used in this study assumed a high friction factor, \( m = 0.8 \), at the bottom mold surface adjacent to the rib entrance on either side. All other molding conditions were the same as the regular molding described in the previous chapter.

Figure 5.16 illustrates the calculated velocity distribution in the charge. The velocity distribution indicated that flow into the rib was relatively low before the plate was completely filled. This flow pattern was similar to that for a low friction under regular molding conditions. However, this pattern did not agree with the trend reported by Xu, et al. [1992]. The discrepancy is believed to be due to the non-isothermal molding condition used in the theoretical calculation, whereas an isothermal condition was used by Xu, et al. [1992]. As explained previously, the friction does not play an important role in non-isothermal molding of SMC. The hotter resin at the mold surface has a lower viscosity and essentially serves as a lubricant. Although the friction does not promote flow into the rib, the difference in the flow pattern across the thickness does influence the resin/fiber separation distribution. As shown in Figure 5.17, the tendency of resin/fiber
separation at the center was lower than that in the regular molding situation.

The predicted depth of the sink mark which resulted from the higher friction on the mold surface had the same depth as that of the regular molding situation, as shown in Figure 5.18. It is noted, however, that the implied high friction factor in the theoretical calculation does not precisely play the same role of the "saw tooth" used in the experiment [Xu et al., 1992]. Therefore, this calculated result could not be used to explain the sink mark reduction achieved with a mold having a saw tooth surface. The improvement of sink mark depth by the saw tooth around the rib was explained by Jutte [1973] as follows. The small ribs (i.e. saw tooth ridges) parallel to the main rib caused the material flow into the rib at a much sharper angle, thus restricting the formation of the resin rich area above the rib.
Figure 5.16. Calculated velocity plot of the charge with high friction at bottom mold surface (mold temperature = 150 °C, mold closing speed = 8.47 mm/sec., free resting period = 10 seconds).
Figure 5.17. Calculated resin content distribution around the rib entrance with high friction at the bottom mold surface at the end of filling stage (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.18. Comparison of predicted top surface profiles under normal mold and mold with high friction at the bottom mold surface (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
5.3 Back Pressure

Back pressure during molding was suggested by Hirai and Yamabe [1990] to reduce the sink marks. Back pressure is provided at the rib to prevent the charge from flowing into the rib before the plate and the web are completely filled. Then, the back pressure is reduced to allow the charge to flow into the rib. However, a lower pressure still acts on the rib to prevent a void from forming at the top surface of the plate as shown in Figure 5.19a. In the present study, the mold was assumed to have no rib before the plate area was completely filled. Then, the mold with a rib cavity was used in the subsequent portion of the mold filling simulation as shown in Figure 5.19b.

Our calculation indicated that no void was formed at the top surface, although there was no back pressure applied during the filling of the rib area. This result contradicts the observation of Hirai and Yamabe [1990]. This discrepancy may result from different analytical approaches. Hirai and Yamabe used the Eulerian approach and divided the mold filling stage into 3 steps to investigate the filling pattern. In the present study, an updated Lagrangian approach was used. The filling stage was divided into several hundred steps. Therefore, a better result is expected from the present model. On the other hand, the anisotropic formulation used in Hirai and Yamabe's work may in itself lead to a different prediction.

The calculated resin content distribution at the rib entrance is shown in Figure 5.20. There are no major differences between the normal molding situation and molding with back pressure in terms of
the resin content distribution and the formation of the sink mark, as shown in Figure 5.21. This is different from the experimental results reported by Hirai and Yamabe. Again, the discrepancy may result from the differences in formulation and approximation.

In the filling stage, there is no indication of the charge losing contact with the mold surface. However, the charge does lose contact with the mold surface during curing. Due to the different timing in curing, the outer edge solidified first. The top surface above the rib was the last location to solidify among the top plate area. The polymerization shrinkage accompanying solidification caused the top surface above the rib to lose contact with the mold surface. Application of back pressure on the rib during curing to reduce the sink mark is discussed in the next section.
(a) Back pressure during molding suggested by Hirai and Yamabe [1990].

(b) Back pressure approximation used in the simulation

Figure 5.19. Back pressure during molding suggested by Hirai and Yamabe [1990] and approximation used in the simulation.
Figure 5.20. Calculated resin content distribution at rib entrance at the end of the filling stage (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.21. Comparison of sink marks of back pressure molding and normal molding (mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
5.4 Effects of Molding Pressure on Sink Marks

Boyd [1976] suggested using a low curing pressure to achieve smaller sink marks. In the present simulation, the pressure during curing was reduced from 1000 psi to 300 psi to study the influence of pressure during curing on sink mark formation. It was assumed that the pressure did not influence the chemical reaction (curing). Therefore, the results of the curing simulation for the normal molding described in the previous chapter were used. The pressure on the upper mold half was changed in calculating the stress and the sink mark. The resulting sink mark is shown in Figure 5.22. Essentially, no improvement can be seen by changing the pressure during curing.

The effects of pressure release on sink mark formation were experimentally studied by Dziewatkoski, et al. [1992]. In their work, the pressure was released at different times and to different levels during the curing stage. In the present study, the molding pressure was reduced to 200 psi at 10 seconds after curing simulation began. The resulting top surface profile is shown in Figure 5.23. This pressure release showed no reduction in sink depth.

As stated previously, the top surface above the rib and the bottom of the rib may lose contact with the mold surface after a certain portion of the rib is completely cured because of the polymerization shrinkage. A back pressure during curing may prevent the surface on top of the rib from losing contact with the mold surface (see Figure 5.24). In the theoretical calculation, the top surface of the plate and the bottom surface of the rib were subjected to a pressure of 1000 psi
applied by a rigid flat surface during curing. The predicted profile of the top surface is shown in Figure 5.25. The sink mark depth increased as the applied back pressure increased, although the profile outside the rib was smoother.

From the simulations under different pressure conditions, there were no notable changes in the sink mark. These simulation results do not directly agree with the experimental results reported in the literature. There are several possible contributing factors for this discrepancy. First, the numerical simplification of the curing and the stress calculations neglect the effects of shrinkage on the heat transfer. As mentioned previously, polymerization shrinkage will cause local regions to lose contact with the mold surface. Therefore, the IHTC at this area should be reduced to a much smaller value to account for the loss of intimate contact. In the future, a new computation scheme should be developed to combine the curing simulation and the stress calculation. Second, the curing reaction may be a function of pressure. The current curing model does not account for the pressure in the curing stage. New curing models need to be explored to account for the effects of pressure on the curing reaction.
Figure 5.22. Comparison of predicted top surface profiles under normal and low pressure during curing (polymerization shrinkage = 1.5 %, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
Figure 5.23. Comparison of predicted top surface profiles with or without pressure release at 10 seconds after curing starts (polymerization shrinkage = 1.5 %, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
(a) Charge loses contact with mold surface during curing

(b) back pressure to keep rib area in contact.

Figure 5.24. Back pressure during curing.
Figure 5.25. Comparison of predicted top surface profiles with or without back pressure during curing (polymerization shrinkage = 1.5 \%, mold temperature = 150 °C, mold closing speed=8.47 mm/sec., free resting period=10 seconds).
5.5 Concluding Remarks

Different techniques proposed for minimizing the sink mark were compared by numerical simulation. The sink mark depths of the plate molded by different techniques were normalized by dividing them with the sink mark depth under normal molding conditions as described in Section 4.5. As shown in Figure 5.26, molding of a plate with multiple ribs offered the best improvement. Back pressure on the rib during curing showed larger sink marks than normal. Other techniques reported to minimize sink mark were not shown to be significant according to our simulation.
Figure 5.26. Comparison of predicted sink mark depths of different techniques to minimize the sink mark formation, (normal molding = 1).
CHAPTER VI
CONCLUSIONS AND RECOMMENDATIONS

6.1 Concluding Remarks

The objective of this study was to establish a numerical modeling procedure to predict the formation of sink marks and to help eliminate sink mark formation in compression molding of polymeric composites. Numerical simulation of several examples was conducted to determine the most promising techniques to eliminate sink marks. A framework for numerical simulation of sink mark formation in compression molding of polymeric composites was developed. Following are the distinct features in the numerical procedure and the conclusions reached based on the numerical calculations executed in Chapters IV and V.

1. A resin/fiber separation model was developed based on Jeffrey's fiber suspension model to predict the resin content distribution. The model was implemented to work with a commercial finite element package, DEFORM.

2. A computational algorithm was developed to include the polymerization shrinkage during solidification in the deformation analysis.
3. The conclusion from numerical simulation of sink formation was that the resin rich area was the major contributor in sink mark formation.

4. Molding of a multiple-ribbed plate offered the best improvement on sink mark formation due to the shorter rib depth.

6.2 Recommendations for Future Work

The recommendations for future work are:

1. Investigate the flow mechanism of bridging-and-looping in the mold filling stage and the relation between this flow mechanism process variables.

2. Develop resin/fiber separation model considering bridging-and-looping flow mechanism and experimental techniques to verify the resin/fiber separation model.

3. Incorporate anisotropic flow into the mold filling simulation. This will enable the anisotropic analysis in the resin curing and composite cooling stages.

4. Further investigate the changes in physical and mechanical properties during curing. This would result in a more accurate material model used in the simulation of sink mark formation.

5. Combine the curing model into the filling simulation. This would help to obtain more accurate curing information for the molding process with long mold filling times.
6. Develop a new computational scheme to simultaneously calculate the curing reaction and stress efficiently.
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APPENDIX A
PROGRAMS AND EXAMPLES

A.1 Program RESIN for Calculating Resin Content

PROGRAM RESIN
IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)
PARAMETER (MXMNP=1200, XMEL=1000)

DIMENSION NOD(4, XMEL), RZ(2, MXMNP), RATEL(MXMEL),
VELNP(2, MXMNP), VFMIN(2, MXMNP), VELM(2, MXMNP),
VELMP(2, MXMNP), STREL(MXMEL), STRNP(MXMNP), TMPNP(MXMNP),
RZC(2, MXMNP), RATELN(MXMEL), RATNP(MXMNP)

OPEN FILES AND READ NECESSARY INFORMATION

WRITE(*,900)
READ(*,905) FNAM E
OPEN(11, FILE=FNAME, STATUS='OLD', FORM='FORMATTED')
WRITE(*,910)
READ(*,905) FNAM E
OPEN(12, FILE=FNAME, STATUS='OLD', FORM='UNFORMATTED')
WRITE(*,*), ' PLEASE INPUT RESULT FILENAME:
READ(*,905) FNAM E
OPEN(13, FILE=FNAME, STATUS='NEW', FORM='UNFORMATTED')
OPEN(14, FILE='RESIN.PAR', STATUS='OLD',
FORM='FORMATTED')
WRITE(*,*), ' PLEASE INPUT MIN. VEL. FILE:
READ(*,905) FNAM E
OPEN(15, FILE=FNAME, STATUS='OLD', FORM='FORMATTED')
WRITE(*,*), ' FILE CONTAIN INITIAL POINT:
READ(*,905) FNAM E
OPEN(16, FILE=FNAME, STATUS='OLD', FORM='UNFORMATTED')
WRITE(*,*), ' FILE CONATINS DISPLACED POINTS:
READ(*,905) FNAM E
OPEN(17, FILE=FNAME, STATUS='NEW', FORM='UNFORMATTED')

READ(14,*) FORCE, TOL, MAXI, NSEG, ISOTH

WRITE(*,*), ' TIME INCREMENT :'
READ(*,*) DT
READ(11,916) DTYPE,IDUM,IDUM2,NP
DO 5 IP=1,NP
5 READ(11,* ) IDUM,R1,R2,R3
READ(11,916) DTYPE,IDUM,IDUM2,NP
DO 6 IP=1,NP
6 READ(11,* ) R1,R2,R3
READ(11,915) DTYPE,IDUM,NUMNP
DO 10 IP=1,NUMNP
10 READ(11,* ) INP,RZ(1,INP),RZ(2,INP)
READ(11,915) DTYPE,IDUM,NUMNP
DO 11 IP=1,NUMNP
11 READ(11,* ) INP,IDUM,IDUM2
READ(11,915) DTYPE,IDUM,NUMEL
DO 15 IE=1,NUMEL
15 READ(11,* ) IEL,(NOD(IP,IEL),IP=1,4)
READ(11,915) DTYPE,IDUM,IDUM2
DO 20 IP=1,NUMNP
20 READ(11,* ) INP,VELNP(1,INP),VELNP(2,INP)
IF(ISOTH.NE.1) GO TO 40
READ(11,915) DTYPE,IDUM1,IDUM2
DO 30 IP=1,NUMNP
30 READ(11,* ) INP,TMPNP(INP)
40 DO 50 IE=1,NUMEL
50 RATEL(IE)=RAT
READ(15,915) DTYPE,IDUM1,IDUM2
DO 55 IP=1,NUMNP
55 READ(15,* ) INP,VFMIN(1,INP),VFMIN(2,INP)
C INTERPOLATE THE RESIN RATIO AT NODAL POINT FROM
C THE RESIN RATIO AT ELEMENT
CALL CAREA(NOD,RZ,NUMNP,NUMEL,AREL)
CALL AVER(RATEL,RATNP,DUMP,AREL,NOD,RZ,NUMNP,NUMEL)
C INITIALIZE VELOCITY
DO 100 IP=1,NUMNP
DO 100 IDF=1,NDF
VELMP(IDF,IP)=VELNP(IDF,IP)
100 CONTINUE
C CALCUALTE RESIN VELOCITY
DO 300 ITER=1,MAXI
CALL CALSTR(NOD,NUMEL,NUMNP,RZ,STREL,VELMP)
CALL AVER(STREL,STRNP,DUMP,AREL,NOD,RZ,NUMNP,NUMEL)
CALL CALVM(RATNP,NOD,RZ,VELNP,VELF,VELM,FORCE,VFMIN,
$ STRNP,NUMNP,NUMEL,DT,AREL,TMPNP,ISOTH)
CALL UPDATE(XNORM,VELM,VELNP,NUMNP)
WRITE(*,*) ITER,XNORM
IF(XNORM .LT. TOL) GO TO 400

CONTINUE

FORMAT(2F10.3,4X,2F10.3)

CONTINUE

CALL CONT(RATEL,NOD,RZ,VELF,VELNP)

CALL AVER(RATEL,RATNP,DUMP,AREL,NOD,RZ,NUMNP,NUMEL)

DO 500 IE=1,NUMEL

WRITE(13) RATEL(IE)

C

900 FORMAT(' PLEASE INPUT DEFORM DATA FILENAME: ')

905 FORMAT(A80)

910 FORMAT(' PLEASE INPUT RESIN DATA FILENAME: ')

915 FORMAT(A15,215)

916 FORMAT(A15,315)

920 FORMAT(16, 3 E 1 4 .6)

STOP

END

C

SUBROUTINE AVER(VE,VN,SUMA,EAREA,NOD,RZ,NUMNP,NUMEL)

IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)

DIMENSION VE(NUMEL), VN(NUMNP), SUMA(NUMNP)

NOD(4,NUMEL), RZ(2,NUMNP), EAREA(NUMEL)

DO 10 IP=1,NUMNP

SUMA(IP)= 0.0

DO 20 IE=1,NUMEL

DO 20 IP = 1 , 4

NODE=NOD(IP,IE)

SUMA(NODE) =SUMA(NODE)+EAREA(IE)

20 VN(NODE)=VN(NODE)+VE(IE)*EAREA(IE)

DO 30 IP=1,NUMNP

30 VN(IP)=VN(IP)/SUMA(IP)

RETURN

END

C

SUBROUTINE CAREA(NOD,RZ,NUMNP,NUMEL,EAREA)

IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)

DIMENSION EAREA(NUMEL), NOD(4,NUMEL), RZ(2,NUMNP), X(4), Y(4)

DO 20 IEL=1,NUMEL

DO 10 IP=1,4

X(IP)=RZ(1,NOD(IP,IEL))

10 Y(IP)=RZ(2,NOD(IP,IEL))

20 EAREA(IEL)=X(1)*Y(2)+X(2)*Y(3)+X(3)*Y(4)+X(4)*Y(1)

RETURN

END
SUBROUTINE CALVM(RATNP, NOD, RZ, VELNP, VELF, VELM, FORCE, $  
, VFMIN, STR, NUMNP, NUMEL, DT, AREL, TMPNP, ISOTH)
$  
IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)
$  
DIMENSION RATNP(NUMNP), NOD(4, NUMEL), RZ(2, NUMNP)
$  
, VELNP(2, NUMNP), VFMIN(2, NUMNP)
$  
, VELF(2, NUMNP), VELM(2, NUMNP)
$  
, AREL(NUMEL), STR(NUMNP), TMPNP(NUMNP)
$  
DO 500 IP=1, NUMNP
   IF (RATNP(IP).EQ.0.0) GO TO 440
   IF (RATNP(IP).EQ.1.0) GO TO 460
   VCX=VELNP(1, IP)
   VCY=VELNP(2, IP)
   VMINX=VFMIN(1, IP)
   VMINY=VFMIN(2, IP)
   VC=SQRT((VCX**2+VCY**2)
   IF (VC.EQ.0.0) GO TO 450
   IF (ISOTH.EQ.1) THEN
      TMP=TMPNP(IP)
   ELSE IF (ISOTH.EQ.0) THEN
      TMP=25.0
   ELSE
      TMP=ABS(ISOTH)
   ENDIF
   VDIF=(1.0-RATNP(IP))*FORCE/VISM(STR(IP), TMP)
   FAC=SQRT((VCX-VMINX)**2+(VCY-VMINY)**2)
   IF (FAC.EQ.0.0) THEN
      PAR=0.0
   ELSE
      PAR=1.0-RATNP(IP)*VDIF/FAC
   ENDIF
   IF (PAR.LT.0.0) PAR=0.0
   VELF(1, IP)=PAR*VCX+(1.0-PAR)*VMINX
   VELF(2, IP)=PAR*VCY+(1.0-PAR)*VMINY
   VELM(1, IP)=(VCX-(1.0-RATNP(IP))*VELF(1, IP))/RATNP(IP)
   VELM(2, IP)=(VCY-(1.0-RATNP(IP))*VELF(2, IP))/RATNP(IP)
   GO TO 500
   440 VELF(1, IP)=VELNP(1, IP)
   VELF(2, IP)=VELNP(2, IP)
   VELM(1, IP)=VELNP(1, IP)
   VELM(2, IP)=VELNP(2, IP)
   GO TO 500
   450 VELF(1, IP)=0.0
   VELF(2, IP)=0.0
   VELM(1, IP)=0.0
   VELM(2, IP)=0.0
   GO TO 500
   460 VELF(1, IP)=0.0
   VELF(2, IP)=0.0
   VELM(1, IP)=VELNP(1, IP)
   VELM(2, IP)=VELNP(2, IP)
500 CONTINUE
SUBROUTINE CONT(RATEL,NOD,RZ,VELF,VELNP,$
NUMNP,NUMEL,DT,AREL
,RATELN,RZC)
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4(I-N)
DIMENSION RATEL(NUMEL),NOD(4,NUMEL),RZ(2,NUMNP)
$ ,AREL(NUMEL),VELF(2,NUMNP)
$ ,VELNP(2,NUMNP),RZC(2,NUMNP),FCR(2)
$ ,X(4),Y(4),RATELN(NUMEL),RZE(2,4),H(4)
$ ,XP(400),YP(400)
C
C UPDATE THE COORDINATES FOR COMPOSITES AND FIBER
C
DO 10 IP=1,NUMNP
DO 10 ID = 1,2
RZC(ID, IP) =RZ (ID, IP) + VELNP (ID, IP) *DT
10 CONTINUE
C
C *** INITIALIZE FIBER CONTENT VARIABLES
C
DO 20 IEC=1,NUMEL
RATELN(IEC)= 0.0
READ (16) NUMFE
WRITE (17) NUMFE
DO 300 IFE=1,NUMFE
READ (16) NUMPF,FC
WRITE(17) NUMPF,FC
READ (16) (XP(IP),YP(IP),IP=1,NUMPF)
C
C
DO 200 IPF=1,NUMPF
C
XC=XP(IPF)
YC=YP(IPF)
DO 40 IEC=1,NUMEL
DO 30 IP=1,4
ID=NOD(IP,IEC)
X(IP)=RZ (1,ID)
30 Y(IP)=RZ (2,ID)
CALL BBOX(X,Y,XMAX,XMIN,YMAX,YMIN)
IF (INBOX(XC,YC,XMAX,XMIN,YMAX,YMIN).LT.0) GO TO 35
IF (INCHECK(X,Y,XC,YC).GE.0) GO TO 50
35 IF (IEC.EQ.NUMEL) GO TO 65
40 CONTINUE
50 CONTINUE
INEC=IEC
CALL FINDST(X,Y,XC,YC,S,T)
IF(S.GT.1.0 .OR. S.LT.-1.0) GO TO 65
CALL SHAPE(H,S,T)
VFX=0.0
VFY=0.0
DO 60 IP=1,4
   ID=NOD(IP,IEC)
   VFX=VFX+VELF(1,ID)*H(IP)
   VFY=VFY+VELF(2,ID)*H(IP)
60 CONTINUE
GO TO 66
CALL EXPL(VELF,VFX,VFY,RZ,NUMNP,XC,YC)
FCR(1)=XC+VFX*DT
FCR(2)=YC+VFY*DT
   XP(IPF)=FCR(1)
   YP(IPF)=FCR(2)
DO 70 IP=1,4
   X(IP)=RZC(1,NOD(IP,IEC))
   Y(IP)=RZC(2,NOD(IP,IEC))
70 CONTINUE
CALL BBOX(X,Y,XMAX,XMIN,YMAX,YMIN)
IF(INBOX(FCR(1),FCR(2),XMAX,XMIN,YMAX,YMIN).LT.0) $ GO TO 100
IN=INCHECK(X,Y,FCR(1),FCR(2))
IF(IN.LT.0) GO TO 100
IF(IN.EQ.0) THEN
   RATELN(IEC)=RATELN(IEC)+FC/2.0
ELSE
   RATELN(IEC)=RATELN(IEC)+FC
ENDIF
GO TO 200
100 CONTINUE
150 CONTINUE
C PRINT *,XP(4),YP(4)
WRITE(17) (XP(IP),YP(IP),IP=1,NUMPF)
300 CONTINUE
DO 400 IE=1,NUMEL
   FBR=RATELN(IE)/AREL(IE)
IF (FBR .GT. 1.0) FBR = 1.0
400 RATEL(IE) = 1.0 - FBR
RETURN
END

C

SUBROUTINE UPDATE(XNORM, VEL1, VEL2, NUMNP)
IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)
DIMENSION VEL1(2, NUMNP), VEL2(2, NUMNP)
SUM = 0.0
DSUM = 0.0
DO 100 IP = 1, NUMNP
    DO 100 IDF = 1, 2
       SUM = SUM + VEL2(IDF, IP)**2
       DSUM = DSUM + (VEL1(IDF, IP) - VEL2(IDF, IP))**2
100    CONTINUE
IF (SUM .LE. 0.0) GO TO 999
XNORM = DSUM / SUM
RETURN
999 WRITE(*, 1000) SUM
1000 FORMAT(' *** ERROR IN UPDATE *** X N = ', SUM = 1, G12.5)
STOP
END

FUNCTION VISM(STR, TMP)
IMPLICIT REAL*8 (A-H, O-Z)

SUBROUTINE TO EVALUATE THE VISCOSITY OF MATRIX

IF (TMP .LT. 0.0) GO TO 10
T = 1.0 / (TMP + 273.0)
E0 = 574726.6 * EXP(11969.56 * (T - 1.0 / 298))
RSTR = STR * E0 * T
VR = 1.0 / (1.0 + (5.831 * RSTR)**2)**0.3439
VISM = VR * E0 * 1.0E-7
PRINT *, STR, TMP, VISM
VISM = 5.748E-2 / (1.0 + (1.271 * STR)**2)**0.3825
RETURN
10  VISM = ABS(TMP)
END

SUBROUTINE CHECK(NOD, NP1, NP2, NUMEL, IE, ISTAT)
IMPLICIT REAL*8 (A-H, O-Z)
IMPLICIT INTEGER*4 (I-N)
DIMENSION NOD(4, NUMEL)
DO 100 I = 1, NUMEL
    IF (I .EQ. IE) GO TO 10
    DO 10 IP = 1, 4
        IF (NOD(IP, I) .EQ. NP1) GO TO 20
10  CONTINUE
   GO TO 100
20  DO 30 JP=1,4
   IF(NOD(JP,I).EQ.NP2) GO TO 200
30  CONTINUE
100 CONTINUE
   ISTAT=-1
   RETURN
200 ISTAT=1
   RETURN
END

C
C SUBROUTINE SHAPE(H,S,T)
C
C **** SUBROUTINE TO EVALUATE THE SHAPE FUNCTION AT SPECIFIED POINT
C
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DIMENSION H(4)
H(1)=(1.0-S)*(1.0-T)*0.25
H(2)=(1.0+S)*(1.0-T)*0.25
H(3)=(1.0+S)*(1.0+T)*0.25
H(4)=(1.0-S)*(1.0+T)*0.25
RETURN
END

C
C FUNCTION INCHECK(X,Y,XC,YC)
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DIMENSION X(4), Y(4)
C
C *** SUBROUTINE TO CHECK WHETHER POINT (XC,YC)
C IS IN THE ELEMENT FORMED BY (X(I),Y(I))
C RETURN VALUE :
C 1 : IN THE ELEMENT
C 0 : ON THE EDGE
C -1 : NOT IN THE ELEMENT
C
A=X(1)*Y(2)+X(2)*YC+XC*Y(1)
$ -X(1)*YC-X(2)*Y(1)-XC*Y(2)
IF(A.LE.0.0) GO TO 20
C
A=X(2)*Y(3)+X(3)*YC+XC*Y(2)
$ -X(2)*YC-X(3)*Y(2)-XC*Y(3)
IF(A.LE.0.0) GO TO 20
C
A=X(3)*Y(4)+X(4)*YC+XC*Y(3)
$ -X(3)*YC-X(4)*Y(3)-XC*Y(4)
IF(A.LE.0.0) GO TO 20
C
A=X(4)*Y(1)+X(1)*YC+XC*Y(4)
$ -X(4) * YC-X(1) * Y(4)-XC*Y(1)$

IF (A.LE.0.0) GO TO 20
INCHECK=1
RETURN
20 IF (A.EQ.0.0) THEN
   INCHECK=0
ELSE
   INCHECK=-1
ENDIF
RETURN
END

C
SUBROUTINE CALSTR(NOD, NUMEL, NUMNP, RZ, EFSTR, VEL)
IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)
DIMENSION VEL(2, NUMNP), RZ(2, NUMNP), NOD(4, NUMEL), STR(3)
$ , EFSTR(NUMEL), RZEL(2,4), VELEL(2,4), XD(2, 4)
$ , XIP(2), B(3, 2, 4)
DATA NONP, NDF/4.0, 2/
C
EVALUATE STRAIN RATE AT EACH ELEMENT
C
DO 600 IE=1, NUMEL
C
C  TAKE THE ELEMENT COORDINATES AND VELOCITIES FIRST
C
DO 100 IP = 1, NONP
NP=NOD(IP, IE)
DO 100 IDF=1, NDF
RZEL(IDF, IP)=RZ(IDF, NP)
VELEL(IDF, IP)=VEL(IDF, NP)
100 CONTINUE
C
EVALUATE DERIVATIVES
C
WRITE(*, 101) ((RZEL(IDF, IP), IDF=1, 2), IP=1, NONP)
101 FORMAT( 4 (2X, 2G14.5))
CALL JACOB(DXJ, RZEL, XD, XIP)
C
CONSTRUCT B-MATRIX FOR STRAIN RATE EVALUATION
C
DO 110 IP=1, NONP
B(1, 1, IP)=XD(1, IP)
B(1, 2, IP)=0.0
B(2, 1, IP)=0.0
B(2, 2, IP)=XD(2, IP)
B(3, 1, IP)=0.5*XD(2, IP)
B(3, 2, IP)=0.5*XD(1, IP)
110 CONTINUE
C
EVALUATE STRAIN RATE
C
DO 120 IST=1,3
STR(IST)=0.0
DO 120 IP=1,NONP
DO 120 IDF=1,NDF
STR(IST)=STR(IST)+B(IST,IDF,IP)*VELEL(IDF,IP)
CONTINUE
EFSTR(IE)=SQRT((4.0*STR(1)**2+4.0*STR(2)**2
+2.0*STR(3)**2)/3.0)
600 CONTINUE
RETURN
END

SUBROUTINE JACOB(DXJ,RZ,XD,XIP)
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DIMENSION P(2,4),H(4),XD(2,4),XIP(2),XJ(2,2),RZ(2,4)
DATA P/0.25,0.25,-0.25,0.25,
    -0.25,-0.25,0.25,-0.25/
DATA H/0.25,0.25,0.25,0.25/
DATA NDF,NONP/2,4/
C
H(4) : SHAPE FUNCTION
P(2,4) : DERIVATIVES OF SHAPE FUNCTION
XJ(2,2) : JACOBIAN MATRIX
XD(2,4) : DERIVATIVES W.R.T. GLOBAL COORDINATE SYSTEM
DJ : DETERMINANT OF JACOBIAN MATRIX
RZ(2,4) : NODAL POINT COORDINATES OF THE ELEMENT
XIP(2) : COORDINATES OF THE INTEGRATION POINT

EVALUATE THE COORDINATES OF INTEGRATION POINT
DO 10 IDF=1,NDF
XIP(IDF)=0.0
DO 10 IP=1,NONP
XIP(IDF)=XIP(IDF)+H(IP)*RZ(IDF,IP)
CONTINUE

EVALUATE THE JACOBIAN MATRIX

EVALUATE THE DETERMINANT OF THE JACOBIAN AND THE INVERSE JACOBIAN MATRIX
DXJ = XJ(1,1) * XJ(2,2) - XJ(1,2) * XJ(2,1)

IF(DXJ .LE. 0.0) GO TO 9999

TP = XJ(1,1)
XJ(1,1) = TP / DXJ
XJ(2,2) = TP / DXJ
XJ(1,2) = - XJ(1,2) / DXJ
XJ(2,1) = - XJ(2,1) / DXJ

C
C EVALUATE THE DERIVATIVES W.R.T.
C GLOBAL COORDINATE SYSTEM
C
DO 100 IP = 1, NNP
DO 100 IDF = 1, NDF
XD(IDF,IP) = 0.0
DO 100 JDF = 1, NDF
XD(IDF,IP) = XD(IDF,IP) + P(JDF,IP) * XJ(JDF,IDF)
100 CONTINUE
RETURN

9999 WRITE(*,10000)
10000 FORMAT(1*** PROGRAM STOP DUE TO NEGATIVE
$ JACOBIAN ***')
STOP
END

C
C SUBROUTINE BBOX(X,Y,XMAX,XMIN,YMAX,YMIN)
IMPLICIT REAL*8 (A-H,0-Z), INTEGER*4 (I-N)
DIMENSION X(4), Y(4)
XMAX = X(1)
XMIN = X(1)
YMAX = Y(1)
YMIN = Y(1)
DO 10 IP = 2, 4
IF (X(IP) .GT. XMAX) XMAX = X(IP)
IF (X(IP) .LT. XMIN) XMIN = X(IP)
IF (Y(IP) .GT. YMAX) YMAX = Y(IP)
IF (Y(IP) .LT. YMIN) YMIN = Y(IP)
10 CONTINUE
RETURN
END

C
C FUNCTION INBOX(X,Y,XMAX,XMIN,YMAX,YMIN)
IMPLICIT REAL*8 (A-H,0-Z), INTEGER*4 (I-N)
IF (X.GT.XMAX) GO TO 20
IF (X.LT.XMIN) GO TO 20
IF (Y.GT.YMAX) GO TO 20
IF (Y.LT.YMIN) GO TO 20
INBOX = 1
RETURN
20 INBOX = -1
RETURN
SUBROUTINE FINDST(X,Y,XC,YC,S,T)
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DATA EPS/1.0E-6/

SUBROUTINE TO CALCULATE THE LOCAL COORDINATE
OF A GIVEN POINT IN THE ELEMENT

DIMENSION X(4),Y(4)
XMIN=1.0+EPS
A1=X(1)-X(2)+X(3)-X(4)
IF(ABS(A1).LE.EPS) A1=0.0
A2=Y(1)-Y(2)+Y(3)-Y(4)
IF(ABS(A2).LE.EPS) A2=0.0
B1=-X(1)+X(2)+X(3)-X(4)
IF(ABS(B1).LE.EPS) B1=0.0
B2=-Y(1)+Y(2)+Y(3)-Y(4)
IF(ABS(B2).LE.EPS) B2=0.0
C1=-X(1)-X(2)+X(3)+X(4)
IF(ABS(C1).LE.EPS) C1=0.0
C2=-Y(1)-Y(2)+Y(3)+Y(4)
IF(ABS(C2).LE.EPS) C2=0.0
D1=X(1)+X(2)+X(3)+X(4)-4.0*XC
IF(ABS(D1).LE.EPS) D1=0.0
D2=Y(1)+Y(2)+Y(3)+Y(4)-4.0*YC
IF(ABS(D2).LE.EPS) D2=0.0
F1=-C1*A2+C2*A1
F2=-D1*A2+D2*A1+B1*C2-B2*C1
F3=B1*D2-B2*D1
AF1=ABS(F1)
IF(AF1.LT.EPS) THEN
  T=-F2/F2
  CALL FINDS(S,T,A1,A2,B1,B2,C1,C2,D1,D2)
  IF(S.GT.1.0 .OR. S.LT.-1.0) RETURN
ELSE
  R=SQR(T(F2*F2-4.0*F1*F3)
  R1=-(F2+R)/(2.0*F1)
  R2=-(F2-R)/(2.0*F1)
  AR1=ABS(R1)
  IF(AR1.LT.XMIN) THEN
    T=R1
    CALL FINDS(S,T,A1,A2,B1,B2,C1,C2,D1,D2)
    IF(S.GT.1.0 .OR. S.LT.-1.0) RETURN
  ELSE IF(R2.LT.1.0 .AND. R2.GT.-1.0) THEN
    T=R2
    CALL FINDS(S,T,A1,A2,B1,B2,C1,C2,D1,D2)
  ELSE
    S=10.
    T=10.
  RETURN
SUBROUTINE FINDS(S,T,A1,A2,B1,B2,C1,C2,D1,D2)
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DATA EPS/1.0E-6/
F=A1*T+B1
AF=ABS(F)
IF (AF.GT.EPS) THEN
  S = (-C1*T-D1)/F
ELSE
  F=A2*T+B2
  AF=ABS(F)
  IF(AF.GT.EPS) THEN
    S = (-C2*T-D2)/F
  ELSE
    S=-10.
    T=-10.
  ENDIF
ENDIF
RETURN
END

SUBROUTINE EXPL(VO,VX,VY,RZ,NUMNP,X,Y)
IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DIMENSION VO(2,NUMNP), RZ(2,NUMNP)
RAD=1.0
VEX1=0.0
VEX2=0.0
DSUM=0.0
DO 100 IP=1,NUMNP
  D = (X-RZ(1,IP))*2+(Y-RZ(2,IP))*2
  IF (D.GT.RAD) GO TO 100
  IF (D.NE.0.0) THEN
    P=1.0/D
    VEX1=VEX1+P*VO(1,IP)
    VEX2=VEX2+P*VO(2,IP)
    DSUM=DSUM+P
  ELSE
    VX=VO(1,IP)
    VY=VO(2,IP)
  ENDIF
CONTINUE
100 IF (DSUM.LE.0.0) THEN
    RAD=RAD*4.0
RETURN
END
GO TO 10
ELSE
   VX=VEX1/DSUM
   VY=VEX2/DSUM
RETURN
ENDIF
END

A.2 Example Input File for Program RESIN

DIEGEO  2  1  2
1 0.0000000E+00 0.1023306E+02 0.0000000E+00
2 0.5080000E+02 0.1023306E+02 0.0000000E+00
DIEGEO  3  1  7
1 0.5080000E+02 0.1000000E+02 0.0000000E+00
2 0.5080000E+02 -0.1001993E-14 0.1000000E-02
3 0.1587500E+02 -0.1451331E-13 0.5000000E+00
4 0.1587500E+02 -0.9675000E+01 0.1000000E+00
5 0.9525000E+01 -0.9675000E+01 0.1000000E+00
6 0.9525000E+01 0.2081668E-16 0.5000000E+00
7 0.0000000E+00 0.0000000E+00 0.0000000E+00
RZ    1  540
1 0.0000000E+00 -0.1496550E-07
2 0.0000000E+00 0.7320067E+00

/* NODAL COORDINATES */

BCCDEF  1  540
1 1 -3

/* DEFORMATION BOUNDARY CONDITION FROM DEFORM */

ELMCON  1  490
1 14 15 29 30
2 15 13 28 29

/* ELEMENT CONNECTION */

URZ    1  540
1 0.0000000E+00 -0.7482752E-05
2 0.0000000E+00 -0.6803272E-01

/* NODAL VELOCITY FROM DEFORM */

NDTMP  1  540
A.3 ABAQUS Program for Heat Transfer Including Curing

*HEADING
YOUR PROGRAM TITLE
*NODE, SYSTEM=R, NSET=NS1
  1,-1.7392E-13,-1.7780E+01, 0.0000E+00

/* PUT YOUR NODAL COORDINATES HERE */

*ELEMENT, TYPE=DC2D4 , ELSET=ES1
  1 151 145 150 152

/* PUT YOUR ELEMENT CONNECTION HERE */

*NSET, NSET=NMIN
  59,65,455,456,461,462
*SOLID SECTION, ELSET=ES1, MATERIAL=M1
*MATERIAL, NAME=M1
*CONDUCTIVITY
  0.41404
*DENSITY
  1.9865
*SPECIFIC HEAT
  1.027026
*HEAT GENERATION
*DEPVAR
  5
*INITIAL CONDITION, TYPE=TEMPERATURE
  1,0.3359209E+02

/* PUT YOUR INITIAL NODAL TEMPERATURE HERE */

*USER SUBROUTINE
  SUBROUTINE HETVAL(CMNAME, TEMP, TIME, DTIME,
   $ SVAR, FLUX, PREDEF)
  IMPLICIT REAL*8 (A-H, O-Z)
  CHARACTER*8 CMNAME
  DIMENSION SVAR(1), PREDEF(1)
  DATA CONINH, CONINI, EFFINI, AD, EDR, AP, EPR, HRM/
$ 7.21E-7, 3.66E-5, 1.0, 7.82E13, 16054., 1.71E13, 8410., 80. /
DATA TI, TZ/0.02, 1. E9/
TEMPK=TEMP+273.

C *** SET INITIAL CONDITION

IF (TIME.LT.TI) THEN
  SVAR(4)=T2
  SVAR(5)=CONINI
  SVAR(3)=0.0
  SVAR(1)=0.0
  SVAR(2)=0.0
ELSE

C *** INHIBITION PERIOD

SVAR(3)=SVAR(3)+AD*EXP(-EDR/TEMPK)*DTIME
EKD=EXP(-SVAR(3))
IF (TIME.LT.SVAR(4)) THEN
  CSMINI=2.0*EFFINI*CONINI*(1.0-EKD)
  IF (CSMINI.GT.CONINH) THEN
    SVAR(4)=TIME
    SVAR(5)=CONINI*EKD
    SVAR(3)=0.0
  END IF
RETURN
ENDIF

C *** PROPOGATION PERIOD

AKP=AP*EXP(-EPR/TEMPK)
SVAR(1)=SVAR(1)+DTIME*SVAR(2)
SVAR(2)=2.0*EFFINI*SVAR(5)*AKP*(1.0-SVAR(1))*(1.0-
EKD)
IF (SVAR(1).GT.1.0) THEN
  SVAR(1)=1.0
  SVAR(2)=0.0
ENDIF
IF (SVAR(2).LT.0.0) SVAR(2)=0.0
FLUX=HRM*SVAR(2)
RETURN
END

*STEP, INC=2000, CYCLE=30
*HEAT TRANSFER, TMTOL=1., DELTMX=20.0.
0.01, 300., 0.001, 0.5
*FILM, OP=NEW
  2, F3, 130.0, 5.0000E-01

/* PUT YOUR CONVECTION BOUNDARY CONDITION HERE */
A.4 ABAQUS Program Used in Displacement Analysis

*HEADING
  SINK MARK SIMULATION OF PI-SHAPE, MOLD TEMP=150C
*NODE, SYSTEM=R, NSET=NS1
  1, 0.0000000E+00, 0.0000000E+00
/* PUT YOUR NODAL COORDINATES HERE */

*ELEMENT, TYPE=CPE4, ELSET=ES1
  1, 5, 9, 10, 4
/* PUT YOUR ELEMENT CONNECTION HERE */

*NSET, NSET=NDMIN
  4, 276, 570
*ELSET, ELSET=ELMIN
  1, 189, 196, 490
*ELSET, ELSET=EC1
  1, 2, 3, 4, 5, 6, 7, 8, 12, 19,
/* PUT ELEMENTS WITH THE SAME PROPERTIES (RESIN CONTENT) IN ONE GROUP */

*ELSET, ELSET=ELMIN
  1, 198, 490
*NSET, NSET=NCT
  1, 2, 3, 4, 5
*NSET, NSET=NDMIN
  1, 4, 118, 275, 360, 572, 576
*SOLID SECTION, ELSET=EC1, MATERIAL=M1
*MATERIAL, NAME=M1
/* PUT YOUR MATERIAL PROPERTIES OF EACH GROUP HERE */

*INITIAL CONDITION, TYPE=FIELD
  1, 0.50496E+00
/* PUT THE PAPAREMETER FOR MATERIAL PROPERTIES HERE */

*INITIAL CONDITION, TYPE=STRESS
  1,-0.54448E+01,-0.65639E+01,-0.59513E+01,-0.52607E-02

/* PUT THE STRESSES FROM PREVIOUS STEP HERE */

*INITIAL CONDITION, TYPE=TEMPERATURE
  1,-0.73818E+02

/* PUT THE EQUIVALENT TEMPERTAURE INCREMENT HERE */

*STEP, INC=1, CYCLE=20
*STATIC, PTOL=6.
  0.00001, 0.00001, 0.00001, 0.000021
*BOUNDARY
NCT, 1, 1

/* PUT THE PROPER BOUNDARY CONDITION HERE */

*NODE PRINT, NSET=NDMIN
U
*EL PRINT, ELSET=ELMIN
S
*END STEP
*STEP, INC=100, CYCLE=20
*STATIC, PTOL=6.
  1.0, 10., 0.1, 1.0
*TEMPERATURE, AMPLITUDE=STS
*NODE PRINT, NSET=NDMIN, FREQ=100
U
*EL PRINT, ELSET=ELMIN, FREQ=100
S
*EL FILE, ELSET=ES1, FREQ=20
S
*NODE FILE, NSET=NS1, FREQ=20
U
*END STEP

A.5 Pre-processing Program for Abaqus Displacement Analysis

PROGRAM ABPRE
PARAMETER (MXMNP=1200, MXMEL=1000)
IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)
CHARACTER FNAME*60, DTYPE*15
DIMENSION NOD(4,MXMEL), CONVN(MXMEL), CONVO(MXMEL),
$ DTEMP(MXMNP), DUMP(MXMNP), EAREA(MXMEL), EI(MXMEL),
$ EIP(MXMNP), RAT(MXMEL), STSN(4,MXMEL), STSO(4,MXMEL),
$ STNOP(MXMNP), TEMPN(MXMNP), TEMPO(MXMNP),
$ TEQ(MXMEL), TEQP(MXMNP), DISP(2,MXMNP), RZ(2,MXMNP)
DIMENSION H(4), E(4), Y(4), SS(4), DS(4)
DATA E /73000., 100., 2750.0, 7.3E4/
DATA Y /70.0, 10., 35., 70.0/
DATA EL, PL /6.95, 0.49/
DATA EXP1, EXP2 /35.E-6, 1.E-6/
REWIND 20
REWIND 21
REWIND 23
REWIND 25
REWIND 26
REWIND 14
REWIND 15
C
C *** READ POLYMERIZATION SHRINKAGE
C
READ (*,*) FAC
C
C *** READ OLD MESH DATA
C
READ(20,*) NUMNP
DO 10 IP=1,NUMNP
READ(20,*) INP, RZ(1,INP), RZ(2,INP)
10 CONTINUE
READ(20,*) NUMEL
DO 20 IE=1,NUMEL
READ(20,*) IEL, (NOD(IP,IEL), IP=1,4)
20 CONTINUE
READ(*,*) NSTEP
IF(NSTEP.LE.1) GO TO 25
DO 22 ISTEP=1, NSTEP-1
READ(21,21) FNAM
21 FORMAT(A60)
DO 22 IP=1, NUMNP
READ(21,21) FNAM
22 CONTINUE
READ(21,21) FNAM
DO 30 IP=1, NUMNP
READ(21,*) INP, TEMPO(INP)
30 CONTINUE
READ(21,21) FNAM
DO 40 IP=1, NUMNP
READ(21,*) INP, TEMPN(INP)
40 CONTINUE
IF(NSTEP.LE.1) GO TO 45
DO 42 ISTEP=1, NSTEP-1
READ(23,21) FNAM
42 CONTINUE
READ(23,21) NAME
DO 50 IEL=1,NUMEL
READ(23,*) IE,CONVO(IE)
50 CONTINUE
READ(23,21) NAME
DO 60 IEL=1,NUMEL
READ(23,*) IE,CONVN(IE)
60 CONTINUE
DO 70 IEL=1,NUMEL
READ(25,*) IE,RAT(IE)
70 CONTINUE
DO 80 IEL=1,NUMEL
READ(26,*) IE,(STSO(IS,IE),IS=1,4)
80 CONTINUE
C DO 90 IP=1,NUMNP
C90 READ(27,*) IPP,DISP(1,IPP),DISP(2,IPP)
C DO 100 IP=1,NUMNP
C READ(28,*) IPP,DP1,DP2
C DISP(1,IPP)=DISP(1,IPP)+DP2
C100 DISP(2,IPP)=DISP(2,IPP)+DP2
DO 110 IP=1,NUMNP
DTEMP(IP)=TEMPN(IP)-TEMPO(IP)
110 CONTINUE
C C
C INTERPOLATE THE MECHANICAL PROPERTIES BETWEEN
C 5% CONVERSION AND 80% CONVERSION
C
CV=(CONVN(IEL)-0.05)/0.75
IF(CV.LT.0.0) CV=0.0
IF(CV.GT.1.0) CV=1.0
CALL SHAPE(RAT(IEL),CV,H)
DO 150 IS=1,4
150 SS(IS)=STSO(IS,IEL)
EC=0.0
YC=0.0
DTEMPE=0.0
DO 200 IP=1,4
EC=EC+E(IP)*H(IP)
YC=YC+Y(IP)*H(IP)
DTEMPE=DTEMPE+DTEMP(NOD(IP,IEL))
200 CONTINUE
C EI(IEL)=(EC-E(2))/(E(4)-E(2))
EI(IEL)=(CONVO(IEL)+CONVN(IEL))*0.5
POI=EI*0.34-0.25+0.25
EXPAN=RAT(IEL)*(EXP1-EXP2)+EXP2
DTEMP=DTEMPE/4.0
DEV=(FAC*(CONVN(IEL)-CONVO(IEL))*RAT(IEL)+EXPAN*DTEMPE)
TEQ(IEL)=DEV/EXP1
CALL YIELD(DS, SS, SEQ, SMEAN)

IF(SEQ.GE.YC) GO TO 300

GO TO 500

300 HP=EC/99.

WRITE(*, 309) IEL, YC, SEQ

309 FORMAT(' ELM IN PLASTIC: ', I4, 'YS & SEQ: ', 2E14.5)

CONTINUE

CALL CAREA(NOD, RZ, NUMNP, NUMEL, EAREA)

CALL AVER(EI, EIP, DUMP, EAREA, NOD, RZ, NUMNP, NUMEL)

CALL AVER(TEQ, TEQP, DUMP, EAREA, NOD, RZ, NUMNP, NUMEL)

C OUTPUT FOR ABAQUS

DO 700 IP=1, NUMNP

WRITE(14, 920) IP, EIP(IP)

920 FORMAT(I5, ' ', E12.5)

700 CONTINUE

DO 710 IP=1, NUMNP

WRITE(15, 920) IP, TEQP(IP)

710 CONTINUE

STOP

END

SUBROUTINE SHAPE(S, T, H)

*** SUBROUTINE TO EVALUATE THE SHAPE FUNCTION

AT SPECIFIED POINT

IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)

DIMENSION H(4)

H(1) = (1.0 - S) * (1.0 - T)

H(2) = S * (1.0 - T)

H(3) = S * T

H(4) = (1.0 - S) * T

RETURN

END

SUBROUTINE AVER(VE, VN, SUMA, EAREA, NOD, RZ, NUMNP, NUMEL)

IMPLICIT REAL*8 (A-H, O-Z), INTEGER*4 (I-N)

DIMENSION

VE(NUMEL), VN(NUMNP), SUMA(NUMNP), EAREA(NUMEL)

$ , NOD(4, NUMEL), RZ(2, NUMNP)

DO 10 IP=1, NUMNP

SUMA(IP) = 0.0

10 VN(IP) = 0.0

DO 20 IE=1, NUMEL

DO 20 IP=1, 4

NODE = NOD(IP, IE)

SUMA(NODE) = SUMA(NODE) + EAREA(IE)

20 VN(NODE) = VN(NODE) + VE(IE) * EAREA(IE)
DO 30 IP=1,NUMNP
IF(SUMA(IP).LE.0.0) GO TO 999
30 VN(IP)=VN(IP)/SUMA(IP)
RETURN
999 WRITE(*,900) IP
900 FORMAT(2X,'*** AREA AROUND POINT NO.:',I5)
STOP
END

SUBROUTINE CAREA(NOD,RZ,NUMNP,NUMEL,EAREA)

*** SUBROUTINE TO CALCULATE AREA OF EACH ELEMENT

IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DIMENSION EAREA(NUMEL),X(4),Y(4)
$ ,NOD(4,NUMEL),RZ(2,NUMNP)
DO 20 IEL=1,NUMEL
  DO 10 IP=1,4
    X(IP)=RZ(1,NOD(IP,IEL))
  10 Y(IP)=RZ(2,NOD(IP,IEL))
  20 EAREA(IEL)=X(1)*Y(2)+X(2)*Y(3)+X(3)*Y(4)+X(4)*Y(1)
  $ -X(2)*Y(1)-X(3)*Y(2)-X(4)*Y(3)-X(1)*Y(4)
RETURN
END

SUBROUTINE YIELD(D,S,SEQ,SMEAN)

IMPLICIT REAL*8 (A-H,O-Z), INTEGER*4 (I-N)
DIMENSION S(4),D(4)
SMEAN=(S(1)+S(2)+S(3))/3.0
D(1)=S(1)-SMEAN
D(2)=S(2)-SMEAN
D(3)=S(3)-SMEAN
D(4)=S(4)
VAR=D(4)*D(4)+0.5*(D(1)*D(1)+D(2)*D(2)+D(3)*D(3))
SEQ=SQRT(3.0*VAR)
RETURN
END
APPENDIX B
MOLDING OF BUMPER BEAMS

B.1 Introduction

The bumper of a passenger vehicle is a system to provide protection against damage affecting the safety components of the vehicle during low-speed impacts as required by Federal Motor Vehicle Safety Standard (FMVSS) 215 [Kowalski, 1982]. The standard requires that a vehicle be subjected to a series of 5 mph impacts with a pendulum test device, shown in Figure B.1. The mass of the pendulum is made equal to the mass of the vehicle under test. One of the most popular systems consists of fascia and a bumper beam as a structural element to withstand the impacts. Bumper beams made from SMC not only provide good stiffness and corrosion resistance, but also cost less and need less time to assemble than conventional metal bumper systems [Reinforcement Digest, 1992].

Molding of SMC bumper beams require large amount of development effort to design a suitable set of SMC raw material, initial charge pattern, and molding conditions in order to produce sound parts which meet the Federal safety requirement. Hundreds of trials may be needed for a process to be adopted in production. The problems in the molding of thick parts may include long curing times,
suitable charge design, and SMC ply delamination. Some of these problems encountered in the trials may not be obvious from the molding samples. Using numerical simulation technique could assist the polymer engineer in identifying potential problems. It is expected that numerical simulation would accelerate the development of a new bumper beam, thus lowering its overall life-cycle cost.

The objective of this study was to investigate the filling and curing patterns of the molding process using an industrially relevant part. In this chapter, molding experiment and simulation of bumper beam, shown in Figure B.2, are discussed. The bumper beam was 1.5 m (59 in) in length and 0.16 m (6.3 in) in width. The thickest part of the cross section was 11 mm (0.43 in). The molding experiment was conducted on a production press equipped with thermal couples and data acquisition system. The temperature measured by instrumentation
Figure B.1. FMVSS 215 impact pendulum device profile [Kowalski, 1982].

Figure B.2. Isometric view of bumper beam.
B.2 Molding Experiment

The molding experiment was carried out at member company of the Engineering Research Center for Net Shape Manufacturing. The SMC raw material used in the experiment was a vinyl ester compound with an average thickness of 2.11 mm (0.083 in) off the SMC roll. The material composition of the SMC is listed in Table B.1. The charge pattern used in the molding was 5 plies of 178 mm x 1397 mm (7 in x 55 in) SMC. The mold conditions were: (1) mold temperature: 149 °C (300 °F), (2) mold closing speed: 0.7 mm/sec. (0.185 in/sec.), (3) press tonnage: 600 tons.

The temperature was measured by inserting a thermocouple in the charge. The thermocouple was located between the second layer and the third layer, and at a distance approximately 300 mm from one end of the charge. Figure B.3 shows the temperature histories of two repeating runs. From this figure, one can see that the cure started at 70 to 80 seconds after the mold started closing. The peak exotherm occurred at 80 and 88 seconds with temperatures at 203 °C and 227 °C, respectively. The discrepancy of these two runs might result from the positioning and translation of the thermocouples during molding. Sample B showed a faster heat transfer and curing with a lower peak temperature. This reveals that the thermocouple at sample B might be located closer to the mold surface.
Table B.1. Composition of SMC used in bumper beam molding experiment.

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>glass fiber</td>
<td>60%</td>
</tr>
<tr>
<td>resin</td>
<td>35.95%</td>
</tr>
<tr>
<td>thickener</td>
<td>2.25%</td>
</tr>
<tr>
<td>mold release</td>
<td>0.53%</td>
</tr>
<tr>
<td>low profile additive</td>
<td>0.53%</td>
</tr>
<tr>
<td>pigment</td>
<td>0.36%</td>
</tr>
<tr>
<td>promoter</td>
<td>0.36%</td>
</tr>
<tr>
<td>inhibitor</td>
<td>0.04%</td>
</tr>
</tbody>
</table>
Figure B.3. Temperature histories of two molding samples.
B.3 Simulation of Mold Filling

The simulation is carried out under the assumptions that the SMC charge has homogenous and isotropic physical and mechanical properties. The deformation is assumed to be plane strain which is the case only at the center cross section for the bumper beam. The flow properties of the SMC is assumed to be rigid-viscoplastic. This approach has been successfully used by Fan, et al. [1988]. The length of the charge is 1397 mm (55 in) whereas that of the mold cavity is 1500 mm (59 in). Because the charge covered 93% of the mold in the length direction, there was very little flow in that direction. Therefore, the material flow is assumed to be plane strain in the molding simulation and the cross section at the center of the bumper beam is analyzed. The geometry of the cross section at the center is shown in Figure B.4. From the standpoint of SMC practices, the part is relatively thick with the thickest wall at 11 mm (0.43 in). The fillet and corner radii are 3 mm (0.12 in) and 6 mm (0.24 in), respectively.

The free resting period of the molding process was neglected because the charge and the mold cavity had very limited contact area as shown in Figure B.5. This limited contact area also arose numerical difficulty in filling simulation. A convergent solution for the first step was not possible to obtain with this initial charge geometry. Therefore, the charge was slightly modified to increase the contact area. The finite element mesh of the modified charge is shown in Figure B.6. The initial temperature of the charge and mold are 25 °C (77 °F) and 150 °C (302 °F), respectively. Further, the mold temperature is assumed to
be constant (150 °C) in the entire process. The material properties used in the filling simulation is listed in Table B.2. During the filling stage, the core is moving downward at a constant speed of 4.7 mm/sec. (0.185 in/sec.).

<table>
<thead>
<tr>
<th>Table B.2</th>
<th>Physical and mechanical properties used in SMC molding simulation [Fan, et al., 1988]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho ) (g/ml)</td>
<td>1.89</td>
</tr>
<tr>
<td>( C_p ) (N-mm/kg-°C)</td>
<td>1.083</td>
</tr>
<tr>
<td>( k ) (N-mm/mm-s-°C)</td>
<td>0.3864</td>
</tr>
<tr>
<td>( h ) (N-mm/mm²-s-°C)</td>
<td>0.5</td>
</tr>
<tr>
<td>( \bar{\sigma} ) (N/mm)</td>
<td>( \sigma_0 + k\varepsilon^{0.155} )</td>
</tr>
</tbody>
</table>

\( \sigma_0 = 0.0532 \exp[3010.0(1/ T - 1/295)] \) .

\( \kappa = 2.4574 \exp[8809(1/ T - 1/295)] \)
Figure B.4. Central cross section of the bumper beam.
Figure B.5. Schematic of initial SMC charge plies rest on the mold cavity. Two upper corners of the mold cavity contact with SMC charge.
Figure B.6. Finite element mesh of the charge.
Figure B.7 shows the finite element mesh at time = 10.33 seconds. At this stage, two distinct phenomena can be seen, namely folding and necking. There is no reports about folding and necking from the molding engineers. These may be artifacts due to the numerical modeling. Nevertheless, these could serve as potential problematic sites in the molding. These would help molding engineer in identifying the defects related to the molding process. Followings are explanation of causes of these defects based on the simulation results.

Figure B.8 shows the necking area at the right vertical wall. This occurrence of necking can be explained as follows. The whole charge tilts to the right hand side when the left end of the core squeezes down the charge. Therefore, there is more material accumulated at right corner of the cavity. As the core moves down further, the excessive material at this corner prevents the charge from being pulled down. As a consequence, the charge is locked at the right shoulder of the cavity and necking occurs. The charge after necking would break into two pieces from the original one piece charge. These two charge may be met together before the end of the filling stage and form a weld line.

An approximation was made at this stage to simplify the problem. The smaller part of the charge was removed from the charge and a new FEM mesh was generated for the rest of the charge. This would result in a charge smaller than the original one. The time to fill up the mold cavity is extended longer than original one. With this simplification, the information about curing can be obtained for reference purpose.
Folding occurs at right corner of the core, as detailed in Figure B.9. This is related to the spatial variation of flow stress described as follows. In compression molding of SMC, the temperature of the mold is higher than the temperature of the charge in order to promote the chemical reaction (curing). The charge in contact with mold surface has a higher temperature than that in the inner part of the charge. Hence, the outer edge of the charge which comes in contact with the mold surface has a lower flow stress. The spatial variation of flow stress creates a different flow pattern in comparison with the isothermal case. Figure B.10 illustrates four different flow patterns in a simple upsetting of a material whose flow stress is assumed to be a function of temperature only. When there is no friction, the velocity distribution is uniform in the isothermal case as shown in Figure B.10a. The friction at the interface resists the flow in the vicinity of the interface. Therefore, the charge at interface has a lower velocity as shown in Figure B.10b. In the non-isothermal cases (Figure B.10c), we can see that the charge at the interface has a higher velocity due to the lower flow stress caused by the higher temperature. Although the friction decreases the velocity at the interface, the velocity at the interface is still higher than that in the center area, as shown in Figure B.10d. In the numerical simulation, the interface friction is usually assumed to be a fraction of flow stress at the interface. Therefore, the effects of the friction in the non-isothermal case are not as significant as the one in the isothermal case.
Figure B.7. Finite element mesh at time = 10.33 seconds.
Figure B.8. Finite element mesh in the necking area at time = 10.33 seconds.

Figure B.9. Finite element mesh in the folding area at time = 10.33 seconds.
Figure B.10. Velocity distributions in simple upsetting. (a) isothermal without interface friction, (b) isothermal with interface friction, (c) non-isothermal without interface friction, (d) isothermal with interface friction.
In the simulation, the tilting of the charge toward the right hand side also fills the right hand side cavity earlier than the left hand side. As shown in Figure B.11, the right hand side is filled after 22.87 seconds. At this time, there is still a large cavity to be filled over the left hand side. Consequently, the material near the right side wall has a longer contact time than that near the left side wall. Therefore the material temperature near the right side wall is slightly higher than that near the left side wall, see Figure B.12. Generally speaking, the side walls of the workpiece have higher temperatures than those at the bottom web due to the longer contact time. These high temperature areas will result in a faster curing at the later stage of molding.
Figure B.11. Finite element mesh at time = 22.87 seconds.
Figure B.12. Calculated temperature distribution of bumper beam after complete filling.

Temperature
1: 40 °C
2: 55 °C
3: 70 °C
4: 85 °C
5: 100 °C
6: 115 °C
Curing simulation was carried out after mold cavity has been complete filled. The temperature distribution at the end of the filling stage is used as the initial temperature of the curing simulation. The curing model used in this simulation is the model proposed by Stevenson [1980, 1986] and Lee [1981]. This model did not require to assume that the useful curing reaction begins when the number of developed initiator radicals equals the effective number of inhibitor molecules initially present. The SMC material cure reaction can be described as a combination of three steps: initiation, inhibition, and propagation. The governing equations for each of these three steps can be written as

Initiation:
\[
\frac{dI}{dt} = -k_d I \tag{B.1}
\]

or

\[
\frac{d[R\bullet]}{dt} = 2fk_d I - qk_z Z[R\bullet] \tag{B.2}
\]

where

- $I$ = concentration of initiator
- $Z$ = concentration of inhibitor
- $k_d$ = rate constant of initiator decomposition
- $k_z$ = rate constant of inhibitor decomposition
- $A_d = A_d \exp(-E_d/RT)$
\[= A_z \exp(-E_z/RT)\]

\([R\bullet]\) = concentration of free radical

\(f\) = initiator efficiency

\(q\) = inhibitor efficiency

Inhibition:
\[\frac{dZ}{dt} = -k_z[Z[R\bullet]] \quad (B.3)\]

Propagation:
\[\frac{dM}{dt} = -k_p[M[R\bullet]] \quad (B.4)\]

or
\[-\frac{1}{M_0} \frac{dM}{dt} = \frac{d\alpha_c}{dt} = k_p(1 - \alpha_c)[R\bullet] \quad (B.5)\]

where

\(M\) = monomer concentration

\(M_0\) = initial concentration of the total C=C bond

\(k_p\) = rate constant of monomer propagation

\[= A_{po} \exp(-E_{po}/RT)(1 - \alpha_c / \alpha_f)^{m'}\]

\(\alpha_c\) = fractional conversion.

\(\alpha_f\) = final conversion

\(m'\) = parameter.
The parameters of this model are listed in Table B.3. These curing model parameters are obtained from experimental data based on three isothermal DSC measurements. Figure B.13 shows the comparison of the fractional conversions from experiments and the present numerical model.

Figure B.14 shows the calculated temperature distribution of the bumper beam at 71.9 seconds. About one-third of the cross-sectional area is at a temperature higher than the mold temperature, 150 °C. This indicates that these areas already passed the peak exotherm by this time. From Figure B.15, we can see that the fractional conversions at these high temperature areas are greater than 90%. Although the initial temperature near the left side wall before curing is only slightly lower than that near the right side wall, the curing reaction is much slower near the left side due to its larger wall thickness.

Figures B.16 and B.17 show the calculated temperature and fractional conversion distributions at 109.8 respectively. The lower left corner cured last, as shown in B.17, due to the lower initial temperature and the larger mass inertia. Figure B.16 also shows that the thinner wall will cool down faster than the thicker one, as we compare the temperature near the left side wall with that near the right side wall.

Figure B.18 shows both the calculated and measured temperature history of a point at the center of the left side web. The temperature calculated by numerical model rises up and cools down slower than the measured data. This may result from the difference of the
thermocouple positions in experiments and calculation. In the experimental molding, the thermal couple was placed near the end of the beam where the wall thickness is uniform at 6 mm. The simulation was at the center of the beam with wall thickness varied from 9 mm to 11 mm.

Table B.3. Kinetic parameters of curing model B used in curing simulation of bumper beam [Muzumdar, 1992].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{p0}$</td>
<td>$1.901 \times 10^7$</td>
</tr>
<tr>
<td>$E_{p0}$ (KJ/mole)</td>
<td>38.46</td>
</tr>
<tr>
<td>$A_z$</td>
<td>$3.846 \times 10^{10}$</td>
</tr>
<tr>
<td>$E_z$ (KJ/mole)</td>
<td>52.101</td>
</tr>
<tr>
<td>$A_d$</td>
<td>$1.398 \times 10^{12}$</td>
</tr>
<tr>
<td>$E_d$ (KJ/mole)</td>
<td>117.35</td>
</tr>
<tr>
<td>$m$</td>
<td>1.025</td>
</tr>
</tbody>
</table>
Figure B.13. Comparison of DSC data and computation data from curing model at three different temperatures, (a) 95 °C, (b) 105 °C, (c) 115 °C.
Temperature
1: 105 °C
2: 120 °C
3: 135 °C
4: 150 °C
5: 165 °C
6: 180 °C

Figure B.14. Calculated temperature distribution in the central cross section of the bumper beam at time = 71.9 seconds.
Figure B.15. Calculated fractional conversion distribution in the central cross section of the bumper beam at time = 71.9 seconds.
Figure B.16. Calculated temperature distribution in the central cross section of the bumper beam at time = 109.8 seconds.
Fractional Conversion
1: 0.10
2: 0.26
3: 0.42
4: 0.58
5: 0.74
6: 0.90

Figure B.17. Calculated fractional conversion distribution in the central cross section of the bumper beam at time = 109.8 seconds.
Figure B.18. Comparison of temperature histories obtained from simulation with that obtained from molding experiment.
B.4 Molding Multi-Layered Charge

In the molding of SMC parts, the charge usually consist of several plies. The bonding between plies is a critical issue for a SMC structural part. There has been some parts showing delamination after impact test. It is not clear at this time how this would have happen. It is the objective of this study to investigate the possibility of ply delamination during molding.

As it is convenient to assume that the charge is single-layered with the total thickness of the actual charge, in reality, the charge consists of multiple plies of SMC. In this study, a multiple-layered charge was used to investigate the delamination during molding. The term "layer" is used in this dissertation to describe the finite element mesh group used in the calculation. One or more plies may be grouped as a single layer in this study. In the following, we used a simplified approach to investigate the molding of a charge made of multiple plies. The five-ply charge used in the molding is assumed to be consisted of a thin layer and a thick layer in the simulation. These two layers represent the top ply and the bottom four plies. The finite element meshes of these two layers are shown in Figure B.19.

It is assumed that the plies are stacked together at the beginning of the filling stage. However, there is no cohesion between two layers. Therefore, delamination between layers will occur if there is any tensile force at the interface. There will be only free convection between layers if the layers are separated. Therefore, the localization of heat transfer will be reinforced due to the separation between layers.
The interfacial heat transfer coefficient between two plies depends strongly on the pressure between plies. Future effort is needed to investigate the interface heat transfer coefficient as a function of pressure, charge material, surface condition and temperature. However, this is not the major objective of the present study. The interfacial heat transfer coefficient between two plies is assumed to be the same as the one between the charge and the mold surface. The geometry of the charge and the calculated temperature distribution are shown in Figure B.20. In two-layered charge, the interfacial heat transfer coefficient is not high enough to have the same heat transfer properties as single-layered charge. Therefore, the heat from the mold surface can not penetrate through the whole thickness, as shown in Figure B.20.

It should be noted that the top right part of the first layer also has necking during the molding simulation and a smaller portion of the charge has been removed from the FEM model as a simplification. This phenomenon from numerical calculation may increase the in-plane compression acting of the top layer.

An important issue in the molding of SMC is the void formation in the part. The charge is designed to have enough flow and pressure during filling stage to expel the voids in and between the sheets. However, according to the calculated results (see Figure B.20), the separation between layers will create large voids. The ply delamination of charge during molding result from the combinal effects of bending, in-plane compression, and the normal force from the hump of the
lower mold. This indicates that if these voids can not be sealed after
the mold is completely closed, the concave profile in the cavity should
be avoided. If it is necessary to have concave profile in the cavity, the
molding pressure should be high enough to seal the voids created by
the separation between layers. Although the delamination during the
molding process has not been report, it is possible that this could be a
site for poor bonding that initiate the delamination during the impact
test. More detail investigations need to be done on this issue.
Figure B.19. Finite element meshes of two-layered charge used in filling simulation of molding of bumper beam.
Figure B.20. Geometry and calculated temperature distribution of two-layered charge at step no. 355 (time: 7.06 sec.).
B.5 References


*Reinforcement Digest*, 1992, pp. 22-23, No. 49.

SAE, 1971, SAE J980a, Bumper Evaluation Test Procedure - Passenger Cars.
