IN-MOLD COATING OF THERMOPLASTIC AND COMPOSITE PARTS: MICROFLUIDICS AND RHEOLOGY

DISSERTATION

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

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2006

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ABSTRACT

The main technical issues in developing the in-mold coating (IMC) process of polymer and composite parts include: (i) flow pattern, (ii) injection pressure, and (iii) mold deflection. The injection pressure is greatly influenced by the flow field and rheological properties of the coating material. Due to the very small length scale of the IMC flow (15 \( \mu m \) to 125 \( \mu m \)), “apparent” wall slip at the solid-fluid interface occurs in the IMC flow. The high shear rates encountered in the microchannels make it necessary to include the higher shear rate plateau in the viscosity models. Including these two factors is critical in developing a predictive model of the IMC flow. For closed mold IMC, such as in injection molding and resin transfer molding (RTM), predicting the pressure is critical in designing a successful coating process. Mold deflection is also important in RTM as most molds are less rigid than in thermoplastic injection molding.

Flow models based on the slip boundary conditions have been developed to determine the viscosity of microfluidics. A customized microslit rheometer – a slit rheometer with micrometer-sized channels of 4-mil (101.6-\( \mu m \)) and 1-mil (25.4-\( \mu m \)) gaps – was built to measure the viscosity at the microscopic level and at various temperatures. The viscosity data of the coating material was verified by the viscosity measurement from the commercial parallel-disc rheometer at high shear rates. The reduced viscosity of
the coating material was found in the 1-mil (25.4-μm) channel gap, which indicated the apparent wall slip in the flow system. The developed rheological models were used to analyze the experimental results and determine the slip parameter known as slip length. The average value of the slip length obtained from the experiment was then used in modeling the slip flow to predict the pressure. Furthermore, the apparent slip often found in polymer dispersion systems was discussed and used to model the IMC flow.

The numerical solutions based on (i) the viscosity models: the power law and the Carreau viscosity models, and (ii) boundary conditions: no-slip, true slip, and apparent slip were compared with the experimental results. It was found that the Carreau viscosity model of the coating material improved the pressure prediction of the IMC flow while the slip boundary condition was important to accurately predict the pressure in the 1-mil (25.4-μm) channel gap. The work of this dissertation makes it now possible to predict the pressure for IMC of thermoplastics.

The last technical issue, the mold deflection, was studied in IMC of RTM. Simple mathematical models of IMC of RTM were derived to determine the pressure and hydraulic force. The effect of the mold deflection due to the injection pressure was integrated into the model in terms of the compressibility of the mold. The effect of the compressibility of both the substrate and mold on the pressure and hydraulic force is discussed in a case study. In addition, preliminary results of the mold deflection during IMC processing were simulated using commercial finite element method (FEM) packages. These should serve as a basis for developing a model of IMC for RTM.
Dedicated to my family
ACKNOWLEDGMENTS

First of all, I would like to express my deepest gratitude to my adviser, Dr. Jose M. Castro, for all of his guidance, continuous support and encouragement throughout my Ph.D. study. I am thankful to him for a great opportunity to work in the field of polymer processing.

I am very grateful to Dr. L. James Lee for his inspiring guidance, helpful advice, and an excellent opportunity to explore the world of nanotechnology.

I would like to thank Dr. Allen Yi for serving on my dissertation committee and Dr. Blaine Lilly for serving on my Ph.D. candidacy examination committee. Their experienced advice is precious to me. I also thank Dr. Kurt W. Koelling for his useful suggestions and constructive comments on my rheology-related work.

I greatly acknowledge the financial support from the Thai government, the Department of Industrial Engineering at Kasetsart University (KU), Thailand, the Department of Industrial, Welding and Systems Engineering (IWSE) at the Ohio State University (OSU), and the National Science Foundation (NSF), the United States.

Special thanks go to Elliott Straus of OMNOVA Solutions for supplying the IMC coating materials, technical information, and his constructive comments. I also would like to thank Dr. Nick Triantafillopoulos of OMNOVA Solutions for his comments related to the slip phenomena.
I thank Mary Hartzler, Bob Miller, and the staff of the machine shop as well as Cedric Sze and the staff of the computer laboratory at the Department of Industrial, Welding and Systems Engineering, OSU for helping me with machining and computer equipment.

I thank my research group members, especially Mauricio Cabrera Rios, Narayan Bhagavatula, and Yunior Hioe, for their assistance and friendship throughout my study.

Finally, I would like to thank my parents and my sister for their unwavering support during my graduate study. Without them, my dissertation would not have succeeded.
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CHAPTER 1

INTRODUCTION

1.1 Polymers and Polymeric Composites

Polymers and polymeric composites have been used in various industries including aerospace, automotive, construction, electrical and electronics, marine, textile, transportation, as well as other major industries (Astrom, 1997; Brydson, 1999). According to the Society of the Plastics Industry, the U.S. plastics industry employed approximately 2.2 million workers nationwide – about 2 percent of the U.S. workforce – and generated nearly $393 billion in total annual shipments in 2002. The plastics industry remains the nation’s fourth largest manufacturing industry in terms of shipments after the following manufacturing industries: motor vehicles and equipment, petroleum refining, and electronic components and accessories.

A polymer is a compound consisting of repeating structural units called mers that form large chain-like molecules, sometimes called macromolecules, held together by primary covalent bonding. The molecules are connected together within the aggregate material by secondary van der Waals bonding, in particular, hydrogen bonding (Grulke, 1994).
Polymers are usually classified into (i) plastics, which consist of thermoplastics and thermosets, and (ii) elastomers or rubbers. The molecules of thermoplastics consist of long chains of \textit{mers} in a linear or branched structure. Thermoplastics can be heated and cooled repeatedly without substantial change to their molecular structure or significant degradation of the polymers. Common thermoplastics include polyethylene, polystyrene, and polyvinylchloride. In contrast to thermoplastics, thermosets, when reheated, degrade rather than soften. When thermosets are initially heated at an elevated temperature, the molecules transform (or cure) into a rigid three-dimensional (3-D) cross-linked structure due to chemical reaction. Common thermosets are amino resins, epoxies, and phenolics. Elastomers have a 3-D cross-linked molecular structure similar to thermosets but the degree of cross-linking is substantially below that of thermosets. When subjected to a relatively low mechanical load, elastomers exhibit large elastic deformation. Natural rubber, neoprene, and silicone are examples of elastomers.

Polymers provide numerous competitive advantages over other engineering materials such as metals and ceramics. These advantages include: (i) plastics can be formed easily and economically at relatively low temperatures into complicated part geometries usually without further processing required; (ii) polymers have a wide range of mechanical properties and they can be either flexible or rigid; (iii) polymers have high chemical and corrosion resistance but low electrical and thermal conductivity; (iv) polymers are light in weight and they are usually lighter than metals and ceramics; (v) some plastics are transparent and can be colored as desired, which can give them desirable optical properties; (vi) polymers are inexpensive materials and can be reused and recycled by numerous methods; (vii) polymers are biocompatible; and (viii)
elastomers offer excellent elastic properties (Groover, 2002). Numerous manufacturing processes can be used to form polymers into useful products. Examples of polymer processing include injection molding, extrusion, blow molding, thermoforming, and compression molding. Details of these manufacturing techniques can be found in Osswald et al (2001), Rauwendaal (2001), Rosato et al (2003), Throne (1996), and Johnson (2001).

On the other hand, polymers in general have the following limitations: (i) polymers have low strength, modulus of elasticity, and stiffness relative to metals and ceramics; (ii) operating temperatures are limited to only a few hundred degrees because of the low melting (or glass transition) temperature of thermoplastics and the degradation of thermosets; and (iii) some polymers degrade when exposed to sunlight and other forms of radiation.

Polymeric composite materials are developed to improve and enhance the low strength and stiffness of polymers. A composite material is a material system composed of two or more physically distinct phases whose mixture exhibits combined properties that are different from those of its constituents. A polymeric composite consists of a polymer primary phase in which a secondary phase is imbedded in the form of fibers, particles, or flakes. Examples of polymeric composites include rubbers reinforced with carbon black and fiber-reinforced polymers (FRPs), for which thermosetting resins are commonly used and mixed with fiber reinforcement (Groover, 2002).

FRPs have a number of advantages and disadvantages. The outstanding properties of FRPs include: (i) high strength-to-weight ratio; (ii) high modulus-to-weight ratio; (iii) low specific gravity; (iv) good fatigue strength and toughness; (v) good corrosion
resistance; and (vi) low thermal expansion leading to good dimensional stability. However, FRPs have disadvantages and limitations as summarized in the following: (i) their mechanical properties (e.g. modulus of elasticity) are anisotropic – the properties depend on the directions of fiber reinforcement; (ii) they are subject to attack by chemicals, solvents, and radiation; and (iii) they are generally expensive due to the cost of the materials and manufacturing processes.

FRPs can be manufactured by several processes including hand lay-up, spray-up, reactive liquid molding (e.g. resin transfer molding, reinforced/structural reaction injection molding), compression molding (e.g. sheet molding compound, bulk molding compound), filament winding, and pultrusion. Details of manufacturing techniques to form FRPs can be found in Kai (1993), Peters (1998), Mazumdar (2001), and Gay et al (2002).

1.2 Processing of Polymers and Polymeric Composites

The coating operations discussed in this research are mainly related to three manufacturing processes of polymers and polymeric composites: (i) injection molding of thermoplastics, (ii) compression molding of sheet molding compound, and (iii) resin transfer molding.

1.2.1 Injection molding of thermoplastics

Injection molding is the most widely used molding process for thermoplastics. It is particularly well suited for mass production because the conversion of the raw material into a final product usually requires only a single operation. Moreover, little or no finishing process is required and complicated part geometries can be produced in a single
operation. Some thermosets and elastomers can also be injection molded with modifications in equipment and operating parameters to allow the cross-linking of these materials.

The processing steps of the injection molding are described as follows: The raw material is fed into the hopper on the injection molding machine as shown in Figure 1.1. The material is then conveyed, melted, and mixed thoroughly by the rotating screw within the heated barrel. In the filling stage, the molten plastic (or melt) is injected into the mold cavity under high pressure. After the mold cavity is completely filled, the injection pressure is switched to a packing (or holding) pressure in the packing stage and applied into the mold cavity to compensate for the shrinkage of the plastic material while cooling down. Figure 1.2 shows a typical cavity pressure trace for the injection molding process (Malloy, 1994). The applied pressure ends as soon as the sprue is solidified. Once the plastic melt has solidified, the mold opens and the final product is removed from the mold. The injection molding cycle of thermoplastics is illustrated in Figure 1.3 (Michaeli, et al, 2001).

1.2.2 Compression molding of sheet molding compound

Sheet molding compound (SMC) is the most common thermoset-based molding compound. Manufacturing of SMC usually consists of two distinctive steps: (i) compounding of a resin paste and (ii) molding of the SMC sheet. In the compounding process, all ingredients – including thermosetting resins, fillers, thickeners, low profile additives, initiators, color pigments, and mold release agents – are mixed together to create a resin paste. The premixed resin paste is then metered into a Doctor box where the
resin paste is uniformly spread on a carrier film. At the same time, the fibers are fed into the chopper and cut into lengths of 10 to 50 mm. The chopped fibers fall in a random pattern onto a moving conveyor of the resin paste on the bottom carrier film and are sandwiched between two carrier films to form the SMC sheet as illustrated in Figure 1.4. The fiber content varies between 25% and 40% by volume. The SMC sheet then passes through the compaction rolls to impregnate the fiber. The SMC sheet is finally rolled and stored to mature for up to a week before it is ready to be used. During the maturation period, the compound thickens (but does not cure) to a moldable viscosity.

The second step, the molding process of the SMC sheet (typically from 4 to 6 mm thick), takes place in the compression mold under heat and pressure as illustrated in Figure 1.5 (Davis et al, 2003). A charge is formed by cutting two to four SMC sheets of the desired shape and size and stacking them on a heated mold, typically 150°C (300°F). The SMC charge generally covers from 30% to 70% of the mold surface. As the mold compresses, the charge flows and deforms to the mold shape. After the mold is completely filled (only a few seconds), the curing stage begins and requires between one and three minutes. Once the resin has sufficiently cured, the part is stiff enough so that the mold can be opened and the final part removed. The typical compression molding cycle of the SMC sheet is shown in Figure 1.6.

1.2.3 Resin transfer molding

Resin transfer molding (RTM) is a closed mold process to form large fiber-reinforced polymeric composite parts. In the RTM process, a gel coat is usually applied to a mold cavity. A reinforcement preform is then placed in the gel-coated mold. Once
the mold has been closed, a thermosetting resin is injected into the mold cavity under relatively low pressure to impregnate the reinforcement. After the mold filling is completed, the resin is cured, which can take anywhere from minutes to hours, and the final part is removed from the mold. The typical processing cycle of RTM is shown schematically in Figure 1.7.

The advantages of RTM result from the low in-mold pressure (typically 350-700 kPa), which means that lower-cost equipment and composite molds can be used for prototypes and low-volume production (10,000 to 50,000 parts per year). In addition, inserts, fasteners, and cores can be integrated into the reinforcement to produce sandwich components. The total cycle time can be reduced by using higher mold temperatures or highly reactive mixing-activated resin systems; in this case, the process is known as high speed resin transfer molding (HSRTM) (Castro, 1996).

A variation of the traditional RTM is vacuum-assisted resin transfer molding (VARTM). In VARTM, a vacuum bag is employed as a soft upper mold instead of a steel or composite mold. This reduces the cost of the mold. A vacuum system is applied to assist liquid resin flow into the preform. An improvement on VARTM is the Seemann composite resin infusion molding process (SCRIMP). The idea of SCRIMP is to use either a highly permeable layer called resin distribution medium (RDM) or a foam core to facilitate the resin flow under the application of a vacuum system. RTM parts are used as components in numerous industries such as aerospace, automotive, and marine. These resulting consumer products include car body panels, boats, bath tubs, and sporting goods.
In the RTM process, gel coating is generally required to provide a good surface finish, protection from ultraviolet rays, as well as a primer layer for painting. However, a gel coat, typically consisting of polyester or vinyl ester resins mixed with styrene and/or pigments, releases harmful volatile organic compounds (VOCs) into the environment. The environmental problem arises from styrene emission. Styrene is very volatile, easily evaporated and becomes an inhalation hazard. Styrene exposure can cause irritation of eyes, nose, and respiratory system as well as headaches, nausea, and dizziness. The U.S. Occupational Safety and Health Administration (OSHA) strictly regulates the amount of styrene exposure in the industry. The average limit, which varies from state to state, is 50 part per million (ppm) on an eight-hour working day or a forty-hour working week Time Weighted Average (TWA) and 100 ppm on a fifteen-minute Short-Term Exposure Limit (STEL) (Julius et al, 2000 and Astrom, 1997).

1.3 Environmentally Friendly In-Mold Coating

In many applications, particularly for automotive components, molded plastic and composite parts need to be coated to eliminate surface defects (e.g. porosity, sink marks, waviness), to promote paint adhesion, and/or to provide better surface qualities in terms of appearance, durability, and weather resistance. These necessary requirements of the products lead to a development of the coating process called in-mold coating.

In-mold coating (IMC) of RTM parts, for instance, is an attractive alternative to gel coating because it not only serves the same functions as the gel coating, but also eliminates VOCs. IMC is an environmentally friendly process since the cured coating is 100% solid. The entire coating process occurs in the mold and avoids emission of VOCs.
In addition, the IMC coating layer is about 3-5 mils while the gel coating layer is typically 10 mils or thicker. The weatherability of the in-mold coated parts has been tested and found to be superior to that of the gel-coated parts as shown in Figure 1.8 (Straus et al, 1997). As a short-term approach, IMC can be used instead of gel coating to partially reduce the emission of VOCs in the process. However, a long-term approach is to replace both gel coating and painting (or top coat) with IMC. This ultimate goal will completely eliminate the emission of VOCs in the process as illustrated schematically in Figure 1.9. One of the benefits of replacing painting with IMC also involves the significant cost reduction of painting-related operations: reduction in capital investments, reduction in floor space for painting lines, reduction in manpower supporting painting operations, and reduction of emissions control equipment.

1.4 Research Objectives

Implementing the IMC process for plastic and polymeric composite parts is a challenging job. A predictive flow simulation package is critical to the successful development of the technology. In this way, the injection location can be properly selected and the press size is suitably chosen to avoid coating leakage. Three technical issues related to the coating flow are shown in Table 1.1. These issues include: (i) flow pattern of the coating material during mold filling, (ii) the pressure required to inject the coating material, and (iii) mold deflection due to the injection pressure of IMC.

The first issue – flow pattern – is important in the development of IMC of SMC, thermoplastic, and RTM parts. The flow pattern is related to several factors including the flow field, rheological properties of the coating material, and most importantly the
substrate thickness and its compressibility. It was reported by Chen (2004) that the substrate thickness plays a significant role in determining the flow pattern. The prediction of the IMC flow pattern helps locate the injection nozzle to achieve 100% coverage and minimize defects, such as trapped air and weld lines.

The second issue is concerned with the injection pressure of the coating material and hydraulic force generated by the injection pressure during IMC processing. It is necessary to determine the injection pressure and hydraulic force in order to find out the required capacity of a clamping tonnage of the machine. If the clamping tonnage is not sufficient, the mold will open resulting in the leakage of the coating material. Therefore, the injection pressure of the coating material needs to be considered, particularly in the closed mold processes (such as injection molding and RTM), to prevent the leakage of the coating material. On the contrary, in the case of SMC, accurate prediction of the pressure is not critical because the shear edges of the compression mold remain engaged even if the mold is opened and no leakage occurs.

The injection pressure is significantly affected by the flow field and rheological properties of the coating material. A study of the flow field in the IMC process is quite challenging because of the very small length scale of the channel gap. The IMC flow at the microscale level leads to several unusual microscopic phenomena, especially the wall slip at the fluid-solid interface. This wall slip phenomena affects the flow field in microchannels and leads to the invalidity of the conventional no-slip boundary conditions. Understanding the slip flow, effects of the wall slip on the flow field, and rheological properties of the coating material are essential in modeling the microflow and predicting the injection pressure in the IMC process. Therefore, a large portion of this
work is focused on the study of the slip phenomena in the microflow, effects of the wall slip on the flow field, and rheology of the IMC material.

The last issue deals with the mold deflection due to the injection pressure of the coating material. The effects of the mold deflection is more significant in IMC of RTM than IMC of SMC and thermoplastics because the RTM mold is typically made of inexpensive low-strength materials while the compression mold of SMC and the injection mold of thermoplastics are generally made of high-strength tool steels. Therefore, it is important to consider the effect of the mold deflection and the compressibility of the mold in the model, particularly in IMC of RTM.

1.5 Organization of the Dissertation

This dissertation is organized as follows:

Chapter 2 reviews previous research work on IMC processing and applications for plastic and composite parts, IMC materials, and IMC flow modeling.

Chapter 3 focuses on background of microfluidics, basic modeling of fluid flows based on the continuum models, and the constitutive equations of both Newtonian and non-Newtonian fluids.

Chapter 4 discusses the effects of wall slip on the flow field of IMC coating materials, reviews the wall slip phenomena in the microflow, and derives rheological models for slit rheometers based on (i) no-slip and (ii) slip boundary conditions.

Chapter 5 describes an experimental setup of a customized microslit rheometer developed in this work to study the slip phenomena in the microflow, presents the
experimental results of the viscosity measurement, and analyzes the viscosity data to
determine the slip parameter, known as slip length, for IMC materials.

Chapter 6 describes the governing equations used to predict the pressure drop in
the fluid flow based on various viscosity models and boundary conditions. The numerical
results of the pressure drop are compared with the experimental results to validate the
flow models of microfluidics.

Chapter 7 describes mathematical models in the filling and packing stages of IMC
of RTM parts. The effect of the mold deflection due to the injection pressure was
integrated into the model in terms of the compressibility of the mold. The effect of the
compressibility of both the substrate and mold on the pressure and hydraulic force is
discussed in a case study.

Chapter 8 summarizes the results, key research contributions, and suggestions for
future works.
Figure 1.1 A typical injection molding machine (Photo Arburg).
Figure 1.2 A typical cavity pressure trace for the injection molding process of thermoplastics (Molloy, 1994).
Figure 1.3 The injection molding cycle of thermoplastics (Michaeli et al, 2001).
Figure 1.4 Schematic representation of the production line of the SMC sheet.
Figure 1.5 The SMC compression molding process (Davis et al, 2003).
Figure 1.6 The SMC compression molding cycle (Davis et al, 2003).
Figure 1.7 A typical processing cycle of the RTM process: a) spraying a gel coat, b) curing a gel coat, c) placing a reinforcement preform, d) filling a resin, e) curing the resin, and f) removing the part.
Figure 1.8 The gloss retention of gel coated and colorcoat IMC coated panels subjected to accelerated weathering according to the UV stability per SAE J 1960, Jun 89 (Straus et al, 1997).
Figure 1.9 A schematic diagram of (a) the current RTM process, (b) the short term approach: using IMC instead of gel coating, and (c) the long term approach: replacing both gel coating and painting with IMC.
Table 1.1 The main technical issues in developing the in-mold coating (IMC) process of sheet molding compound (SMC), thermoplastic, and resin transfer molding (RTM) parts.

<table>
<thead>
<tr>
<th>Material / Process</th>
<th>Coating Thickness</th>
<th>Main Technical Issues</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression-Molded Sheet Molding Compounds (SMC)</td>
<td>30 mils 3-5 mils</td>
<td>***</td>
</tr>
<tr>
<td>Injection-Molded Thermoplastics</td>
<td>0 3-5 mils</td>
<td>*** *** ***</td>
</tr>
<tr>
<td>Resin Transfer Molding (RTM)</td>
<td>0 3-5 mils</td>
<td>*** *** ***</td>
</tr>
</tbody>
</table>
Chapter 2 reviews previous research work on IMC processing and applications, IMC materials, and IMC flow modeling. Processing of IMC applications for compression-molded sheet molding compound and injection-molded thermoplastics is described in detail. This chapter also addresses the main technical issues in IMC processing of those materials, explains IMC materials including formulations and kinetics, and summarizes modeling and analysis of the IMC flow.

2.1 Processing of In-Mold Coating Applications

2.1.1 In-mold coating of sheet molding compound

Sheet molding compound (SMC) parts usually have surface defects such as porosity, waviness, and sinks. For many years, in-mold coating (IMC) has been commercially applied to SMC as an environmentally friendly way to minimize problems with porosity. IMC also improves the surface quality of SMC parts in terms of functional and cosmetic requirements as well as provides a surface protection. IMC can be used either as a conductive primer-like layer for a subsequent painting operation or it can be used as a topcoat, providing a paint-like surface. In the IMC process, a liquid coating
material is injected onto the surface of the SMC substrate at the end of the molding process while the part is still in the mold. After the coating material has been cured by chemical reaction, the coated SMC part is removed from the mold. Cured IMC is a 100% solid material and, therefore, no volatile chemicals are released during the process. Nowadays, the IMC process is considered an integral part of the molding cycle in the production of compression-molded SMC exterior automotive body panels. Figure 2.1 depicts all stages of the SMC compression molding/in-mold coating (SMC/IMC) process.

The IMC application to SMC parts is classified according to the way of applying the coating material into the mold or the amount of pressure required to inject the coating material: (i) the press-opened coating (POC) process, sometimes referred as low pressure IMC and (ii) the injection-opened coating (IOC) process, commonly called high pressure IMC (Castro and Griffith, 1993). In the POC or low pressure IMC process, once the SMC has been cured to the point that it cannot be damaged by mold separation, the clamping force is reduced in a decompression step and the mold is slightly opened (approximately 1 mm) to make room for the coating material while the shear edges of the mold remain engaged. After the desired volume of the coating material is injected into the mold, the clamping force is reapplied in a compression step. The mold is then closed, which spreads the coating material over the entire part. After the curing of the coating is completed, the final part is removed from the mold as shown schematically in Figure 2.2. Older generation presses can considerably increase the cycle time due to the decompression and compression steps in the process (Castro and Griffith, 1993).

In the IOC or high pressure IMC process, once the SMC has been cured to a certain degree that it cannot be damaged by the injection pressure, the coating material is
injected into the mold where the clamping force remains constant during the process. There are no decompression and compression steps in this process. It, therefore, requires higher pressure to inject the coating material and takes a longer time to fill the mold. The coating material flows by compressing the substrate until the hydraulic force generated by the flowing IMC material exceeds the clamping force at which the press opens but the shear edges remain engaged preventing leakage. The compressibility of the substrate significantly affects the amount of injection pressure. After the coating is completely cured by chemical reaction, the final part is removed from the mold. Figure 2.3 shows schematic representation of the IOC or high pressure IMC process.

2.1.2 In-mold coating of thermoplastics

In many applications, thermoplastic products are required to be subsequently painted to improve surface finish and surface quality as well as to provide surface protection. For example, in the automotive industry, injection-molded thermoplastic parts such as automotive body panels and bumpers are required to have a “class A” surface finish while most thermoplastic surfaces do not meet that requirement. It is also difficult to paint thermoplastic surfaces because they have low surface energy.

Because of the potential advantages of IMC and its successful application to SMC, IMC has been developed by OMNOVA Solutions Inc. located in Akron, Ohio – the leading supplier of IMC materials for SMC products – to achieve the adhesion of coatings to the injection-molded thermoplastic parts. Honda Manufacturing has shown interest in using IMC as a substitute for the adhesion promoter used in their current
painting operation. If the surface quality is satisfactory, they will employ IMC as an alternative to painting (Chen, 2003).

An injection molding process typically consists of three processing steps: filling, packing, and cooling. In the filling stage, thermoplastic is heated and injected to fill up the cavity. In the packing stage, the pressure is increased to inject more plastic melt to compensate for the material shrinkage due to the solidification. In the cooling stage, the mold is cooled down and the part solidifies. Similar to injection molding, IMC of thermoplastics consists of three processing steps: filling, packing, and curing. However, the reactive coating material solidifies by chemical reaction in the curing stage. To perform in-mold coating, once the substrate is solidified and rigid enough to withstand the coating pressure, the coating material is injected onto the substrate while the part still remains in the mold. The coating material flows to cover the entire surface of the part by compressing the substrate in the filling stage. This is similar to the IOC or high pressure IMC process of SMC parts; however, the hydraulic force can not exceed the clamping force to avoid leakage. More coating material is injected into the cavity in the packing stage to achieve the desired coating thickness. The coating material is completely solidified in the curing stage and the final part is ejected from the mold. The thermoplastic injection molding integrated with IMC process is illustrated in Figure 2.4.

The timing control on the coating injection is very critical and was studied by Chen (2003). The coating material should be injected into the mold during the cooling stage of thermoplastics. The later the coating material is injected into the mold, the lower the pressure required to inject the coating material and the lower the substrate temperature. The lower substrate temperature decreases the chemical reaction rate and,
consequently, increases the cycle time. Therefore, the injection pressure of the coating material needs to be compromised with the substrate temperature in order to obtain an adequate curing rate and good adhesion of the coating.

2.1.3 Technical challenges in IMC of SMC and IMC of thermoplastics

Unlike IMC of SMC, one of the technical challenges in IMC of thermoplastics is to avoid the leakage of the coating material in the process. SMC parts are formed by compression molding where a mold with shear edges is used. The shear edge feature of the mold allows the mold to be partially opened. As long as the shear edges remain engaged, there is no leakage of the coating material. On the other hand, thermoplastic parts are formed by injection molding where a land mold is used. The mold is kept closed by clamping the mold halves at the parting line and has no shear edge. Any opening of the closed mold caused by the injection of the coating material will result in coating leakage. To avoid this problem, the clamping tonnage needs to be greater than the hydraulic force generated by the injected coating material at any time. This is also the case in IMC of RTM. The estimation of the hydraulic force generated by the coating material in IMC of RTM is described in detail in Chapter 7. The mold configurations of both the compression mold for SMC and the closed mold for thermoplastics and RTM are illustrated in Figure 2.5.

Another challenge of IMC of thermoplastics is the relatively low processing temperature. The typical mold temperature of SMC processing is approximately 150°C (300°F) or higher. At this temperature, the coating can be cured at an adequate rate. In thermoplastic processing, the mold temperatures are varied and mostly lower than 150°C,
depending on the type of thermoplastics. For example, the mold temperatures of thermoplastics, commonly used in the automotive industry, are as follows: 125°C (257°F) for Polyethylene Terephthalate (PET), 88°C (190°F) for Polycarbonate Acrylonitrile Butadiene Styrene (PCABS), 58°C (136°F) for Acrylonitrile Butadiene Styrene (ABS), and 45°C (113°F) for Thermoplastic Polyolefin (TPO).

This lower mold temperature increases the cure time of the coating material as well as the cycle time of the entire process. In some cases of low temperature thermoplastics, the cure time could possibly be as long as 350 seconds or more, which is not suitable for industrial manufacturing (Zuyev, 2004). Other coating systems applied for thermoplastics such as a mixing-activated two-component system can be an effective alternative to the thermally-activated one-component system employed in the coating systems for SMC. Formulations and kinetics of the coatings for SMC and thermoplastics are described in more detail in Section 2.2.

2.2 Coating Materials

2.2.1 Formulation of the coatings

The coatings formulation is designed to meet surface finish requirements, to provide the desired functional properties, and to pass the customer application tests. In the automotive industry, for instance, the coating must provide a smooth surface and gives a distinctness of image (DOI) of 95 and a 60° gloss reading of 70. The coating layer must be stronger than the substrate so that any mechanical failure originates in the substrate rather than the coating. The coating layer must have a pencil hardness of H and conductivity of at least 165 Ransburg units at 0.0635-mm thickness. Hardness must also
be adequate for handling without damage when removing from the hot mold and during subsequent operations. Coated parts must give a gravelometer adhesion test rating of at least 8 and pass water immersion, accelerated and outdoor weathering, and other tests commonly used to qualify paints (Castro and Griffith, 1993).

Viscosity is one of the most important properties of the coating material. It influences the flow of the coating material in the mold. For non-reactive systems, the viscosity generally depends on temperature and rate of deformation. Reactive systems such as IMC are more complicated by the considerable increase in viscosity resulting from chemical reaction. For typical IMC systems, there is no significant increase in viscosity until all inhibitors are consumed. After all inhibitors are consumed, the viscosity increases significantly as shown in Figure 2.6. The time available for the flow of the coating material is typically designed to coincide with the time required for the inhibitors to be consumed to avoid the difficulty of highly increased viscosity. Thus, the chemical reaction can be neglected when modeling the filling stage. The viscosity of the coating material without catalysts for thermoplastics was measured and described in detail in Chapter 5.

The IMC coating material was first commercialized for SMC parts in the late 1970s. The coating material was a two-component reactive liquid containing unsaturated polyester and isocyanate to provide outstanding adhesion to the substrate. Later on, a one-component reactive system based on free radical reaction-based unsaturated oligomers and monomers was developed and also has excellent adhesion to the substrate. Compared to two-component systems, one-component systems are more commonly used.
because they are less sensitive to moisture and can be employed without any difficulties of metering and mixing (Castro and Griffith, 1993).

The IMC materials are formulated to provide both good coating performance and good molding capabilities. For example, the thermally-activated one-component coating material for SMC parts consists of (i) unsaturated oligomers and monomers to provide good hot hardness and adhesion to the substrate; (ii) peroxides to control the filling time and curing rate as desired; (iii) benzoquinone for longer shelf life and increased flow time; (iv) carbon black to enhance the conductivity of the coatings, which is desired for subsequent electrostatic painting, and to improve the mechanical properties of the coatings; (v) polyvinylacetate to provide better paint adhesion; (vi) fillers to increase hardness and reduce shrinkage; and (vii) a mold release agent to help remove the final part from the mold.

An example of the thermally-activated one-component coating material for thermoplastics is Stylecoat, which has been developed by Omnova Solutions Inc. The main components of Stylecoat are composed of unsaturated polyester, styrene, and catalysts: initiator and inhibitor. Tetra Butyl Perbenzoate (TBPB) is successfully used as an initiator in Stylecoat to coat high temperature thermoplastics such as PET and PCABS. The minimum recommended cure temperature of the coating material to achieve reasonable cure times is 90°C. Additionally, Cobalt Octoate (CoOct), 2,4-Pentanediione (2,4-P), and Methyl Ethyl Ketone Peroxide (MEKP) can possibly be used as initiators to coat low temperature thermoplastics, such as ABS and TPO, since they activate the chemical reaction at lower temperatures. However, this formulation causes a problem due
to its short shelf life. Shelf life and cure time of Stylecoat at different catalyst levels were studied by Zuyev (2004).

Another possible solution for coating low temperature thermoplastics is to use a mixing-activated two-component system. Similar to reaction injection molding (RIM), the concept of the method is to activate the chemical reaction when two reactive components (e.g. isocyanate and polyol) are mixed together. The system, therefore, eliminates the limitation due to low temperature processing of thermoplastics and the limited shelf life as found in one-component systems. In this system, two components are contained in separate temperature-controlled tanks. They are delivered through supply lines to metering equipment for precise measuring and then transported to a mixing head where they are mixed and injected into the mold. An example of the mixing-activated two-component system is shown in Figure 2.7. The main disadvantage of the mixing-activated two-component system is that mixing needs to occur on-line with molding. This makes the process much more challenging.

2.2.2 Kinetics of the coating materials

A study of the cure kinetics of the coating materials is necessary to characterize a reactive system and represent the IMC cure. The cure reaction of IMC materials is fundamentally a free radical polymerization. Heat development and structure build-up are the main consequences of the polymerization reaction. A series of kinetic models for free radical polymerization of IMC coating materials has been developed by Stevenson (1986) to describe the reaction mechanism including initiation, inhibition, and propagation steps.
The kinetic models were simplified to use in process modeling and proposed by Castro and Lee (1987).

The assumptions of the proposed model are summarized as follows:

1. Only one initiator and one inhibitor are used in the system.
2. No monomer reacts until the number of free radicals created by initiators is equal to the effective number of inhibitor molecules initially present.
3. A single reaction rate constant characterizes all propagation reactions.
4. Monomer diffusion control is less important.
5. Free radical termination is negligible.

Based on the above assumptions, the governing equations for the free radical mechanism under isothermal conditions can be written as follows:

1. In the initiation step, the initiator ($I$) decomposes to give two free radicals ($R\cdot$):

$$I \rightarrow 2R\cdot$$

Those free radicals ($R\cdot$) react with molecules of the inhibitor ($Z$) present in the system:

$$R + Z \rightarrow RZ\cdot$$

Until the time when all inhibitor molecules ($Z$) are consumed, which is called the inhibition time ($t_z$), all free radicals produced are inactivated instantaneously.

For $t < t_z$,

$$-\frac{dC_I}{dt} = k_d C_I$$

(2.1)
For isothermal conditions, the concentration of the initiator \( C_I \) at a given time \( t \) can be obtained as follows:

\[
C_I = C_{Io} \exp(-k_d t)
\]  

(2.2)

where \( C_{Io} \) is the initial concentration of the initiator, \( k_d \) is a kinetic rate constant for the decomposition at a given temperature \( T \).

At time \( t = t_z \) when all inhibitors are consumed, the initial concentration of the inhibitor \( (C_{zo}) \) can be determined as:

\[
(2.3a)\quad (2C_{zo} - C_I(t_z))
\]

By applying Equation 2.2 and introducing \( f \) and \( q \), we obtain the following equation for isothermal conditions:

\[
(2.3b)\quad qC_{zo} = 2fC_{Jo} \left[1 - \exp(-k_d t_z)\right]
\]

where \( C_I(t_z) \) is the concentration of the initiator at the inhibition time \( t_z \), \( f \) is the initiator efficiency, and \( q \) is the inhibitor efficiency. The values of \( f \) and \( q \) are between zero and one. \( f \) and \( q \) are introduced in the model because of the following reasons: (i) not every molecule of the initiator produces a free radical and (ii) not every molecule of the inhibitor can react with a free radical.

2. In the propagation step \( (t > t_z) \), free radicals \( (R\cdot) \) react with molecules of monomer \( (M) \):
\[ R \cdot + M \rightarrow k_p RM \cdot \]

For \( t > t_Z \),

\[
\frac{dC_M}{dt} = -k_p C_M C_{R*} \tag{2.4}
\]

where \( C_M \) is the concentration of monomer at a given time \((t, t > t_Z)\), \( C_{R*} \) is the concentration of the free radicals at a given time \((t, t > t_Z)\), \( k_p \) is a kinetic rate constant for the propagation at a given temperature \((T)\).

The concentration of the free radicals \((C_{R*})\) at a given time \((t, t > t_Z)\) for isothermal conditions can be estimated from the following equations:

\[
C_{R*} = 2[C_{i0} - C_i(t)] - C_{ZO} \tag{2.5a}
\]

or

\[
C_{R*} = 2fC_{i0}[1 - \exp(-k_d t)] - qC_{ZO} \tag{2.5b}
\]

By substituting Equation 2.3b into Equation 2.5b, we obtain

\[
C_{R*} = 2fC_{i0}\left[\exp(-k_d t_z) - \exp(-k_d t)\right] \tag{2.6}
\]

A kinetic rate constant for the decomposition \((k_d)\) at a given temperature and a kinetic rate constant for propagation \((k_p)\) at a given temperature can be respectively represented by the Arrhenius-type temperature-dependent equation as follows:
\[ k_d = k_{d0} \exp \left( -\frac{E_d}{RT} \right) \] (2.7a)

\[ k_p = k_{p0} \exp \left( -\frac{E_p}{RT} \right) \] (2.7b)

where \( k_{d0} \) is a frequency factor for the decomposition, \( E_d \) is the activation energy of the decomposition, \( k_{p0} \) is a frequency factor for the propagation, \( E_p \) is the activation energy of the propagation, \( R \) is an ideal gas constant, and \( T \) is temperature. These kinetic parameters, which include \( k_{d0}, E_d, k_{p0}, \) and \( E_p \), are determined experimentally from isothermal differential scanning calorimeter (DSC) measurement.

By substituting Equation 2.7a into Equation 2.3b and solving the equation, the inhibition time \( (t_z) \) can be estimated as follows:

\[ t_z = -\frac{1}{k_{d0}} \exp \left( \frac{E_d}{RT} \right) \ln \left[ 1 - \frac{qC_{Z0}}{2fC_{f0}} \right] \] (2.8)

In addition, by substituting Equation 2.6 into Equation 2.4, we obtain

\[ \frac{dC_M}{dt} = -2k_{p0}fC_{f0} \exp(-k_dt_z)C_M \exp \left( -\frac{E_p}{RT} \right) \left[ 1 - \exp \left( -k_d(t-t_z) \right) \right] \] (2.9)

By introducing \( A = 2k_{p0}fC_{f0} \exp(-k_dt_z) \), Equation 2.9 becomes

\[ \frac{dC_M}{dt} = -AC_M \exp \left( -\frac{E_p}{RT} \right) \left[ 1 - \exp \left( -k_d(t-t_z) \right) \right] \] (2.10)
By integrating Equation 2.10 for a constant temperature, the concentration of the monomer \(C_M\) at a given time \((t > t_d)\) can be determined as:

\[
C_M = C_{MO} \exp \left\{ \frac{A}{k_d} \exp \left( -\frac{E_p}{RT} \right) \left[ 1 - k_d(t - t_d) - \exp(-k_d(t - t_d)) \right] \right\} \tag{2.11}
\]

where \(C_{MO}\) is the initial concentration of the monomer.

The extent of the chemical reaction, which is called conversion \((c^*)\), is defined as follows:

\[
c^* = \frac{C_{MO} - C_M}{C_{MO}} = 1 - \frac{C_M}{C_{MO}}
\]

Therefore,

\[
c^* = 1 - \exp \left\{ \frac{A}{k_d} \exp \left( -\frac{E_p}{RT} \right) \left[ 1 - k_d(t - t_d) - \exp(-k_d(t - t_d)) \right] \right\} \tag{2.12}
\]

According to the equations derived earlier, the time period when the coating material can flow in the mold without the significant increase of the viscosity due to the chemical reaction can be estimated by Equation 2.8. In addition, the conversion of the chemical reaction at a given time can also be determined by Equation 2.12.

2.3 Modeling and Analysis of the IMC Flow

Castro and Griffith (1990) first proposed a mathematical model of the IMC flow for SMC parts. They developed the model for high pressure IMC where there is no mold
opening during IMC injection. As IMC is injected into the mold, it compresses the SMC substrate and spreads over the surface until the force generated by the coating liquid equals the imposed tonnage. An illustration of IMC filling is shown in Figure 2.8.

Assumptions of the model including isothermal conditions, quasi-steady-state flow with inertial terms neglected were made. Lubrication approximation was also assumed. In addition, an empirical equation was used to describe the relationship between the coating thickness \( h \) and the coating injection pressure \( p \):

\[
h = C(p - p_r)
\]

where \( C \) is the compressibility of the SMC substrate and \( p_r \) is the average mold clamping pressure on the uncoated part.

From experiments, the viscosity of typical IMC can be represented by the power law viscosity model:

\[
\eta = K \left[ \frac{1}{2} \mathbf{I}_\Delta \right]^{\frac{1}{n-1}}
\]

where \( K \) and \( n \) are the power law constants and \( \mathbf{I}_\Delta \) is the second invariant of the rate-of-deformation tensor.

By applying the above assumptions and using the symmetry condition, the momentum balance equation in a cylindrical coordinate system was simplified to:

\[
\frac{\partial p}{\partial r} = \frac{\partial}{\partial z} K \left( \frac{\partial v_r}{\partial z} \right)^n
\]

with boundary conditions:
z = 0; \quad v_r = 0

z = \frac{h}{2}; \quad \frac{\partial v_r}{\partial z} = 0

By integrating Equation 2.15 with respect to \( z \) and applying the above boundary conditions, the velocity of the coating material flow could be calculated by:

\[
v_r = \frac{1}{K^{1/(n+1)}} \left( -\frac{\partial p}{\partial r} \right)^{1/n} \left( \frac{h}{2} \right)^{(1/n)+1} \left( \frac{h}{2} - z \right)^{(1/n)+1}
\]

(2.16)

From Equation 2.16, the volumetric flow rate was obtained as:

\[
Q = \frac{2\pi r}{(1/n+2)K^{1/n}} \left( -\frac{\partial p}{\partial r} \right)^{1/n} \left( \frac{h}{2} \right)^{1/(n+2)}
\]

(2.17)

The relationship between the pressure drop and the flow rate was represented as:

\[
\frac{\partial p}{\partial r} = -\frac{Q' \left(1/n + 2\right)^r K}{(2\pi)^{r/(h/2)^{1+2n}}}
\]

(2.18)

By substituting Equation 2.13 into Equation 2.18 and then integrating it, the injection pressure of the coating material at different distances \( r \) is represented by Equation 2.19 and the spreading velocity of the coating material could then be calculated. However, as the mold opens when the hydraulic force generated by the injection pressure exceeds the clamping force, the spreading velocity calculated in this way would be smaller than the actual case because the additional flow caused by the mold opening was not taken into account. In the case of the mold opening before the coating injection where
the gap is known and constant, Equation 2.18 can be integrated directly to predict the fill pressure.

\[
p = p_T + \left( \frac{n^{1/2 + 2/n} C^{1 + 2/n}}{(2\pi)^n} \right) \left( \frac{2 + 2n}{1 - n} \right) \left( R^{1 - n} - r^{1 - n} \right)
\]  

(2.19)

A flow simulation program based on the generalized Hele-Shaw model was also used to predict the low pressure IMC flow. The generalized Hele-Shaw model for compression molding was represented by

\[
\frac{\partial}{\partial x} \left( \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial p}{\partial y} \right) = \frac{\partial h}{\partial t}
\]  

(2.20)

and

\[
\bar{u} = -\frac{S \frac{\partial p}{\partial x}}{h}
\]  

(2.21)

\[
\bar{v} = -\frac{S \frac{\partial p}{\partial y}}{h}
\]  

(2.22)

where \( \frac{\partial h}{\partial t} \) is the closing speed of the press, \( \bar{u} \) and \( \bar{v} \) are the gap-wise average velocities in the x and y directions respectively, \( p \) is the pressure, and \( S \) is the flow conductance defined as:

\[
S = \int \frac{\left( z - \frac{h}{2} \right)^2}{\eta} dz
\]  

(2.23)
The predicted mold filling showed a good agreement with the short shot experiments for IMC coating an automotive hood panel. However, the compressibility of the substrate was not taken into account in the simulation. Only the IMC flow caused by the mold closing was considered while the flow caused by compressing the substrate was neglected. To predict the IMC flow accurately, it is necessary to take the compressibility of the substrate into account, particularly in the case of the high injection pressure IMC process.

Chen (2003) developed a computer code for the two dimensional (2-D) IMC flow to predict the fill pattern of the coating material and the injection pressure for injection molded thermoplastic parts. The governing equations, based on the generalized Hele Shaw approximation, were solved by control volume based finite element method (CV/FEM). The compressibility of the thermoplastic substrate was modeled by the two-domain Tait PVT equation. The power law viscosity model was used to predict the rheological behavior of the coating material and no-slip boundary conditions were assumed in the flow model. It was found experimentally that the fill pattern of the coating material was successfully predicted by the numerical results; however, the prediction of the injection pressure was quite different from the experimental results as shown in Figure 2.9. More research works on the flow field at the microscale level and the improved viscosity models at high shear rates, such as the Carreau viscosity model, of the coating material need to be studied in order to better predict the pressure in the IMC process.
Figure 2.1 A schematic diagram of the SMC compression molding/in-mold coating (SMC/IMC) process (Zuyev, 2004).
Figure 2.2 Schematic representation of the press-opened coating (POC) or low pressure IMC process (Castro and Griffith, 1993).
Figure 2.3 Schematic representation of the injection-opened coating (IOC) or high pressure IMC process (Castro and Griffith, 1993).
Figure 2.4 A schematic diagram of the thermoplastic injection molding/in-mold coating (IM/IMC) process (Chen, 2003).
Figure 2.5 The mold configurations used in IMC of SMC and IMC of thermoplastics and RTM.
Figure 2.6 Typical viscosity changes of the coating material while IMC undergoes during typical processing.
Figure 2.7 Schematic representation of a mixing-activated two-component reactive system.
Top view of IMC and SMC during Injection

Section AA view

Figure 2.8 Schematic representation of the IMC flow before the mold opens (Castro and Griffith, 1990).
Figure 2.9 Comparison of the injection pressure between experimental and numerical results (Chen, 2003).
CHAPTER 3

BACKGROUND OF MICROFLUIDICS

Chapter 3 focuses on background of microfluidics, basic modeling of fluid flows based on the continuum models, and the constitutive equations of both Newtonian and non-Newtonian fluids.

3.1 Introduction to Microfluidics

Microfluidics is a new research discipline dealing with transport phenomena of fluid flows in fluid-based devices at microscopic length scales, typically 1 to 100 μm (Gravesen et al, 1993). In recent decades, microfluidics has become a popular and promising research topic due to the development of microelectromechanical systems (MEMS) technology and biochemical lab-on-a-chip devices. Microfluidic devices provide benefits over macroscopic devices such as lower material consumption, faster response/reaction time, better portability, and the possibly new functionality. In addition to microfluidic devices, material processing such as the in-mold coating (IMC) process is also a good example of microfluidics. The flow of the coating materials in IMC occurs in a channel gap ranging mostly from 15 μm to 125 μm, which is the final thickness of the IMC coating, as discussed in Chapter 2. The understanding of the flow behavior in
microchannels is essential in designing, analyzing, and modeling microfluidic devices and material processing such as IMC.

3.2 Microscopic Phenomena and Characteristics of Microfluidics

As the length scale of the fluid flow reaches the microscale level (1-100 μm) and below, several unusual phenomena that are not observed at the larger scales appear. The significant changes due to the very small length scale are summarized as follows (Conlisk and Singer, 2005):

- Fluid properties: Properties of fluids – particularly transport properties such as viscosity and diffusion coefficient – are different from their bulk values.

- Fluid-solid boundary: Fluids may slip at the fluid-solid interface leading to the invalidity of the no-slip boundary condition. This boundary condition is commonly assumed in conventional flow modeling. The significance of the wall slip in the microflow depends on several factors including the size of the channel gaps and type of fluids (e.g. simple Newtonian fluids, complex non-Newtonian fluids, or colloidal fluids). The wall slip occurring in the microflow leads to the apparent reduced viscosity of fluids. Details of the wall slip phenomena in the microflow are discussed in Chapter 4.

- Effects of surface properties: Physical, electrical, and chemical properties of the channel’s surface – such as roughness, electrical charge, hydrophobicity and hydrophilicity – become very important and significantly affect the fluid flow at the microscale level and below it. The significant effect of electrically-charged surfaces leads to two useful electrokinetic phenomena known as: (i)
electrophoresis – where the applied electrical field generates the motion of the charged surface relative to the stationary liquid – and (ii) electro-osmosis – where the applied electrical field generates the motion of ionized liquid relative to the stationary charged surface.

These microscopic phenomena can possibly be explained by characteristics of the microflow. These unique characteristics – due mainly to the very small length scale of the flow – include: (i) high surface-to-volume ratio leading to the significance of surface forces, (ii) high rate-of-deformation (e.g. high shear rate and high extensional rate), (iii) high heat and mass transfer rate as well as evaporation rate, and (iv) low Reynolds number ($Re$).

- High surface-to-volume ratio

This ratio determines the significance of the surface forces in the system, which can be demonstrated by the characteristic length $L$ of the surface area and volume as follows:

$$\frac{\text{Surface Area}}{\text{Volume}} = \frac{L^2}{L^3} = \frac{1}{L}$$

(3.1)

According to Equation 3.1, the surface-to-volume ratio for a channel with a characteristic length of 1 m is 1 m$^{-1}$ while that ratio for a microchannel having a size of 1 μm is 10$^6$ m$^{-1}$. The million-fold increase in the surface area and the very small mass of the fluid substantially affect the transport of mass, momentum, and energy. It is found that
the smaller the length scale, the higher the surface-to-volume ratio and the greater significance of the surface forces. Such surface forces include the long-ranged van der Waals attractive forces and shorter-ranged steric or electrostatic repulsive forces.

At very small scales, the surface forces become increasingly dominant over the body forces (e.g. gravitational and electromagnetic force), viscous force, and inertial force. The ratio of either the gravitational force, viscous force, or inertial force to the surface force can be determined by the following dimensionless numbers, respectively:

The Bond number: \[ Bo = \frac{\text{Gravitational Force}}{\text{Surface Tension Force}} \]

The Capillary number: \[ Ca = \frac{\text{Viscous Force}}{\text{Surface Tension Force}} \] (3.2a)

The Weber number: \[ We = \frac{\text{Inertial Force}}{\text{Surface Tension Force}} \]

In the case of a drop of water moving at 10 mm/s inside a 100 μm diameter tube, these dimensionless numbers can be obtained as follows:

\[ Bo = \frac{\rho g d^2}{\sigma} \approx 10^{-3} \]

\[ Ca = \frac{\mu U}{\sigma} \approx 10^{-4} \] (3.2b)

\[ We = \frac{\rho d U^2}{\sigma} \approx 10^{-4} \]

where \( \sigma \) is the surface tension force, \( g \) is the gravitational constant, \( d \) is the characteristic length, \( \mu \) is the viscosity of the liquid, and \( U \) is the characteristic velocity.
• High heat and mass transfer rate as well as evaporation rate

The large surface-to-volume ratio and small diffusion distance in microfluidic devices lead to the high heat and mass transfer rates in microfluidic systems. These high heat and mass transfer rates increase the yield and efficiency of thermal systems. These provide the advantages of microscale thermal devices (e.g. microheat exchangers and microreactors) over conventional scale thermal devices. Additionally, the microflow with a large free surface area under a high-temperature environment can cause a problem due to the fast evaporation. Consequently, the rate of evaporation should be taken into account in open-channel experiments and high temperature applications.

• High rate-of-deformation (e.g. high shear rate and high extensional rate)

For a simple drag flow of a liquid between two parallel plates with a distance $H$ (e.g. $10 \, \mu m$) and the upper plate moves at the velocity $V$ (e.g. 100 mm/s), the shear rate $\dot{\gamma}$ can be determined as:

$$\dot{\gamma} = \frac{V}{H} \approx 10^4 \, s^{-1} \quad (3.3)$$

According to Equation 3.3, the shear rate is inversely proportional to the distance between parallel plates $H$. Therefore, the flow in microchannels typically experiences the high shear rate ($>10^4 \, s^{-1}$). Moreover, such high shear rate is not achievable in macrochannels before the flow becomes turbulent. This high shear rate of the flow in microchannels significantly affects the viscosity of non-Newtonian fluids such as IMC coating materials, polymer melts and solutions. The measurement at the high shear rate of
rheological properties of the IMC coating materials is performed in this work and described in Chapter 5. Moreover, in many biofluids, this high rate-of-deformation may potentially cause the damage to the bioactivity of biomolecules such as protein, cells, and DNA.

- Low Reynolds number \((Re)\)

The relatively small channel dimensions and low flow velocities in microfluidic applications limit the liquid flows to small \(Re\), where \(Re\) is defined as the ratio of the inertial force to the viscous force as expressed in Equation 3.3. In the case of a water flow at the average velocity of 1 mm/s in a channel with a 100 \(\mu m\) hydraulic diameter, the Reynolds number can be approximated as:

\[
Re = \frac{\rho U D_H}{\mu} \approx 0.1
\]

where \(\rho\) is the density of the fluid, \(U\) is the average velocity of the fluid flow, \(D_H\) is the hydraulic diameter of the flow, and \(\mu\) is the viscosity of the fluid.

Due to the very small characteristic length in microfluidics, \(Re\) is usually less than one. This low \(Re\) indicates that the laminar flow is often found in the microflow. The laminar flow is commonly used in fluid dynamics to simplify the governing equations. Modeling of pressure-driven flow based on the continuum hypothesis is described in detail in Section 3.3.2.
3.3 Modeling of Fluid Flows

3.3.1 Classification of fluid flow modeling

A fluid flow can be modeled based on two approaches: (i) continuum hypothesis and (ii) molecular theory. A classification of flow models is displayed schematically in Figure 3.1 (Gad-el-Hak, 1999). In the continuum hypothesis, a fluid is assumed to be a continuous medium – which is describable in terms of the spatial coordinate (space) and time variations of macroscopic flow quantities such as density, pressure, velocity, and temperature – and cannot be divisible, in which the molecular structure and forces (e.g. intermolecular forces) of a fluid are ignored. Principles of mass, momentum, and energy balance (also commonly called conservation of mass, momentum, and energy) lead to a set of nonlinear partial differential equations such as Navier-Stokes and Euler equations.

The continuum models are generally easier to solve mathematically at a relatively low cost and short time and are more familiar to engineers compared to the molecular models. Therefore, continuum models should be used as long as they are applicable. However, in cases when the continuum models fail to accurately predict the fluid flow at the microscale, high-cost molecular models are the only approach available to determine the fluid flow in microchannels.

The molecular theory distinguishes the fluid as a collection of discrete particles to represent molecules, atoms, ions, and electrons. The macroscopic properties at any location in the flow are suitably averaged from a sufficient number of the discrete particles within the smallest significant volume of a flow. The final objective is to determine the position, velocity, and state of all particles at all times. Molecular-based flow models include molecular dynamics (MD), direct simulation Monte Carlo (DSMC)
and Boltzmann equations as shown in Figure 3.1. Molecular modeling of fluid flows is not the scope of this work. More details in molecular modeling can be found in Allen and Tildesley (1987) and Haile (1993).

3.3.2 The continuum hypothesis

Conceptually, the continuum hypothesis is valid and leads to accurate predictions as long as local properties of the fluid, such as density and velocity, can be defined as averages over elements. These elements are large compared to the molecular structure, but small enough compared to the macroscopic length scale, which allows the use of a mathematical differentiation to represent them. In addition, the flow condition must be near thermodynamic equilibrium. The averaged-property condition is almost always satisfied while the near-equilibrium condition mostly limits the validity of the continuum models (Gad-el-Hak, 2000).

The mechanism of transporting mass, momentum, and energy in gases and liquids are different. In dilute gases, the molecules spend most of their time in free flight with abrupt changes in their directions and speeds due to intermolecular collisions. The random molecular motion of gases plays a significant role in transport processes. On the other hand, the liquid molecules are closely packed and experience collisions with large intermolecular forces. The transport processes in liquids occur mainly due to the intermolecular forces. For gases, the near-equilibrium condition of the flow can be described by the Knudsen number $Kn$, which is defined as the ratio between the mean free path $\lambda$ and the characteristic length of the flow $L$: 
The mean free path λ is the average distance traveled by molecules between collisions, which can be determined from the well-defined molecular theory of gases, known as the kinetic theory. The mean free path indicates a length scale of fluidic and thermal transport for gases because the momentum and energy transfers occur within the gas-wall and intermolecular collisions. At standard temperature (T = 288 K) and pressure (p = 1.01x10^5 N/m^2), the mean free path of air is approximately 65 nm. For macroscopic flows, Kn is very small. The surrounding air can be considered a continuous medium. However, in microscopic flows, Kn can be fairly large due to the small length scales of channels.

The value of Kn in a particular gas flow determines the degree of rarefaction and the degree of validity of the continuum models. The continuum hypothesis is valid when Kn < 0.1 in which the mean free path of gas molecules is smaller than one tenth of a characteristic flow dimension. As Kn increases, the effects of rarefaction become more significant and the continuum assumptions finally break down. When Kn ≥ 0.1, the flow is no longer near equilibrium and both the linear relation between stress and shear (strain) rate and the conventional no-slip boundary conditions are no longer valid. The equations applicable in different ranges of Kn are illustrated in Figure 3.2 and can be summarized in the following (adapted from Gad-el-Hak, 2000):

\[ Kn = \frac{\lambda}{L} \] 

(3.5)
Continuum equations with no-slip boundary conditions

\( \text{Kn} < 10^{-3}, \quad \text{Continuum equations with no-slip boundary conditions} \)

\( 10^{-3} \leq \text{Kn} < 10^{-1}, \quad \text{Continuum equations with slip boundary conditions} \)

\( 10^{-1} \leq \text{Kn} < 10, \quad \text{Transition regime} \)

\( \text{Kn} \geq 10, \quad \text{Free-molecular flow} \)

According to Bridgeman (1923), the lattice spacing \( (\delta) \) in liquids may be used to describe the near-equilibrium condition similar to the mean free path \( (\lambda) \) of gases. The lattice spacing \( (\delta) \) is defined as follows (Probstein, 1994):

\[
\delta = \left( \frac{V_i}{N_A} \right)^{\frac{1}{3}}
\]

(3.6)

where \( V_i \) is the molar volume and \( N_A \) is Avogadro’s number.

Because liquids have higher density than gases, the spacing between molecules in liquids is less than the spacing in gases. The lattice spacing for water, for example, is about 0.3 nm. Following the Knudsen number regime as shown in Figure 3.2, continuum equations – with slip boundary conditions – may possibly be used to model the water flow in channels as small as 3 nm. Additionally, because of the long-ranged interaction forces between liquid molecules, continuum-based hydrodynamics can provide a useful description at nanoscale. For example, Stokes’ classical result for drag on a sphere is applied to particles whose diameters are well below 100 nm (Sharp et al, 2002).
3.3.3 Continuum models of fluid flows

Continuum models are usually derived from the conservation of mass, momentum, and energy, which are also called mass, momentum, and energy balances. The conservation of mass, momentum, and energy can be expressed at every point in space \((x, y, z)\) and time \((t)\) as a set of partial differential equations as follows (Dantzig and Tucker, 2001):

- Mass balance equation, which is also known as the continuity equation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (3.7a)
\]

or

\[
\frac{D \rho}{Dt} + \rho (\nabla \cdot \vec{v}) = 0 \quad (3.7b)
\]

where \(\rho\) is the density of fluid, \(t\) is time, and \(\vec{v}\) is the velocity vector \((v_x, v_y, v_z)\).

Because liquid molecules are closely packed, the density of a liquid in the channel flow remains nearly constant along the channels. Therefore, for liquid flows, the flow is sometimes referred to as the incompressible flow, in which the density is constant, allowing the continuity equation to be reduced to:

\[
\nabla \cdot \vec{v} = 0 \quad (3.8a)
\]

or

\[
\frac{\partial v_i}{\partial x_i} = 0 \quad (3.8b)
\]

where \(\vec{v}\) is the velocity vector \((v_x, v_y, v_z)\) and \(x_i\) is the coordinate for a spatial description \((x, y, z)\).
• Momentum balance equation, which is also called the equation of motion

The general form of the momentum balance equation is shown as follows:

\[
\rho \frac{D\vec{v}}{Dt} = -\nabla p + \nabla \cdot \vec{\tau} + \rho \vec{b}
\]  

(3.9)

where \( \rho \) is the density of fluid, \( \vec{v} \) is the velocity vector \((v_x, v_y, v_z)\), \( t \) is the time, \( p \) is the pressure, \( \vec{\tau} \) is the (extra) stress tensor, and \( \vec{b} \) is the body force vector.

In some situations, such as the inviscid flows of high-velocity gases, the viscosity of the fluid is very small and can be neglected over the flow domain. The equation of motion can be reduced by dropping the \( \nabla \cdot \vec{\tau} \) term, which results in the following Euler equation:

\[
\rho \frac{D\vec{v}}{Dt} = -\nabla p + \rho \vec{b}
\]  

(3.10)

• Energy balance equation

The general form of the energy balance equation is written as follows:

\[
\rho C_p \frac{DT}{Dt} + \rho L_p \frac{Dp}{Dt} = \nabla \cdot \left( \tilde{\tau} \cdot \nabla T \right) + \tilde{\tau} : \tilde{D} + \rho \dot{R}
\]  

(3.11)

where \( \rho \) is the density of fluid, \( C_p \) is the specific heat at constant pressure, \( T \) is temperature, \( t \) is time, \( L_p \) is the latent heat of pressure change, \( \tilde{k} \) is the thermal conductivity tensor, \( \tilde{\tau} \) is the extra stress tensor, \( \tilde{D} \) is the rate-of-deformation tensor, and \( \dot{R} \) is the rate of internal heat generation.
For a fluid with constant density and constant isotropic thermal conductivity, the general form of energy balance equation can be simplified by dropping the \( \rho L_p \frac{Dp}{Dt} \) term and rewriting the \( \nabla \cdot \left( \tilde{k} \cdot \nabla T \right) \) term, which results in the following simplified equation:

\[
\rho C_p \frac{dT}{Dt} = k \nabla^2 T + \tilde{\tau} : \tilde{D} + \rho \tilde{R} \tag{3.12}
\]

In addition to the balance equations, a constitutive equation that describes the response of the material to applied stress is also required to solve problems of the fluid flow. Constitutive relations can be determined from numerous approaches including experimental observations and correlations, phenomenological theories, and molecular theories. A good model must use constitutive relations that accurately describe the material behavior under the applied stress.

3.3.4 The constitutive equations of fluids

- The constitutive relation of Newtonian fluids (e.g. air, water), where the viscosity \( \mu \) is constant, is shown as follows:

\[
\tilde{\tau} = 2 \mu \tilde{D} \tag{3.13a}
\]

or

\[
\tau_{ij} = 2 \mu D_{ij} \tag{3.13b}
\]

where \( \tilde{\tau} \) is the extra stress tensor, \( \mu \) is the constant viscosity of a Newtonian fluid, and \( \tilde{D} \) is the rate-of-deformation tensor.
When the material is a Newtonian fluid with constant density, the \( \tau \) term in Equation 3.9 – the general form of the momentum balance equation – is replaced by Equation 3.13a – the Newtonian constitutive equation. The resulting equation is known as the Navier-Stokes equation as shown below:

\[
\rho \frac{D\vec{v}}{Dt} = -\nabla p + \nabla \cdot (2\mu \vec{D}) + \rho \vec{b} \tag{3.14a}
\]

Since the viscosity \( \mu \) of Newtonian fluids is constant, Equation 3.14a can be further simplified by using the continuity equation. The result yields:

\[
\rho \frac{D\vec{v}}{Dt} = -\nabla p + \mu \nabla^2 \vec{v} + \rho \vec{b} \tag{3.14b}
\]

- The constitutive equation for non-Newtonian fluids

The constitutive relation for non-Newtonian fluids, such as polymer melts and solutions, can be represented by the generalized Newtonian fluid (GNF) model, where the viscosity \( \eta \) is a function of three invariants of the rate-of-deformation tensor (Dantzig and Tucker, 2001). The equation can be written as shown below:

\[
\vec{\tau} = 2\eta \left(I_{\vec{D}}, II_{\vec{D}}, III_{\vec{D}}\right) \vec{D} \tag{3.15}
\]

For a simple shear flow of a constant density fluid – which is mostly the case for a liquid flow in a channel, the first and third invariants of the rate-of-deformation tensor \( \left(I_{\vec{D}}, III_{\vec{D}}\right) \) can be neglected. Therefore, the viscosity \( \eta \) is only a function of the second invariant of the rate-of-deformation tensor, \( \eta = \eta \left(II_{\vec{D}}\right) \). Thus,

\[
\vec{\tau} = 2\eta \left(II_{\vec{D}}\right) \vec{D} \tag{3.16}
\]
For convenience, the second invariant is replaced by the scalar shear (strain) rate \( \dot{\gamma} \), which is defined as:

\[
\dot{\gamma} = \sqrt{2 \overline{I_2}} = \sqrt{2 D_{ij} D_{ji}}
\]

(3.17)

With the first and third invariants neglected and the second invariant replaced by shear rate \( \dot{\gamma} \), the constitutive equation for the generalized Newtonian fluid (GNF) model can be written as follows:

\[
\overline{\tau} = 2 \eta(\dot{\gamma}) \overline{\dot{D}} = \eta(\dot{\gamma}) \dot{\gamma}
\]

(3.18)

The important viscosity models – commonly used for non-Newtonian fluids – include (i) the power law model, (ii) the Sisko model, (iii) the Cross model, and (iv) the Carreau model.

The power law model: \[ \eta(\dot{\gamma}) = m |\dot{\gamma}|^{n-1} \]

(3.19)

The Sisko model: \[ \eta(\dot{\gamma}) = m |\dot{\gamma}|^{n-1} + \eta_\infty \]

(3.20)

The Cross model: \[ \eta(\dot{\gamma}) = \frac{\eta_0}{1 + (\frac{\eta_0 \dot{\gamma}}{\tau})^{1-n}} \]

(3.21)

The Carreau model: \[ \frac{\eta(\dot{\gamma}) - \eta_\infty}{\eta_0 - \eta_\infty} = \left[1 + (\lambda \dot{\gamma})^2\right]^{\frac{n-1}{2}} \]

(3.22)

where \( m \) and \( n \) are material parameters, \( m \) is called the consistency index, and \( n \) is called the power law index, \( \eta_\infty \) is the infinite-shear-rate viscosity, \( \eta_0 \) is the zero-shear-rate viscosity, \( \tau \) is a time constant in the Cross model, and \( \lambda \) is a time constant in the Carreau model.
The fitted shear rate range of the following viscosity models: (i) the power law model, (ii) the Sisko model, and (iii) the Carreau model for non-Newtonian fluids (e.g. polymer melts and solutions) are illustrated in Figures 3.3a, 3.3b and 3.3c, respectively.
Figure 3.1 Molecular and continuum flow models (Gad-el-Hak, 1999).
Figure 3.2 Knudsen number regimes of fluid flows (Gad-el-Hak, 1999).
Figure 3.3 The fitted shear rate range of the following viscosity models: (a) the power law model, (b) the Sisko model, and (c) the Carreau model for non-Newtonian fluids.
CHAPTER 4

SLIP PHENOMENA AND RHEOLOGICAL MODELS

Chapter 4 discusses the effects of wall slip on the flow field of IMC coating materials, reviews the wall slip phenomena in the microflow, and derives rheological models for slit rheometers based on (i) no-slip and (ii) slip boundary conditions.

4.1 Effects of Wall Slip on the Flow Field of IMC Coating Materials

IMC coating materials are dilute colloidal dispersions (or suspensions) in which solid particles of fillers (e.g. carbon blacks and silicas) are suspended in a highly viscous liquid mixture. These solid particles provide distinctive physical properties required in the coating applications as discussed in Chapter 2. A colloidal stabilization helps maintain the homogeneous distribution of these particles throughout the coating material. In general, the colloidal particles tend to attract each other and aggregate into large particle clusters due to the influence of long-ranged van der Waals attractive forces. The colloidal stabilization is needed to prevent the particles’ aggregation by modifying the particles’ surfaces in order to compensate the attractive forces with the repulsive forces. These shorter-ranged repulsions can be carried out by either deformable macromolecules via steric stabilization or electric charge via electrostatic stabilization (Witten and Pincus,
The topic of surface forces and stabilization is out of the scope of this work but can be found in Israelachvili (1991).

The flow of the coating material in IMC processing occurs at the microscale level and exhibits the unique characteristics of microfluidics as discussed in Chapter 3. These characteristics – including high surface-to-volume ratio resulting in the domination of surface forces and high shear rate – lead to the unusual slip phenomena in the microflow. The slip phenomena also affect the flow field of microfluidics.

4.2 Causes of the Wall Slip Phenomena

The slip flow in polymer systems, such as polymer melts and solutions as well as macromolecule dispersed systems, can be classified into two modes according to Cohen (1986), Cohen and Metzner (1985): (i) true slip and (ii) apparent slip. The true slip occurs when the shear stresses are large enough to overcome the static friction between the wall and the flowing material. The true slip is usually found in polymer melts and highly cross-linked polymer systems and can occur as either a steady state phenomenon or an unsteady phenomenon – such as slip-stick or melt distortion in the extruded material. The onset of this melt distortion has been found at the shear stress in the order of $10^5$ Pa independent of the polymer type, temperature, or chain length (Tadmor and Gogos, 1979).

The second mode of the wall slip, the apparent slip, is revealed through the observation of abnormally low apparent viscosities of the fluids. This mechanism is applicable to both polymer solutions and suspensions. The apparent slip is primarily the result of depletion of the polymeric or dispersed components near the wall region, which
leads to the formation of a fluid layer of lower viscosity near the wall. The remainder of the fluid then may appear to slip through the flow channel even though the more dilute, less viscous solution near the wall does not violate the usual no-slip boundary condition.

The migration or diffusion of polymeric or dispersed components away from the wall in the apparent slip flow may be explained by one or both of the following reasons: (i) inhomogeneous stress fields in the flow field or deformation-induced migration and (ii) the presence of fluid-wall interactions or repulsive wall forces. In the former, the higher shear stress near the wall creates the distortion of the macromolecules, in which the entropy is at a lower level, compared to those located away from the wall where the shear stress is lower. Spatial entropy variations induce concentration changes as the system tends toward equilibration of the free energy gradients implied by deformation-induced entropy gradients. In the latter, these fluid-wall interactions or repulsive forces – including steric forces, hard-core or electrostatic repulsions – are more significant and most likely influential in the microflow.

For the pressure-driven flow in a circular channel, indirect measurement of the wall slip may be obtained by using a series of channels with the same length-to-radius ratio ($L/R$) but varied radius ($R$) to measure the apparent shear rate ($\dot{\gamma}_A$) at a given pressure drop as explained by Cogswell (1981). The slip velocity ($v_s$) can be determined by using the following equations as proposed by Mooney (1931):
\[ Q = \frac{\pi R^3}{4} \dot{\gamma}_{true} + \pi R^2 v_s \]  
(4.4)

\[ \frac{4Q}{\pi R^3} = \dot{\gamma}_{true} + \frac{4v_s}{R} \]  
(4.5)

where \( Q \) is the volumetric flow rate, \( \dot{\gamma}_{true} \) is the true shear rate, and \( \dot{\gamma}_A = \frac{4Q}{\pi R^3} \) is the apparent shear rate.

Following Equation 4.5, when the apparent shear rate \( \dot{\gamma}_A = \frac{4Q}{\pi R^3} \) is plotted against the inverse radius \( \frac{1}{R} \), a linear relationship between these two parameters can be found as shown in Figure 4.1. The slip velocity can be obtained from the slope and the true shear rate can be derived from the y-intercept of the fitted line. This determination depends on the assumption that the slip velocity is a unique function of the true shear rate at the die wall and must be treated with caution (Cogswell, 1981).

4.3 Mathematical Expression of Boundary Conditions

In general, the boundary conditions in the fluid flow problems may be either kinematic boundary conditions, where the velocity must be continuous at a boundary, or dynamic boundary conditions, which follow from the continuity principle of stress across a boundary (Middleman, 1977). In this study, two types of kinematic boundary conditions commonly found in simple shear flow problems are discussed. These boundary conditions are: (i) no-slip and (ii) slip boundary conditions.
The no-slip boundary condition (Figure 4.2a) assumes that there is no relative motion at the solid-fluid boundary. This means that the velocity of the fluid at the wall-fluid interface is the same as the velocity of the wall. In the pressure-driven flow, where the fluid flow is due only to the pressure difference with no motion of the wall, the no-slip condition assumes that the velocities of the fluid at the wall equal zero. This is shown as follows:

\[ v_x = 0, \quad v_y = 0 \]  \hspace{1cm} (4.1)

where \( v_x \) and \( v_y \) is the velocity of the fluid in the flow direction (\( x \)) and the perpendicular flow direction (\( y \)), respectively, as shown in Figure 4.2a.

On the other hand, the slip boundary condition (Figure 4.2b), which is related to the hydrodynamic friction assumption, is motivated by the motion of a thin film or a thin layer of fluid – of thickness infinitely small compared with its lateral dimensions – in contact with the solid wall. This slip condition is represented by the following relation (Lamb, 1932):

\[ \tau_w = \lambda v_x \]  \hspace{1cm} (4.2)

where \( \tau_w \) is the shear stress at the wall, \( \lambda \) is the friction coefficient (sometimes called slip coefficient) at the wall, and \( v_x \) is the slip velocity in the flow direction at the wall.

Therefore, we obtain
\[ v_s = \frac{\eta}{\lambda} \left. \frac{dv_x}{dx} \right|_w \]  

(4.3a)

\[ v_s = \beta \left. \frac{dv_x}{dx} \right|_w \]  

(4.3b)

where \( \eta \) is the fluid viscosity, \( \frac{dv_x}{dx} \) is the velocity gradient, and \( \beta = \frac{\eta}{\lambda} \) is the slip parameter known as slip length.

In Section 4.4, the slip velocity defined by Equation 4.3b will be used to derive the rheological models for slit rheometers.

4.4 Rheological Models for Slit Rheometers

A slit rheometer is suitable for the rheological measurement of microfluidics, particularly IMC coating materials, because it can measure the viscosity at high shear rate, it is geometrically and fundamentally similar to the relevant flow, and it is relatively easy to fabricate a micrometer-sized channel gap. In this study, a customized slit rheometer was built and used to measure rheological properties of two different types of fluids at the microscale level. Details of the experimental setup of the microslit rheometer are explained in Chapter 5.

The concept of the slit rheometer is based on the pressure-driven flow of a fluid between two stationary parallel plates. The fluid flows due only to the pressure drop across the channel (\( \Delta p = p_1 - p_2 \)) at a given volumetric flow rate (\( Q \)) in a rectangular channel with width (\( W \)), length (\( L \)), and height (\( H \)) as shown in Figure 4.3.
rheological models for the slit rheometer – including shear stress \( \tau_w \) and shear rate \( \dot{\gamma}_w \) at the wall – are derived as shown in the following:

Basic assumptions – including (i) fully developed, laminar flow and isothermal flow and (ii) incompressible, quasi-steady state flow – are made to simplify the mass and momentum balance equations. According to the basic assumptions, the momentum balance equation is simplified as follows.

**X-component:**

\[
0 = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xz}}{\partial z} \tag{4.4}
\]

\[
\frac{\partial \tau_{xz}}{\partial z} = \frac{\partial p}{\partial x}
\]

\[
\int_0^\zeta \partial \tau_{xz} = \int_0^\zeta \frac{\partial p}{\partial x} \partial z
\]

Thus,

\[
\tau_{xz} = \frac{dp}{dx} \cdot z \tag{4.5}
\]

Also, at the wall

\[
\tau_w = \frac{dp}{dx} \cdot \frac{H}{2} \tag{4.6}
\]

From Equations 4.5 and 4.6, we obtain the following relation:

\[
\frac{\tau_{xz}}{\tau_w} = \frac{z}{H/2}
\]

or

\[
z = \frac{H}{2\tau_w} \cdot \tau_{xz} \tag{4.7}
\]
Force balance equation at the wall:

\[ \tau_w \cdot (2 WL) = \Delta P \cdot (WH) \]

Thus, the shear stress at the wall is obtained as:

\[ \tau_w = \frac{H}{2L} \Delta P \] (4.8)

The volumetric flow rate \( Q \) is determined by:

\[ Q = 2W \int_0^{H/2} v_x \, dz \] (4.9)

By integrating by part, Equation 4.9 can be rewritten as

\[ \frac{Q}{2W} = [v_x \cdot z]_0^{H/2} - \int_0^{H/2} z \frac{dv_x}{dz} \, dz \] (4.10)

Next, Equation 4.10 will be solved by applying two different boundary conditions as follows:

(i) No-slip boundary condition: \( v_x \left( z = \frac{H}{2} \right) = 0 \),

Equation 4.10 becomes

\[ \frac{Q}{2W} = -\int_0^{H/2} z \frac{dv_x}{dz} \, dz \] (4.11-NS)

By substituting Equation 4.7, Equation 4.11-NS becomes

\[ \frac{Q}{2W} = -\int_0^{\tau_w} \left( \frac{H}{2\tau_w} \cdot \tau_{xz} \right) \frac{dv_x}{dz} \, dz \]
\[
\frac{2Q}{WH^2} \cdot \tau_w^2 = -\int_0^\frac{H}{2} \left( \tau_{xz} \frac{dv_x}{dz} \right) \cdot dz
\]  
(4.12-NS)

By differentiating Equation 4.12-NS with respect to \( \tau_w \), we obtain

\[
\frac{2Q}{WH^2} \cdot 2\tau_w + \frac{2\tau_w^2}{WH^2} \cdot \frac{dQ}{d\tau_w} = \tau_w \cdot \dot{\gamma}_w
\]  
(4.13-NS)

Therefore, the shear rate at the wall with the no-slip boundary condition is derived as:

\[
\dot{\gamma}_w = \frac{2}{WH^2} \left( 2Q + \tau_w \cdot \frac{dQ}{d\tau_w} \right)
\]  
(4.14-NS)

By applying the relationship in Equation 4.8, Equation 4.14-NS becomes

\[
\dot{\gamma}_w = \frac{2}{WH^2} \left( 2Q + \Delta P \frac{dQ}{d\Delta P} \right)
\]  
(4.15-NS)

(ii) Slip boundary condition: \( v_x \left( z = \frac{H}{2} \right) = v_s = \beta \frac{dv_x}{dz} \bigg|_{z=\frac{H}{2}} \)

Equation 4.10 becomes

\[
\frac{Q}{2W} = \frac{H}{2} v_s - \int_0^{\frac{H}{2}} z \frac{dv_x}{dz} \cdot dz
\]

or

\[
\frac{Q}{2W} = \frac{H}{2} \cdot \beta \frac{dv_x}{dz} \bigg|_{z=\frac{H}{2}} - \int_0^{\frac{H}{2}} z \frac{dv_x}{dz} \cdot dz
\]

(4.11-SL)
By substituting Equation 4.7, Equation 4.11-SL becomes

\[
\frac{Q}{2W} = -\frac{H}{2} \beta \dot{\gamma}_w - \int_0^{\tau_w} \left( \frac{H}{2 \tau_{xz}} \cdot \tau_{xz} \right) \frac{dv_x}{dz} \cdot d\left( \frac{H}{2 \tau_{xz}} \cdot \tau_{xz} \right)
\]

\[
\frac{2}{WH^2} (Q + WH \beta \dot{\gamma}_w) \cdot \tau_{xz}^2 = - \int_0^{\tau_w} \left( \tau_{xz} \frac{dv_x}{dz} \right) \cdot d\tau_{xz}
\]  \hspace{1cm} (4.12-SL)

By differentiating Equation 4.12-SL with respect to \( \tau_w \), we obtain

\[
\frac{2}{WH^2} (Q + WH \beta \dot{\gamma}_w) \cdot 2 \tau_w + \tau_w^2 \cdot \frac{2}{WH^2} \frac{dQ}{d\tau_w} = \tau_w \cdot \dot{\gamma}_w
\]

\[
\frac{4Q}{WH^2} + \frac{4\beta}{H} \dot{\gamma}_w + \frac{2\tau_w}{WH^2} \frac{dQ}{d\tau_w} = \dot{\gamma}_w
\]

\[
\dot{\gamma}_w \left( 1 - \frac{4\beta}{H} \right) = \frac{4Q}{WH^2} \frac{dQ}{d\tau_w} \hspace{1cm} (4.13-SL)
\]

Therefore, the shear rate at the wall with the slip boundary condition is derived as:

\[
\dot{\gamma}_w = \frac{2}{WH^2 \left( 1 - \frac{4\beta}{H} \right)} \left( 2Q + \tau_w \frac{dQ}{d\tau_w} \right) \hspace{1cm} (4.14-SL)
\]

By applying the relationship in Equation 4.8, Equation 4.14-SL becomes

\[
\dot{\gamma}_w = \frac{2}{WH^2 \left( 1 - \frac{4\beta}{H} \right)} \left( 2Q + \Delta P \frac{dQ}{d\Delta P} \right) \hspace{1cm} (4.15-SL)
\]
The rheological models for slit rheometers – including the shear stress ($\tau_w$), shear rate ($\dot{\gamma}_w$) at the wall, and shear viscosity ($\eta$) – are summarized in the following:

**No-Slip Boundary**

\[
\tau_w = \frac{H}{2L} \Delta P
\]

\[
\dot{\gamma}_w = \frac{2}{WH^2} \left(2Q + \Delta P \frac{dQ}{d\Delta P}\right)
\]

\[
\eta = \frac{\tau_w}{\dot{\gamma}_w}
\]

**Slip Boundary Condition**

\[
\tau_w = \frac{H}{2L} \Delta P
\]

\[
\dot{\gamma}_w = \frac{2}{WH^2} \left(2Q + \Delta P \frac{dQ}{d\Delta P}\right) \left(1 - \frac{4\beta}{H}\right)
\]

\[
\eta = \frac{\tau_w}{\dot{\gamma}_w}
\]
Figure 4.1 A linear relation between apparent shear rate \( \dot{\gamma}_A = \frac{4Q}{\pi R^3} \) and the inverse radius \((1/R)\), where the slope of the fitted line is \(4 \times v_s\) (Cogswell, 1981).
Figure 4.2 Schematic representation of boundary conditions at the fluid-wall interface: (a) no-slip boundary conditions and (b) slip boundary conditions.
Figure 4.3 A fluid flow due to the pressure drop ($\Delta p = p_1 - p_2$) in a rectangular channel with width ($W$), length ($L$), and height ($H$).
CHAPTER 5

DEVELOPMENT OF MICROSLIT RHEOMETERS AND ANALYSIS OF THE SLIP FLOW

Chapter 5 describes an experimental setup of a customized microslit rheometer developed in this work to study the slip phenomena in the microflow, presents the experimental results of the viscosity measurement, and analyzes the viscosity data to determine the slip parameter, known as slip length, for IMC materials.

5.1 Introduction to the Microslit Rheometer

In this study, the term “microslit rheometer” is used to represent a slit rheometer with a micrometer-sized channel gap to distinguish the flow in microscopic channels and macroscopic channels. The concept of the slit rheometer is based on a pressure-driven flow of a fluid between two stationary parallel plates. Pressure flow rheometers, such as slit and capillary rheometers, offer several advantages in rheological measurements over drag flow (or rotational) rheometers, such as parallel-disc and cone-and-plate rheometers. First, the absence of free surface area in pressure flow rheometers prevents edge failure, which usually limits the maximum shear rate obtainable in drag flow rheometers. Commercial drag flow rheometers typically can only achieve shear rates as high as $10^3 \text{ s}^{-1}$
while pressure flow rheometers can obtain shear rates up to $10^6$ s$^{-1}$ or higher. Second, only a fresh material flows through the channel at a given shear rate in pressure flow rheometers. No shear stress history is accumulated in the fluid. Third, the flow in pressure flow rheometers is fundamentally and geometrically similar to many practical materials processing such as IMC and injection molding. Therefore, the results are directly applicable. In contrast, the main disadvantage of pressure flow rheometers is the inhomogeneous shear stress field. This requires measurement to be conducted in steady state. The existence of the inhomogeneous shear stress affects the distribution of particles or large molecules in the fluid, which tends to migrate away from the higher-stress region near the wall. The formation of a thin layer free of particles or large molecules results in the lower viscosity near the wall and induces the slip flow.

5.2 Experimental Setup of the Microslit Rheometer

An experimental setup of the developed microslit rheometer as shown in Figure 5.1 consists of four main components including: (i) a microslit die, (ii) a high precision syringe pump with an on-pump pressure transducer, (iii) a data acquisition system, and (iv) heating tape for high temperature measurement. The microslit die with a micrometer-sized channel gap was built and connected to the syringe pump via stainless steel tubing (ID = 0.25 in or 6.35 mm). The high precision syringe pump (model 1000D from Teledyne ISCO, Lincoln, Nebraska) was used to drive the fluid through the channel of the microslit die at a given volumetric flow rate. This pump has a flow rate capacity from 0.1 to 408 mL/min and a pressure range from 0 to 13.8 MPa (0 to 2,000 psi). The fluid flowed from the pump into the tubing, then into the channel of the microslit die, and
exited at the end of the die, where the fluid was collected in a container underneath the die as shown in Figure 5.1. The total pressure drop ($\Delta p_{tot}$) in the tubing and the channel was measured by the on-pump pressure transducer and monitored by a data acquisition system (LabView version 7.1 from National Instruments, Austin, Texas) to find out the pressure at steady state. The details on how to calculate the pressure drop across the channel ($\Delta p$) are discussed in Section 5.2.2. For higher temperature testing, heating tape with an adjustable power controller was used and wrapped around the tubing and the die to increase the operating temperatures. The setting temperatures were controlled at the inlet, where the material flows into the die, by a surface thermometer.

5.2.1 Design of the microslit die and channel

The microslit die was built by machining a shim stock of stainless steel following the channel design and clamping it between two die halves (1 in thick each) as illustrated in Figure 5.2. The thickness of the channel gap is then defined by the thickness of the shim stock. A shim stock-based microchannel offers numerous advantages including: (i) low cost in materials and manufacturing, (ii) simple fabrication with short production time, and (iii) uniform channel thickness. However, the channel gap is limited by the thickness of a shim stock because the thinnest shim stock commercially available is 0.5 mil (12.7 $\mu$m) thick.

In this experiment, two differently sized shim stocks were used – 4 mil (101.6 $\mu$m) and 1 mil (25.4 $\mu$m) thick – to study the slip phenomena in the microchannel. The channel was designed with an entrance region to promote a fully developed, laminar flow as shown in Figure 5.3. The minimum length of the entire channel was limited by the size of
the fitting at the inlet. The width \((W)\) and length \((L)\) of the channel were designed to be much greater than the height \((H)\) so that the analysis of the fluid flow can be simplified to a one-dimensional (1-D) flow. The channel design was drawn by Solid Edge (from Integrated Technology Solutions, Elmhurst, Illinois) and fabricated by wired-electrical discharge machining (Wired-EDM). The process of designing and manufacturing was facilitated by computer-aided design (CAD) and computer-aided manufacturing (CAM) systems, which significantly reduce the time in redesign and production. In addition, the die halves were made of 1-inch-thick hardened steel in order to minimize the deformation of the channel gap due to the injection pressure. Analysis of the microslit die deflection is described in detail in Appendix A.

5.2.2 Measurement of the pressure drop across the channel

The pressure drop across the channel \((\Delta p)\), which is used in the viscosity calculation, needs to be determined to obtain the accurate viscosity of the fluid. A significant pressure drop in the end region \((\Delta p_{\text{end}})\), including tubing and entrance region, cannot be neglected. Therefore, the total pressure drop \((\Delta p_{\text{tot}})\), which is collected from the on-pump pressure transducer, needs to be corrected accordingly to determine \(\Delta p\). \(\Delta p_{\text{end}}\) is typically obtained from the Bagley plot (Macosko, 1994). For a slit rheometer, the Bagley plot is drawn between \(\Delta p_{\text{tot}}\) and the varying \(L/H\) ratios, where \(H\) and \(Q\) are kept constant, as illustrated in Figure 5.4. \(\Delta p_{\text{end}}\) is then obtained by extrapolated the fitted line to \(y\)-axis of \(\Delta p_{\text{tot}}\) \((y\)-intercept\). The \(\Delta p_{\text{end}}\) is then subtracted from \(\Delta p_{\text{tot}}\) to determine \(\Delta p\) as shown in the following relation:

\[
\Delta p_{\text{tot}} - \Delta p_{\text{end}} = \Delta p
\]  

(5.1)
The end pressure correction using the Bagley plot was first attempted in this experiment. However, due to the large $L/H$ ratios ($L/H = 150$ and 500), when the fitted line was extrapolated to determine $\Delta p_{\text{end}}$, the possible error was high as shown schematically in Figure 5.4. In this experiment, $\Delta p_{\text{end}}$ was obtained by directly measuring the pressure drop in the channel of the microslit die with only the entrance region of the channel. $\Delta p_{\text{end}}$ is then subtracted from $\Delta p_{\text{tot}}$ to obtain $\Delta p$ as illustrated in Figure 5.5. The results of the calculated viscosity from the microslit rheometer showed a good agreement with the viscosity data at high shear rates measured from the commercial parallel-disc rheometer as described in Section 5.3.

5.3 Results and Discussions of the Viscosity Measurement

The experiments were conducted to measure the shear viscosity of two different types of fluids: (i) a simple Newtonian fluid: antifreeze (Winter-EEZ from South Win, Greensboro, NC) and (ii) a non-Newtonian fluid: Stylecoat – an IMC coating material for thermoplastic parts (from OMNOVA Solutions, Akron, Ohio). To verify the data, the viscosity of both fluids obtained from the microslit rheometer was compared with the data measured from the commercial 1-mm-gap parallel-disc Physica MCR 300 rheometer (from Anton Paar, Ashland, Virginia) at high shear rates.

5.3.1 Viscosity measurement of antifreeze

The viscosity measurement of antifreeze was conducted at room temperature ($25^\circ\text{C}$) and plotted against the shear rate as shown in Figure 5.6. By using the developed microslit rheometer, the viscosity data of the antifreeze – a simple Newtonian fluid – was
obtained at a high shear rate up to $10^6$ s$^{-1}$. There is no indication of shear thinning or a reduced viscosity due to wall slip in both 4-mil (101.6 $\mu$m) and 1-mil (25.4 $\mu$m) channel gaps. The viscosity of the material is constant at low and high shear rates. This implies that, for antifreeze, wall slip does not occur in the channel gaps at either the macroscopic scale (40 mil or 1 mm thick) or the microscopic scale (4 mil or 101.6 $\mu$m, and 1 mil or 25.4 $\mu$m thick).

5.3.2 Viscosity measurement of Stylecoat

Stylecoat (MB99-P3X) was measured in various conditions. Variables used in this experiment include: (i) channel gaps: 40 mil (1 mm), 4 mil (101.6 $\mu$m), and 1 mil (25.4 $\mu$m), (ii) operating temperatures: 25°C and 50°C, and (iii) percentage of carbon black: 0%, 2.8% and 4%. The values of these variables are summarized in Table 5.1.

The viscosity of Stylecoat was first measured using the commercial parallel-disc rheometer at different temperatures: 25°C, 45°C, 65°C, 85°C, and 100°C and displayed in Figure 5.7. The viscosity data was then fitted by the power law and Carreau viscosity models to determine the parameters of these two models at different temperatures. The values of these parameters are summarized in Table 5.2. The microslit rheometer with 4-mil (101.6-$\mu$m) and 1-mil (25.4-$\mu$m) gaps was then used to measure the viscosity of Stylecoat. The viscosity data at 25°C and 50°C from the microslit rheometer are displayed in Figures 5.8 and 5.9, respectively. In addition, the viscosity of Stylecoat with varied percentages of carbon black (0%, 2.8% and 4%) was also tested at room temperature (25°C) and is displayed in Figure 5.10. The experimental results show the
reduced viscosity of Stylecoat in the 1-mil (25.4-μm) channel gap, which indicates wall slip of Stylecoat at this length scale of the channel gap.

5.4 Analysis of the Slip Flow

According to the viscosity data, the reduced viscosity of Stylecoat found in the 1-mil (25.4-μm) channel gap indicates wall slip in the IMC flow. The rheological models derived in Chapter 4 were used to analyze the viscosity data and determine the values of the slip parameter, known as slip length (β), as discussed in Chapter 4. The relative viscosity – the ratio of the reduced viscosity due to wall slip (η_{SL}) to the no-slip viscosity (η_{NS}) – was then used to determine the slip length. The average values of the slip length in the 1-mil (25.4-μm) channel gap at temperatures of 25°C and 50°C are summarized as follows:

<table>
<thead>
<tr>
<th>Channel Gap</th>
<th>Slip Length, Beta</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mil (25.4 μm)</td>
<td></td>
</tr>
<tr>
<td>Temp 25°C</td>
<td>3.0 μm</td>
</tr>
<tr>
<td>Temp 50°C</td>
<td>2.4 μm</td>
</tr>
</tbody>
</table>

The values of the slip length at different temperatures can be predicted by the following equation in the exponential form:

\[
\beta = 3.0 \exp[-8.926 \times 10^3 (T - 298)]
\]  \hspace{1cm} (5.2)

where β is the slip length in μm, and T is temperature in Kelvin.
The wall slip in the microflow affects the flow field and leads to the apparent reduced viscosity of Stylecoat in the 1-mil (25.4-μm) channel gap. The value of the slip length obtained from the experiment is used to correct for wall slip to obtain the true viscosity of Stylecoat, which is independent of the channel size. The true viscosity of Stylecoat at 25°C and 50°C after the slip correction is shown in Figures 5.11 and 5.12, respectively. The value of the slip length is also needed in the numerical solution to accurately predict the pressure flow of the coating material in microchannels.
Figure 5.1 An experimental setup of the microslit rheometer.
Figure 5.2 A shim stock assembly of the microslit die.
Figure 5.3 A channel design ($L = 0.15$ in, $W = 0.1$ in) of the microslit die for testing Stylecoat.
Pressure reading from the syringe

$L/H$ ratio

$Q$ and $H$ are constant.

Figure 5.4 The Bagley plot used to determine the pressure drop in the end region ($\Delta p_{\text{end}}$).
Figure 5.5 The end pressure correction for the microslit rheometer.
Figure 5.6 The viscosity measurement of antifreeze at 25°C using the commercial parallel-disc rheometer and the microslit rheometer with the channels of 4-mil (101.6-μm) and 1-mil (25.4-μm) gaps.
Channel Gaps
1 mil (25.4 μm), 4 mil (101.6 μm)
2 mil (50.8 μm), 5 mil (127 μm)
(a combination of 1 mil and 4 mil)

Operating Temperatures
25°C and 50°C

Carbon Black
0%, 2.8%, and 4%

Table 5.1 The values of the parameters used in the experiment of the microslit rheometer.
Figure 5.7 The viscosity of Stylecoat measured using the commercial parallel-disc rheometer and predicted by the Carreau viscosity model at different temperatures: 25°C, 50°C, and 100°C.
Table 5.2 Summary of the fitted parameters of the Carreau viscosity model for Stylecoat at the temperatures of 25°C, 45°C, 65°C, 85°C, and 100°C.

<table>
<thead>
<tr>
<th>Temp (deg C)</th>
<th>Eta zero (Pa.s)</th>
<th>Eta infinity (Pa.s)</th>
<th>(1-n)</th>
<th>n</th>
<th>Lamda (second)</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>4.27</td>
<td>0.989</td>
<td>0.2805</td>
<td>0.7195</td>
<td>9.42</td>
<td>2</td>
</tr>
<tr>
<td>45</td>
<td>3.96</td>
<td>0.327</td>
<td>0.4803</td>
<td>0.5197</td>
<td>9.42</td>
<td>2</td>
</tr>
<tr>
<td>65</td>
<td>3.77</td>
<td>0.133</td>
<td>0.6432</td>
<td>0.3568</td>
<td>9.42</td>
<td>2</td>
</tr>
<tr>
<td>85</td>
<td>3.54</td>
<td>0.0647</td>
<td>0.7141</td>
<td>0.2859</td>
<td>9.42</td>
<td>2</td>
</tr>
<tr>
<td>100</td>
<td>2.85</td>
<td>0.0408</td>
<td>0.7438</td>
<td>0.2562</td>
<td>9.42</td>
<td>2</td>
</tr>
</tbody>
</table>
Figure 5.8 The viscosity measurement of Stylecoat at 25°C using the commercial parallel-disc rheometer and the microslit rheometer with 4-mil (101.6-\(\mu\)m) and 1-mil (25.4-\(\mu\)m) channel gaps.
Figure 5.9 The viscosity measurement of Stylecoat at 50°C using the commercial parallel-disc rheometer and the microslit rheometer with 4-mil (101.6-μm) and 1-mil (25.4-μm) channel gaps.
Figure 5.10 The viscosity measurement of Stylecoat with varied percentages of carbon black (0%, 2.8%, and 4%) at 25°C.
Figure 5.11 The true viscosity of Stylecoat after the slip correction at 25°C.
Test Fluid: Stylecoat (MB99-P3X) 2.8% CB
Temperature 50°C

Figure 5.12 The true viscosity of Stylecoat after the slip correction at 50°C.
In Chapter 6, the IMC flow with slip boundary conditions is modeled to predict the pressure drop ($\Delta p$) in the flow at steady state. The slip boundary conditions used in the flow model are described by two different mechanisms: (i) true slip, where the fluid velocity at the wall defined by the slip velocity ($v_s$) and (ii) apparent slip, where the lower-viscosity layer is present near the wall region. In addition, the Carreau viscosity model is used to represent the viscosity data at high shear rates. The predicted pressure from the flow models with various viscosity models (including the power law and Carreau viscosity models) and boundary conditions (including no-slip, true slip, and apparent slip boundary conditions) are then compared with the experimental results.

6.1 Governing Equations of the Continuum Flow Models

Basic assumptions – including (i) fully developed, laminar, isothermal flow and (ii) incompressible, quasi-steady state flow – are made to simplify the mass and momentum balance equations.
According to the assumptions, the momentum balance equation is simplified to:

\[
\frac{\partial \tau_{xz}}{\partial z} = \frac{\partial p}{\partial x}
\]  

(6.1)

Applying the symmetry condition \(\frac{dv_x}{dz} = 0\) at \(z = 0\) and integrating Equation 6.1,

\[
\int_{0}^{z} \tau_{xz} \, dz' = \int_{0}^{z} \frac{dp}{dx} \, dz'
\]

\[
\tau_{xz} = \left( \frac{dp}{dx} \right) \cdot z
\]

(6.2)

Therefore,

\[
\eta(z) \frac{dv_x}{dz} = \left( \frac{dp}{dx} \right) \cdot z
\]

or

\[
\frac{dv_x}{dz} = \left( -\frac{\Delta p}{L} \right) \cdot \frac{z}{\eta(z)}
\]

(6.3)

Next, we apply the following boundary conditions: (i) no-slip, (ii) true slip, and (iii) apparent slip as shown schematically in Figure 6.1a, 6.1b, and 6.1c, respectively, and integrate Equation 6.3 to obtain the governing equations:

6.1.1 The no-slip boundary conditions (Figure 6.1a)

The no-slip boundary condition at the wall \((z = h = H/2)\) is described as:

\[
v_x(z = h) = 0
\]

(6.4)
By applying the no-slip boundary condition (Equation 6.4) and integrating Equation 6.3, Equation 6.3 becomes

\[ \int_{v_x}^{0} d\nu_x = \left( -\frac{\Delta p}{L} \right) \int_{0}^{h} \frac{z'}{\eta(z')} d\nu_x \]

\[ v_x = \left( \frac{\Delta p}{L} \right) \int_{0}^{h} \frac{z'}{\eta(z')} d\nu_x \quad (6.5) \]

The volumetric flow rate \( Q \) is determined by

\[ Q = 2W \int_{0}^{h} v_x \, dx \quad (6.6) \]

By applying Equation 6.5, Equation 6.6 becomes

\[ \frac{Q}{2W} = \left( \frac{\Delta p}{L} \right) \int_{0}^{h} \frac{z'}{\eta(z')} d\nu_x \, dz \]

\[ \frac{Q}{2W} = \left( \frac{\Delta p}{L} \right) \int_{0}^{h} \left( \int_{0}^{\nu_x} \frac{z'}{\eta(z')} \, dz' \right) d\nu_x \, dz' \]

\[ \frac{Q}{2W} = \left( \frac{\Delta p}{L} \right) \int_{0}^{h} \frac{z^2}{\eta(z)} \, dz \quad (6.7) \]

Therefore,

\[ \Delta p = \frac{Q}{2W} \cdot L \int_{0}^{h} \frac{z^2}{\eta(z)} \, dz \quad (6.8) \]
6.1.2 The true slip boundary conditions (Figure 6.1b)

The true slip boundary condition at the wall \((z = h = H/2)\) is defined as:

\[
v_s = v_s(z = h) = \beta \frac{dv_s}{dx}\bigg|_w
\]

(6.9)

where \(v_s\) is the slip velocity, \(\beta\) is the slip length, and \(\frac{dv_s}{dx}\bigg|_w\) is the velocity gradient at the wall.

By applying the true slip boundary condition (Equation 6.9) and integrating Equation 6.3, Equation 6.3 becomes

\[
\int_{v_s}^v dv = \left(-\frac{\Delta p}{L}\right) \int_{z}^{h} \frac{z'}{\eta(z')} dz'
\]

(6.10)

The volumetric flow rate \((Q)\) is determined by:

\[
Q = 2W \int_{0}^{h} v_s dx
\]

(6.11)

By applying Equation 6.10, Equation 6.11 becomes

\[
\frac{Q}{2W} = v_s h + \left(\frac{\Delta p}{L}\right) \int_{0}^{h} \left(\int_{0}^{z} \frac{z'}{\eta(z')} dz\right) dz'
\]

\[
\frac{Q}{2W} = v_s h + \left(\frac{\Delta p}{L}\right) \int_{0}^{h} \left(\int_{0}^{z} \frac{z'}{\eta(z')} dz\right) dz'
\]
\[
\frac{Q}{2W} = v_s h + \left( \frac{\Delta p}{L} \right) \int_0^h \frac{z^2}{\eta(z)} \, dz
\]

(6.12)

Therefore,

\[
\Delta p = \frac{\left( \frac{Q}{2W} - v_s h \right) \cdot L}{\int_0^h \frac{z^2}{\eta(z)} \, dz}
\]

(6.13)

6.1.3 The apparent wall slip (Figure 6.1c)

The apparent slip is caused by the presence of a layer (δ) of a lower Newtonian viscosity (μ) near the wall (region 2) where the non-Newtonian viscosity (η) exists in the core (region 1) as shown in Figure 6.1c. The boundary conditions of the apparent slip are defined as follows:

Region 1: at \( z = 0 \),

\[
\frac{d v_{x1}}{d z} = 0
\]

(6.14a)

Region 2: at \( z = h \),

\[ v_{x2} = 0 \]

(6.14b)

At the interface between region 1 and region 2, we have continuity of velocity and stress:

At \( z = h-\delta \),

\[ v_{x1} = v_{x2} = v_{AS} \]

(6.14c)

At \( z = h-\delta \),

\[ \tau_{x1} = \tau_{x2} \]

(6.14d)
Region 1: non-Newtonian fluid,

By applying the boundary condition (Equation 6.14c) and integrating Equation 6.3, Equation 6.3 becomes

\[
\int_{v_{x1}}^{v_{x1}'} dv_x = \left( -\frac{\Delta p}{L} \right) \int \frac{z'}{\eta(z')} dz' \\
v_{x1} = v_{x1}' + \left( -\frac{\Delta p}{L} \right) \int \frac{z'}{\eta(z')} dz' 
\]

(6.15)

Region 2: Newtonian fluid,

The Navier-Stokes equation for Newtonian fluids is simplified to:

\[
\frac{\mu}{\eta} \frac{\partial^2 v_{x2}}{\partial z^2} = \frac{\partial p}{\partial x}
\]

(6.16)

\[
\frac{d^2 v_{x2}}{dz^2} = \frac{1}{\mu} \left( \frac{dp}{dx} \right) \]

\[
\frac{dv_{x2}}{dz} = \frac{1}{\mu} \left( \frac{dp}{dx} \right) z + C_1
\]

\[
v_{x2} = \frac{1}{2\mu} \left( \frac{dp}{dx} \right) z^2 + C_1 z + C_2
\]

(6.17)

At the interface between region 1 and region 2 \( (z = h-\delta) \), by applying the boundary condition Equation 6.14d, \( \tau_{x1} = \tau_{x2} \), we obtain

\[
\eta \frac{dv_{x1}}{dz} = \mu \frac{dv_{x2}}{dz}
\]

(6.18)

\[
\frac{dp}{dx} (h-\delta) = \frac{dp}{dx} (h-\delta) + \mu C_1
\]
It is found that \( C_1 = 0 \)

Thus, Equation 6.17 becomes

\[
v_{x_2} = \frac{1}{2\mu} \left( \frac{dp}{dx} \right) z^2 + C_2
\]

By applying the boundary condition (Equation 6.14b), at \( z = h \), \( v_{x_2} = 0 \), to Equation 6.19, it is found that

\[
C_2 = -\frac{1}{2\mu} \left( \frac{dp}{dx} \right) h^2
\]

Therefore, Equation 6.19 becomes

\[
v_{x_2} = \frac{1}{2\mu} \left( \frac{dp}{dx} \right) \left[ z^2 - h^2 \right]
\]

or

\[
v_{x_2} = \frac{1}{2\mu} \left( \frac{\Delta p}{L} \right) \left[ h^2 - z^2 \right]
\]

The apparent slip velocity \((v_{AS})\) at the interface is obtained by applying the boundary condition, Equation 6.14c, \( v_{x_1} = v_{x_2} = v_{AS} \) at \( z = h-\delta \), into Equation 6.20. Thus,

\[
v_{AS} = v_{x_2} (z = h-\delta) = \frac{1}{2\mu} \left( \frac{\Delta p}{L} \right) \left[ h^2 - (h-\delta)^2 \right]
\]

\[
v_{AS} = \frac{1}{2\mu} \left( \frac{\Delta p}{L} \right) \left[ 2h\delta - \delta^2 \right]
\]
The volumetric flow rate \( Q \) is determined by

\[
Q = 2W \int_{0}^{h} v_x \, dx
\]

\[
\frac{Q}{2W} = \int_{0}^{h-\delta} v_x \, dz + \int_{h-\delta}^{h} v_x \, dz
\]

\[
\frac{Q}{2W} = \int_{0}^{h-\delta} \left[ v_{AS} + \left( \frac{\Delta P}{L} \right) \int_{z}^{z'} \frac{z'}{\eta(z')} \, dz' \right] \, dz + \int_{h-\delta}^{h} \left[ \frac{1}{2\mu} \left( \frac{\Delta P}{L} \right) \left( h^2 - z^2 \right) \right] \, dz
\]

\[
\frac{Q}{2W} = v_{AS} (h - \delta) + \left( \frac{\Delta P}{L} \right) \left[ \int_{0}^{h-\delta} \frac{z^2}{\eta(z)} \, dz - \frac{\delta^2 (\delta - 3h)}{6\mu} \right]
\]

Therefore,

\[
\Delta P = \left[ \frac{Q}{2W} - v_{AS} (h - \delta) \right] \cdot L
\]

\[
= \left[ \int_{0}^{h-\delta} \frac{z^2}{\eta(z)} \, dz - \frac{\delta^2 (\delta - 3h)}{6\mu} \right]
\]

The following summarizes the governing equations used in this work.

(i) No-slip boundary condition (Figure 6.1a):

Boundary condition: \( v_x (z = h) = 0 \)

Shear rate equation: \( \frac{dv_x}{dz} = \left( -\frac{\Delta P}{L} \right) \cdot \frac{z}{\eta(z)} \)

Pressure governing equation: \( \Delta P = \frac{Q}{2W} \cdot \frac{L}{\int_{0}^{h} \frac{z^2}{\eta(z)} \, dz} \)
(ii) True slip boundary condition (Figure 6.1b)

Boundary condition: \( v_s = v_s(z = h) = \beta \frac{dv_s}{dx} \bigg|_w \)

Shear rate equation: \( \frac{dv_s}{dz} = \left( -\frac{\Delta p}{L} \right) \cdot \frac{z}{\eta(z)} \)

Pressure governing equation: \( \Delta p = \frac{\left( \frac{Q}{2W} - v_s h \right) \cdot L}{\int_0^h \frac{z^2}{\eta(z)} dz} \)

(iii) Apparent slip boundary condition (Figure 6.1c)

Boundary condition: \( v_{AS} = v_{s2}(z = h - \delta) \)

\[ = \frac{1}{2\mu} \left( \frac{\Delta p}{L} \right) [h^2 - (h - \delta)^2] \]

Shear rate equation: \( \frac{dv_s}{dz} = \left( -\frac{\Delta p}{L} \right) \cdot \frac{z}{\eta(z)} \)

Pressure governing equation: \( \Delta p = \frac{\left[ \frac{Q}{2W} - v_{AS}(h - \delta) \right] \cdot L}{\int_0^{h-\delta} \frac{z^2}{\eta(z)} dz - \frac{\delta^2 (\delta - 3h)}{6\mu}} \)

6.1.4 The viscosity models

The viscosity models \( \eta(\dot{\gamma}) \), where \( \dot{\gamma} = \dot{\gamma}(z) \), used in this work are: (i) the power law model and (ii) the Carreau model.
(i) The power law viscosity model:

\[ \eta(\dot{\gamma}) = m|\dot{\gamma}|^{n-1} \quad (6.25) \]

where \( m \) and \( n \) are material parameters, \( m \) is the consistency index, and \( n \) is the power law index, and \( \dot{\gamma} \) is the shear rate.

(ii) The Carreau viscosity model:

\[ \frac{\eta(\dot{\gamma}) - \eta_\infty}{\eta_0 - \eta_\infty} = \left[ 1 + (\lambda \dot{\gamma})^2 \right]^{(\frac{n-1}{2})} \quad (6.26a) \]

or

\[ \eta(\gamma) = \eta_\infty + (\eta_0 - \eta_\infty) \left[ 1 + (\lambda \dot{\gamma})^2 \right]^{\frac{n-1}{2}} \quad (6.26b) \]

where \( \eta_0 \) is the zero-shear-rate viscosity, \( \eta_\infty \) is the infinite-shear-rate viscosity, \( \lambda \) is a time constant, and \( n \) is the power law index.

6.2 Numerical Solutions of the Governing Equations

The governing equations derived in Section 6.1 are solved numerically to determine the pressure drop of the IMC flow. The mathematical formula, known as Weddle’s rule, is used to approximate the integral function of the viscosity models (\( \eta \)). A computer code was implemented to iteratively solve these governing equations. The numerical results are then compared with the experimental results as discussed in Section 6.3.
Weddle’s Rule

Let the values of a function \( f(x) \) be tabulated at points \( x_i \) equally spaced by \( h \) (where \( h = x_{i+1} - x_i \)), so that \( f_1 = f(x_1) \), \( f_2 = f(x_2) \), \( f_3 = f(x_3) \), \( f_4 = f(x_4) \), \( f_5 = f(x_5) \), \( f_6 = f(x_6) \), and \( f_7 = f(x_7) \). Then, Weddle’s rule approximating the integral of \( f(x) \) is given by the following formula:

\[
\int_{x_i}^{x_i} f(x) \, dx = \frac{3}{10} h \left( f_1 + 5f_2 + f_3 + 6f_4 + f_5 + 5f_6 + f_7 \right)
\] (6.27)

6.3 Comparison and Discussions of Experimental and Numerical Results

The numerical solutions of the pressure drop are compared with the results from the experiments in Chapter 5 at various channel gaps: 5 mil (127 \( \mu \)m), 4 mil (101.6 \( \mu \)m), 2 mil (50.8 \( \mu \)m), and 1 mil (25.4 \( \mu \)m). The effects of the viscosity models and the true slip boundary conditions on the pressure prediction are first determined. The numerical results, using (i) the power law and Carreau viscosity models, and (ii) the no-slip and true slip (with \( \beta = 3 \mu m \)) boundary conditions, are compared with the experimental results as shown in Figures 6.2, 6.3, 6.4, and 6.5 for the channel gaps of 5 mil (127 \( \mu \)m), 4 mil (101.6 \( \mu \)m), 2 mil (50.8 \( \mu \)m), and 1 mil (25.4 \( \mu \)m), respectively. It is found that, the Carreau viscosity model gave a better prediction of the pressure than the power law viscosity model in all sizes of the channel gap. Moreover, the slip boundary conditions become very significant in the 1-mil (25.4-\( \mu \)m) channel gap while the no-slip boundary conditions failed to predict the pressure in this length scale as shown in Figure 6.5. Therefore, in order to accurately predict the pressure, the Carreau viscosity model needs
to be used in the model while the slip boundary condition is important in the very small channel gap.

Next, the effects of the true slip (with $\beta = 3 \, \mu m$) and apparent slip boundary conditions are determined. In the apparent slip boundary conditions discussed in Chapter 4, the thin layer ($\delta$) of the lower Newtonian viscosity ($\mu$) near the wall is caused by the migration of the particles away from the wall. Therefore, it is reasonable to estimate the viscosity ($\mu$) by using the viscosity of Stylecoat with 0% carbon black. This viscosity was experimentally tested by the microslit rheometer and varied from 0.6 to 0.8 Pa.s. The particle-free layer ($\delta$) was estimated from the simulation results by Chopra and Larson (2002). This value was found to be approximately 25% of the channel gap, which is around 6 $\mu m$, in the 1-mil (25.4-$\mu m$) channel gap.

The numerical results based on the Carreau viscosity model and the apparent slip boundary conditions (with $\delta = 6 \, \mu m$ and $\mu = 0.6, 0.7$, and 0.8 Pa.s) were modeled and compared with the true slip (with $\beta = 3 \, \mu m$) and no-slip boundary conditions as displayed in Figures. 6.6, 6.7, 6.8, and 6.9 for the channels of 5-mil (127-$\mu m$), 4-mil (101.6-$\mu m$), 2-mil (50.8-$\mu m$), and 1-mil (25.4-$\mu m$) gaps, respectively. It is found that, in the 1-mil (25.4-$\mu m$) channel gap, the slip boundary conditions using (i) the true slip with $\beta = 3 \, \mu m$ and (ii) the apparent slip with $\delta = 6 \, \mu m$ and $\mu = 0.6$ Pa.s showed good agreement with the experimental results.
Figure 6.1 Schematic diagrams of (a) no-slip boundary conditions, (b) true slip boundary conditions, and (c) apparent slip boundary conditions.
Figure 6.2 Comparison of the pressure drop in the 5-mil (127-μm) channel gap between experimental and numerical results of Stylecoat.
Figure 6.3 Comparison of the pressure drop in the 4-mil (101.6-μm) channel gap between experimental and numerical results of Stylecoat.
Figure 6.4 Comparison of the pressure drop in the 2-mil (50.8-μm) channel gap between experimental and numerical results of Stylecoat.
Figure 6.5 Comparison of the pressure drop in the 1-mil (25.4-μm) channel gap between experimental and numerical results of Stylecoat.
Figure 6.6 Comparison of the pressure drop in the 5-mil (127-μm) channel gap between experimental and numerical results of Stylecoat using the Carreau viscosity model and various boundary conditions: no-slip, true slip (with \( \beta = 3 \mu m \)), and apparent slip (with \( \delta = 6 \mu m \) and \( \mu = 0.6, 0.7, \) and 0.8 Pa.s).
Figure 6.7 A comparison of the pressure drop in the 4-mil (101.6-μm) channel gap between experimental and numerical results of Stylecoat using the Carreau viscosity model and various boundary conditions: no-slip, true slip (with $\beta = 3$ μm), and apparent slip (with $\delta = 6$ μm and $\mu = 0.6, 0.7, \text{and} 0.8$ Pa.s).
Figure 6.8 A comparison of the pressure drop in the 2-mil (50.8-μm) channel gap between experimental and numerical results of Stylecoat using the Carreau viscosity model and various boundary conditions: no-slip, true slip (with $\beta = 3 \mu m$), and apparent slip (with $\delta = 6 \mu m$ and $\mu = 0.6$, 0.7, and 0.8 Pa.s).
Figure 6.9 A comparison of the pressure drop in the 1-mil (25.4-μm) channel gap between experimental and numerical results of Stylecoat using the Carreau viscosity model and various boundary conditions: no-slip, true slip (with $\beta = 3 \, \mu m$), and apparent slip (with $\delta = 6 \, \mu m$ and $\mu = 0.6, 0.7,$ and $0.8$ Pa.s).
CHAPTER 7

MATHEMATICAL MODELING OF IN-MOLD COATING (IMC) OF RESIN TRANSFER MOLDING (RTM)

In Chapter 7, one-dimensional (1-D) mathematical modeling of the IMC process of a simple-shaped RTM part in the filling and packing stages is described. The compressibility of both the mold and substrate is taken into account in this model. In addition, a case study of the IMC filling and packing stages is also explained and discussed.

7.1 Modeling of IMC of RTM

For the purposes of analysis and modeling, the IMC process is divided into three main stages: (i) filling, (ii) packing, and (iii) curing as shown in Figure 7.1. In the filling stage, the coating material is injected into the mold and flows by compressing the RTM substrate until it covers the entire part. In the packing stage, the pressure is increased to inject more coating material into the mold until the desired volume is achieved for the prescribed coating thickness. Uniform thickness should be obtained after the coating equilibrates in the mold at the end of packing stage. The part remains in the mold until the coating is completely cured in the curing stage.
7.1.1 Filling stage

The IMC flow in a simple long rectangular cavity with a line source injection can be modeled as a one-directional (1-D) flow as shown in Figure 7.2. By developing a model for a 1-D flow, the model can then be used to test the more complicated models.

Basic assumptions are made to simplify the governing equations. These include:

(i) Isothermal flow due to the very thin cavity (see Appendix B).
(ii) Fully developed, incompressible flow.
(iii) Quasi-steady-state, laminar flow with body forces neglected.
(iv) Lubrication approximation – The thickness of the channel is relatively small compared to the width and length of the channel.
(v) No-slip conditions on the mold wall and surface of the substrate.
(vi) Chemical reaction is neglected during the filling and packing stages.
(vii) The viscosity of the typical coating materials can be represented by the power law viscosity model:

\[ \eta = m|\dot{\gamma}|^{n-1} \]  

(7.1)

where \( \eta \) is viscosity, \( m \) and \( n \) are the power law viscosity constants, and \( \dot{\gamma} \) is the shear rate.

(viii) Viscoelastic and entrance effects are not included. In addition, normal stresses are neglected in comparison with shear stresses.
(ix) Fountain region flow is neglected at the advancing flow front.

(x) Due to the very small thickness of the coating layer (3 to 5 mil or 76.2 to 127 \( \mu m \)), there is a linear relationship between the thickness change of a substrate and the injection pressure (Castro and Griffith, 1990).
The thickness change \((h)\) due only to the compressible substrate (Case I) and the thickness change \((h)\) due to both the compressible substrate and the compressible mold (Case II) can be estimated as follows:

**Case I:** Compressible substrate \((C_1)\) and rigid mold (e.g. a steel mold)

\[
h = C_1 \cdot p
\]  

**Case II:** Compressible substrate \((C_1)\) and compressible mold \((C_2)\) (e.g. a composite mold)

\[
h = C_1 \cdot p + C_2 \cdot p
\]

where \(C_1\) is the compressibility of the substrate, \(C_2\) is the compressibility of the mold, and \(p\) is the injection pressure of the coating material.

The compressibility of the fiber-reinforced composite substrates (e.g. RTM parts) is explained in Appendix C. It can be approximated using Hooke’s law as follows:

\[
\sigma_e = E \cdot e = E' \left( \frac{h_s - h_{sf}}{h_s} \right)
\]

Therefore,

\[
p = \left( \frac{E'}{h_s} \right) \cdot h = \left( \frac{1}{C_1} \right) \cdot h
\]

where \(\sigma_e\) is engineering stress due to the injection pressure of the coating material, \(E\) is modulus of elasticity, \(e\) is engineering strain, \(E'\) is modulus of elasticity perpendicular to the fiber direction, \(h_s\) is the initial thickness of the substrate, \(h_{sf}\) is the final thickness of the substrate due to in-mold coating, and \(h\) is the thickness change of the substrate due to the injection pressure of the coating material \((h = h_s - h_{sf})\).
The illustration of the relationship between $h$, $h_s$, and $h_{sf}$ is displayed in Figure 7.3.

It is found that

$$C_1 = \frac{h_s}{E_s'} \quad (7.4)$$

where $E_s'$ is the modulus of elasticity perpendicular to the fiber direction of the substrate.

Similarly, the compressibility of the mold ($C_2$) also depends on the thickness of the mold ($h_m$) and modulus of elasticity of the mold material ($E_m'$). For convenience, we express $C_2$ as proportional to $C_1$ as:

$$C_2 = \frac{h_m}{E_m'} = C_r \left( \frac{h_s}{E_s'} \right) = C_r \cdot C_1 \quad (7.5)$$

where $C_r$ is the compressibility ratio of $C_2$ and $C_1$ ($C_2 / C_1$).

Alternatively, the compressibility of the mold ($C_2$) can be determined by a computer simulation of the mold deflection due to the applied injection pressure of the coating material. A preliminary study of the mold deflection using commercial finite element method (FEM) packages is explained in Appendix D.

By substituting Equations 7.4 and 7.5 into Equation 7.2 and Equation 7.3, respectively, the thickness change ($h$) becomes

Case I

$$h = C_1 \cdot p$$

$$= \left( \frac{h_s}{E_s'} \right) \cdot p \quad (7.6)$$
Case II

\[ h = (1 + C_r) C_i . p \]
\[ = (1 + C_r) \left( h_s / E_s \right) . p \]  \hspace{1cm} (7.7)

In general, the thickness change (\( h \)) of both cases can be written in the form of

\[ h = (1 + C_r) C_i . p \]
\[ = (1 + C_r) \left( h_s / E_s \right) . p \]  \hspace{1cm} (7.8)

Note: \( C_r = 0 \) if we consider only the compressibility of the substrate (Case I).

According to the assumptions (i) to (ix), the momentum balance equation can be simplified to:

\[
\frac{\partial p}{\partial x} = \frac{\partial}{\partial z} \left[ m \left| \frac{\partial v_x}{\partial z} \right|^{n-1} \frac{\partial v_x}{\partial z} \right] \]  \hspace{1cm} (7.9)

where \( \frac{\partial p}{\partial x} \) is the pressure drop (or pressure gradient), \( \frac{\partial v_x}{\partial z} \) is the velocity gradient, \( m \) and \( n \) are the Power Law viscosity constants.

The boundary conditions are given as:

\[ \text{at } z = 0, \quad v_x = 0 \]
\[ \text{at } z = \frac{h}{2}, \quad \frac{\partial v_x}{\partial z} = 0 \]  \hspace{1cm} (7.10)

By integrating Equation 7.9 with respect to \( z \), the relationship that satisfies the boundary conditions between the pressure drop and volumetric flow rate is:
\[
\frac{dp}{dx} = -m \left[ \frac{1}{n+2} \right]^n 2^{n+1} q_x^n \frac{X_f - x}{h^{2n+1}}
\]  

where \( q_x \) is the volumetric flow rate per width of the part.

The pressure of the coating material at any point \( x \) along the flow when the flow front reaches a given distance \( X_f \) can be obtained by integrating Equation 7.11 with Equation 7.8.

\[
p = \left[ m \left( \frac{1}{n+2} \right)^n 2^{n+2} (n+1) q_x^n \frac{X_f - x}{\left[ (C_r + 1) C_1 \right]^{2n+1}} \right]^{\frac{1}{2n+2}}
\]  

The hydraulic force \( (F) \) generated by the coating material in the filling stage when \( X_f = L \) can be calculated from

\[
F = w \int_0^{X_f} p \, dx
\]  

Thus,

\[
F = \left( \frac{2n+2}{2n+3} \right) w L^{\left( \frac{2n+3}{2n+2} \right)} \left[ m \left( \frac{1}{n+2} \right)^n 2^{n+2} (n+1) q_x^n \frac{1}{\left[ (C_r + 1) C_1 \right]^{2n+1}} \right]^{\frac{1}{2n+2}}
\]  

where \( w \) is the width of the part and \( L \) is the length of the part.
The filling time \( t_{\text{fill}} \) at the location of the flow front \( (X_f) \) can be obtained from the following equation:

\[
\begin{align*}
    t_{\text{fill}} &= \frac{\int_0^{x_f=L} h \, dx}{q_x} \\
    \text{(7.15)}
\end{align*}
\]

Therefore,

\[
\begin{align*}
    t_{\text{fill}} &= \left(\frac{2n + 2}{2n + 3}\right) L \left\{ \frac{m \left( \frac{1}{n + 2} \right)^n 2^{n+2} (n+1)[(C_r + 1) C_1]}{q_x^{n+2}} \right\}^{\frac{1}{2n+2}} \\
    \text{(7.16)}
\end{align*}
\]

### 7.1.2 Packing stage

In this stage, the location of the flow front \( (X_f) \) remains constant and equals the length of the RTM part \( (L) \). However, the pressure at the mold end \( (p_{\text{end}}) \) increases as more coating material is injected into the mold.

The packing pressure at any point \( x \) can be obtained by integrating Equation 7.11.

\[
\begin{align*}
    p &= p_{\text{end}}^{2n+2} + \left[ \frac{m \left( \frac{1}{n + 2} \right)^n 2^{n+2} (n+1) q_x^n (L - x)}{[(C_r + 1) C_1]^{2n+1}} \right]^{\frac{1}{2n+2}} \\
    \text{(7.17)}
\end{align*}
\]

To estimate the value of \( p_{\text{end}} \), we recall that the desired coating thickness should be determined by:
\[ h = \frac{h_{(x=0)} + h_{(x=L)}}{2} \]  

\[ h = \frac{(C_r + 1)C_1}{2} p_{\text{end}}^{2n+2} + \frac{m \left( \frac{1}{n+2} \right)^{2n+2} (n+1) q_x^n}{\left[ (C_r + 1)C_1 \right]^{2n+1} L} \left[ \frac{1}{2n+2} \right] + \frac{(C_r + 1)C_1}{2} [p_{\text{end}}] \]  

By optimizing Equation 7.19, the pressure at the end, \( p_{\text{end}} \), can be determined. In addition, the hydraulic force \( F \) generated by the coating material in the packing stage can also be obtained as discussed in the filling stage. Thus,

\[ F = \left( \frac{2n+2}{2n+3} \right) w \left[ (C_r + 1)C_1 \right]^{2n+1} x \left[ p_{\text{end}}^{2n+2} + \frac{m \left( \frac{1}{n+2} \right)^{2n+2} (n+1) q_x^n}{\left[ (C_r + 1)C_1 \right]^{2n+1} L} \left[ \frac{2n+3}{2n+2} \right] \right] - p_{\text{end}}^{2n+3} \]  

(7.20)

### 7.1.3 Numerical solution for 1-D IMC filling

Because it is easy to use, the finite difference method (FDM) is used to solve the governing equations numerically for 1-D IMC filling. However, FDM cannot easily handle irregular-shaped parts since the coordinate lines of some orthogonal coordinate systems in the solution domains may not coincide with the boundaries of the physical domain. FDM then requires the use of cumbersome boundary-fitted coordinates as shown in Figure 7.4. Therefore, FDM is restricted to solution domains with simple geometry.
For complicated parts, control volume/finite element method (CV/FEM) is preferred because it has the ability to handle the solution domain with arbitrary geometry.

The flow chart for the numerical solution of 1-D IMC filling is shown in Figure 7.5. According to the flow chart, a fixed spatial step is used to track the flow front location. For each time step, the flow front location is advanced by one spatial step. The thickness change and pressure distribution are also updated by an iterative solution of Equations 7.8 and 7.9. The time step can be determined by Equation 7.15. The entire procedure is repeated until the flow front reaches the mold end.

The analytical solution of the 1-D IMC flow can also be used to verify the numerical solution. It is found that there is good agreement of the pressure along the flow path between the analytical and numerical results as shown in Figure 7.6. For complicated flows, the numerical solution is the only option.

7.2 A Case Study of IMC Filling and Packing Stages

A case study of the 1-D IMC filling and packing stages for the RTM substrate is discussed next. A simple rectangular E-glass reinforced polyester part of dimensions – 2 m long \((L)\) x 1 m wide \((w)\) x 0.01 m thick \((h_s)\) – is used as an example. We assume that the same material is also employed to build the mold for Case II. The thickness of the mold \((h_m)\) is assumed to be 0.24 m. Figure 7.7 shows a schematic diagram of the part and mold.

The modulus of elasticity \((E')\) of the composite material perpendicular to the fiber direction is calculated by assuming the percentage by weight \((%w)\) of the fiber glass and the properties of the resin and reinforcement. 30 \%w and 60 \%w of the reinforcement in
the composite part are considered. The coating material is assumed to be injected at the mold temperature of 140°C. The final thickness of the coating is 3 mil (76.2 μm). The values of the parameters and constants used in this case study are summarized in Table 7.1.

7.2.1 Results and discussions

The effects of parameters – including the volumetric flow rate, percentage by weight of the reinforcement, and the compressibility of the mold – on the pressure \( p \) and hydraulic force \( F \) are calculated in both the filling and packing stages. The results are displayed in Figures 7.8, 7.9, 7.10 and Table 7.2. It is found that in the filling stage (Figure 7.8), the flow rate and percentage by weight of the reinforcement affect the pressure. The higher the flow rate and the more reinforcement, the more pressure is required to inject the coating material for a rigid mold (Case I). In the packing stage (Figure 7.9), the required pressure increases as the percentage by weight of the reinforcement increases. However, the packing pressure depends only slightly on the flow rate for a rigid mold. Figure 7.10 shows the pressure required in the filling and packing stages for both cases: a rigid mold (Case I) and a compressible mold (Case II). It was found that the pressure required in the packing stage is much higher than that in the filling stage for a rigid mold. Moreover, the compressibility of the mold significantly reduces the pressure required in both the filling and packing stages. These tendencies are also found in the hydraulic force as shown in Table 7.2, which indicates the required clamping force to avoid the coating leakage.
Figure 7.1 Three stages of the IMC process: (a) filling, (b) packing, and (c) curing.
Figure 7.2 An IMC filling flow in a simple rectangular cavity with a line source injection.
Figure 7.3 The illustration of the thickness change \((h = h_s - h_{sf})\), the initial thickness of the substrate \((h_s)\), and the final thickness of the substrate \((h_{sf})\) due to IMC injection.
Figure 7.4 (a) The coordinate lines of some orthogonal coordinate systems and (b) The boundary-fitted coordinates near the boundary (Blazek, 2001).
Figure 7.5 A flow chart for 1-D IMC filling (Adapted from Chen, 2003).
Figure 7.6 Comparison of the pressure between analytical and numerical solutions along the flow path at the flow rate of $1.617 \times 10^{-6}$ m$^3$/s in the filling stage for a rigid mold.
Figure 7.7 A drawing of the part and mold used as an example in the case study.
<table>
<thead>
<tr>
<th>h (m)</th>
<th>T (°C)</th>
<th>m (Pa.s^n)</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>76.2x10^{-6}</td>
<td>140</td>
<td>1.0685</td>
<td>0.3085</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flow Rate (m^{3}/s)</th>
<th>Glass Fiber</th>
<th>C_r</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>%w1 %w2</td>
<td>C_r1 C_r2</td>
</tr>
<tr>
<td>3.23x10^{-6}</td>
<td>30 60</td>
<td>0*  24**</td>
</tr>
<tr>
<td>Q2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.62x10^{-6}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Case I for a rigid mold
** Case II for a compressible mold

Table 7.1 Summary of constants and parameters used in the case study.
Figure 7.8 The effects of the flow rate and percentage by weight of the reinforcement on the pressure along the flow path in the filling stage for a rigid mold.
Figure 7.9 The effects of the flow rate and percentage by weight of the reinforcement on the pressure along the flow path in the packing stage for a rigid mold.
Figure 7.10 The effects of the compressibility of the mold \((C_r = 24)\) on the pressures along the flow path in the filling and packing stages at the flow rate of \(1.617 \times 10^{-6} \text{ m}^3/\text{s}\) with 60 \%w of the reinforcement.
Table 7.2 Hydraulic force (N) generated by the coating at the flow rate of $1.617 \times 10^{-6} \text{ m}^3/\text{s}$ (Q2) with 30 %w and 60 %w of the reinforcement in the filling and packing stages for a rigid mold (Case I) and a compressible mold (Case II).
CHAPTER 8

CONCLUSIONS AND FUTURE WORKS

8.1 Conclusions

The main technical issues in developing the in-mold coating (IMC) process of polymer and composite parts include: (i) flow pattern, (ii) injection pressure, and (iii) mold deflection. The injection pressure is greatly influenced by the flow field and rheological properties of the coating material. Due to the very small length scale of the IMC flow (15 $\mu m$ to 125 $\mu m$), “apparent” wall slip at the solid-fluid interface occurs in the IMC flow. The high shear rates encountered in the microchannels make it necessary to include the higher shear rate plateau in the viscosity models. Including these two factors is critical in developing a predictive model for the IMC flow. For closed-mold IMC, such as in injection molding and resin transfer molding (RTM), predicting the pressure is critical in designing a successful coating process. The hydraulic force generated by the pressure needs to be calculated to determine the required clamping force of the molding machine; this helps prevent the leakage of the coating material. In addition, mold deflection is also important in RTM as most molds are less rigid than in thermoplastic injection molding.
Previous work found that the substrate thickness plays an important role in the flow pattern (Chen, 2003) while microfluidics and rheology of the coating material play a critical role in the injection pressure in the IMC process. This statement has also been confirmed by Bhagavatula (2006). His computer simulation based on the Carreau viscosity model and the slip boundary conditions using the parameters measured in this work has significantly improved the pressure prediction in the IMC process as shown in Figure 8.1. Microfluidics and rheology of fluids are therefore essential in designing and modeling microfluidic devices and materials processing.

The flow of the coating material in the IMC process mostly occurs at the microscale level from 15 μm to 125 μm (Bhagavatula, 2006) and exhibits the unique characteristics of microfluidics as discussed in Chapter 3. These characteristics – including high surface-to-volume ratio, which results in the domination of surface forces, and high shear rate – lead to the unusual apparent slip phenomena in the microflow. The wall slip changes the flow field in the microflow and subsequently affects the pressure field at the microscale level.

The slip flow in polymer systems is classified into two modes as discussed in Chapter 4: (i) true slip and (ii) apparent slip. The true slip occurs when the shear stresses are large enough to overcome the static friction between the wall and the flowing material. The true slip is usually found in polymer melts and highly cross-linked polymer systems. The second mode of the wall slip, the apparent slip, is revealed through the observation of abnormally low apparent viscosities of the fluids. This mechanism is applicable to both polymer solutions and suspensions. The apparent slip is primarily the result of the depletion of the polymeric or dispersed components near the wall region,
which leads to the formation of a fluid layer of lower viscosity near the wall. The migration or diffusion of polymeric or dispersed components away from the wall in the apparent slip flow may be caused by the following: (i) inhomogeneous stress fields in the flow field or deformation-induced migration and (ii) the presence of fluid-wall interactions or repulsive wall forces, which is the mechanism present in the polymer dispersion systems (Cohen, 1986) such as IMC.

The rheological models based on the true slip boundary condition were developed in Chapter 4 to determine the viscosity at the microscale level. These rheological models based on the no-slip and slip boundary conditions are summarized as follows:

**No-Slip** (at the wall, \( v_x = 0, v_y = 0 \))

\[
\tau_w = \frac{H}{2L} \Delta P
\]

\[
\dot{\gamma}_w = \frac{2}{WH^2} \left( 2Q + \Delta P \frac{dQ}{d\Delta P} \right)
\]

\[
\eta = \frac{\tau_w}{\dot{\gamma}_w}
\]

**True Slip** (at the wall, \( v_y = \beta \frac{dv_x}{dx} \))

\[
\tau_w = \frac{H}{2L} \Delta P
\]

\[
\dot{\gamma}_w = \frac{2}{WH^2} \left( 2Q + \Delta P \frac{dQ}{d\Delta P} \right)^{-1} \left( 2Q + \Delta P \frac{dQ}{d\Delta P} \right)
\]

\[
\eta = \frac{\tau_w}{\dot{\gamma}_w}
\]

A customized microslit rheometer with various channel gaps: 5 mil (127 \( \mu m \)), 4 mil (101.6 \( \mu m \)), 2 mil (50.8 \( \mu m \)), and 1 mil (25.4 \( \mu m \)), was built and developed to measure the viscosity of the IMC material as explained in Chapter 5. The viscosity measurement at temperatures of 25°C and 50°C from the microslit rheometer was conducted. This was
compared with the viscosity measurement from the commercial parallel-disc rheometer at high shear rates to verify the viscosity data. The viscosity measurement using the commercial parallel-disc rheometer was conducted at temperatures of 25°C, 45°C, 65°C, 85°C, and 100°C and fitted by the Carreau viscosity model. The parameters of the Carreau viscosity model of the IMC material were summarized in Table 5.2.

According to the viscosity data measured from the microslit rheometer, the reduced viscosity was found in the 1-mil-gap (25.4-μm-gap) channel at 25°C and 50°C as shown in Figures. 5.7 and 5.8, respectively. This reduced viscosity indicates the wall slip of the IMC material in the 1-mil-gap (25.4-μm-gap) channel. The developed rheological models were used to analyze the viscosity measurement at the differently-sized microchannels (4 mil or 101.6 μm and 1 mil or 25.4 μm gaps) and determine the average values of the slip parameter, known as slip length (β), as shown in the following:

<table>
<thead>
<tr>
<th>Channel Gap</th>
<th>Slip Length, Beta</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mil (25.4 μm)</td>
<td></td>
</tr>
<tr>
<td>Temp 25°C</td>
<td>3.0 μm</td>
</tr>
<tr>
<td>Temp 50°C</td>
<td>2.4 μm</td>
</tr>
</tbody>
</table>

These values of the slip length were then used to predict the pressure drop based on the continuum flow models as described in Chapter 6. The governing equations of the pressure flow based on (i) the viscosity models: the power law and the Carreau models and (ii) the boundary conditions: no-slip, true slip, and apparent slip were derived and numerically solved to predict the pressure drop in the microchannels. It was found that
the pressure prediction was improved when using the Carreau viscosity model compared to the power law viscosity model as shown in Figures 6.2-6.5. The Carreau viscosity model better predicted the pressure drop in the microchannels because of the high shear rate in the microflow. Moreover, the pressure prediction of the IMC flow using the Carreau viscosity model showed good agreement with the experimental results when applying the true slip (with $\beta = 3 \, \mu m$) and the apparent slip (with $\delta = 6 \, \mu m$ and $\mu = 0.6$ Pa.s) boundary conditions as shown in Figure 6.9 while the conventional no-slip boundary condition failed to predict the pressure drop in the 1-mil-gap (25.4-$\mu m$-gap) channel.

The last technical issue, the mold deflection, was discussed in Chapter 7. Simple mathematical models of IMC of RTM were derived to determine the pressure and hydraulic force. The effect of the mold deflection due to the pressure was integrated into the model in terms of the compressibility of the mold. The effect of the compressibility of both the mold and substrate on the pressure and hydraulic force is studied and discussed in Chapter 7. In addition, preliminary results of the mold deflection during IMC processing were simulated using commercial finite element method (FEM) packages as explained in Appendix D. These should serve as a basis for developing a model of IMC of RTM.

8.2 Future Works

The following is recommended for future works:
(i) The rheological and slip flow models developed for the IMC material as well as the experimental setup of the microslit rheometer can potentially be used in modeling and testing other microfluidic systems such as bio-fluidic systems (e.g. protein, DNA, cells).

(ii) The testing flow rate range of the microslit rheometer can be increased by employing a greater pressure capacity of the syringe pump and a better temperature control. In addition, the smaller channel of the microslit die can be obtained by using (a) a thinner shim stock, which is limited to 0.5 mil (12.7 μm) thick, and (b) micro/nanofabrication techniques such as photolithography and micromachining, and other materials such as SU-8.

(iii) The surface properties of the microchannels – including roughness and surface chemistry (e.g. hydrophobicity and hydrophilicity) – can be modified or enhanced to study the effect of these properties in the microflow and to better understand the fluid flow in microchannels.

(iv) Using the preliminary models developed in this work as a basis, a mathematical model to predict IMC of RTM can be developed.
Pressure Comparison for ABS at the Flow Rate of $1.12 \times 10^{-6}$ m$^3$/s

Figure 8.1 A computer simulation of the pressure prediction in the IMC process of thermoplastics (Bhagavatula, 2006).
APPENDIX A

ANALYSIS OF MICROSLIT DIE DEFLECTION
Deflection of the microslit die due to the pressure of the IMC flow was studied and determined by Hooke’s Law:

\[ \sigma = E \varepsilon \]  

(A.1)

\[ p = E \frac{\Delta h}{h_d} \]

Therefore,

\[ \Delta h = \frac{p h_d}{E} \]  

(A.2)

where \( \sigma \) is stress, \( E \) is Young’s modulus of the die material, \( \varepsilon \) is strain, \( p \) is the pressure of the IMC flow, \( \Delta h \) is the deflection of the microslit die due to the pressure \( p \), and \( h_d \) is the thickness of the die half.

An extreme case is shown here to determine the largest deflection of the microslit die. According to the experimental data, the maximum pressure in the 1-mil-thick (25.4-\( \mu \)m-thick) channel, after the end pressure correction, was 5.48 MPa. The microslit die was made of 1-in-thick (25.4-mm-thick) steel block (with \( E = 210 \) GPa). The deflection of the microslit die due to the maximum pressure can be obtained as follows:

\[ \Delta h = \frac{(5.48 \times 10^6)(25.4 \times 10^{-3})}{(210 \times 10^9)} \]

\[ \therefore \) \( \Delta h = 0.66 \times 10^{-6} \text{ m (0.66 \( \mu \)m)} \]

This value represents the largest deflection of the channel near the inlet, which is about 5% of the 1-mil (25.4-\( \mu \)m) channel gap and 1% of the 4-mil (101.6-\( \mu \)m) channel gap, while the smallest deflection of the channel is found at the outlet.
The effect of the die deflection on the pressure was studied and explained in the following. The deflection ($\Delta h$) was first calculated based on the corresponding pressure from the experiments at a given flow rate using Equation A.2. This value represented the largest deflection of the channel near the inlet. Once the pressure decreases along the channel, the deflection of the microslit die also decreases and becomes zero at the outlet. To simplify the problem, the average deflection ($\Delta h/2$) was used to represent the deflection of the entire channel, which was then included in the model. The governing equations based on the average deflection were numerically solved to determine the pressure. A comparison of the experimental and numerical results of the pressure with and without the deflection is shown in Figure A.1 for the 4-mil (101.6-μm) channel gap and Figure A.2 for the 1-mil (25.4-μm) channel gap.

From the results, it was found that the deflection of the channel due to the pressure of the IMC flow reduces the pressure prediction and has the most effect at the highest flow rate. However, when compared with the case with no deflection, the percentage change is less than 1.7% in the 4-mil (101.6-μm) channel gap and less than 7.6% in the 1-mil (25.4-μm) channel gap. Therefore, the effect of the channel deflection can be neglected in the microslit rheometer.
Figure A.1 Comparison of the experimental and numerical results of the pressure with and without the channel deflection for the 4-mil (101.6-μm) channel gap.
Figure A.2 Comparison of the experimental and numerical results of the pressure with and without the channel deflection for the 1-mil (25.4-μm) channel gap.
APPENDIX B

ISOTHERMAL CONDITIONS OF IMC FILLING
There are two extreme cases of filling a mold with a fluid at an initial room temperature different from the mold wall temperature. The first case is when the filling time ($t_f$) is much less than the conduction time ($t_c$). In this case, the temperature of the fluid can be taken as room temperature. The second case is when the filling time ($t_f$) is much greater than the conduction time ($t_c$). In this case, the temperature of the fluid can be taken as the mold wall temperature.

In the IMC process, the conduction time is of the order:

$$t_c = \frac{(h/2)^2}{\alpha} = 0.025 \text{ sec}$$

where $h$ is the coating thickness, which is about 5 mil (0.0127 cm), $\alpha$ is the thermal diffusivity of the IMC material, which is of the order of 0.002 cm$^2$/sec.

Therefore, because the typical conduction time of the IMC process (~0.025 sec) is very small compared to the filling time, the IMC material during the mold filling is assumed to be at the mold wall temperature.
APPENDIX C

THE COMPRESSIBILITY OF FIBER REINFORCED POLYMERS
A fiber reinforced polymer composite, which has all fibers oriented in the same
direction as shown in Figure C.1, is considered as a unidirectional composite. This
unidirectional composite is classified as an orthotropic material, in which the properties
in a particular direction (1-axis) are the same and the properties in all other directions
perpendicular to that direction (2- and 3-axes) are the same, but different from the first
axis.

Assuming a small deformation, the volume change (ΔV) of an orthotropic
material due to an applied pressure (p) in 2-axis is determined by

\[ \Delta V = V_o \left[ \varepsilon_2 (\nu_{21} + \nu_{23} - 1) \right] \]  \hspace{1cm} (C.1)

where \( V_o \) is the original volume of the material, \( \varepsilon_i \) is the strain in \( i \)-axis, and \( \nu_{ij} \) is the
poisson’s ratio defined as \( \nu_{ij} = -\frac{\varepsilon_j}{\varepsilon_i} \).

Applying Hook’s law into Equation C.1, we obtain

\[ \frac{\Delta V}{V_o} = \frac{\sigma_2}{E_2} (\nu_{21} + \nu_{23} - 1) \]  \hspace{1cm} (C.2)

where \( \sigma_2 \) is the stress in 2-axis and \( E_2 \) is Young modulus of the material in 2-axis.

The deformation of the material mainly occurs in 2-axis due to pressure (p) while
the deformation in 1- and 3-axes is relatively small due to the mold constraints as shown
in Figure C.2. Therefore,

\[ \nu_{21}, \nu_{23} \approx 0 \]
Equation C.2 becomes

\[
\frac{\Delta V}{V_o} \approx \frac{\Delta h}{h_s} = -\frac{\sigma_2}{E_2}
\]  \hspace{1cm} (C.3)

where \( \Delta h \) is the thickness change of the material, and \( h_s \) is the original thickness of the material.

By rearranging Equation C.3 and applying pressure \( p \), Equation C.3 becomes

\[
\Delta h = \left( \frac{h_s}{E_2} \right) \cdot p = C \cdot p
\]  \hspace{1cm} (C.4)

where \( C \) is the compressibility of the material.

Therefore, the compressibility of the orthotropic material, such as RTM parts, can be determined by

\[
C = \frac{h_s}{E_2}
\]  \hspace{1cm} (C.5)
Figure C.1 The 1-, 2- and 3-axes are the principal directions of a unidirectional fiber reinforced polymer composite defined as follows: 1- Principal fiber direction, 2- Out-of-plane direction perpendicular to fibers, and 3- In-plane direction perpendicular to fibers.
Figure C.2 Schematic representation of an experimental setup to determine the compressibility of a unidirectional fiber reinforced polymer composite part.
APPENDIX D

SIMULATION OF MOLD DEFLECTION
The purpose of this work is to study the deflection of a rigid mold such as steel mold during the filling stage of the IMC process. The simulation of the mold deflection was performed by using commercial finite element method (FEM) packages, including ABAQUS and IDEAS. A mold made of typical steel (Young modulus = 200 GPa and poisson’s ratio = 0.3) with a mold cavity \((L = 150 \text{ mm}, W = 150 \text{ mm}, H = 2.5 \text{ mm})\) was used in the simulation. The pressure profiles from the analytical solution as derived in Chapter 7 were applied to the mold cavity at different flow fronts \((X_f = L/4, L/2, 3L/4, \text{ and } L)\): 37.5, 75, 100, and 150 mm, respectively.

The filling pressure was obtained from

\[
p = \left[ \frac{m \left( \frac{1}{n} + 2 \right)^n 2^{n+2} (n+1) \left( \frac{Q}{W} \right)^n}{(C_i)^{2n+1}} \right]^{1/(2n+2)} \left( X_f - x \right)^{1/(2n+2)} \quad (D.1)
\]

By using the parameters in the case study in Section 7.2 for a rigid mold, the pressure profile as shown in Figure D.1 was defined by

\[
p = 1.475 \times 10^6 (X_f - x)^{0.3821} \quad (D.2)
\]

where \(p\) is the filling pressure of the IMC material in Pa, \(X_f\) is the flow front of the IMC material (37.5, 75, 100, and 150 mm, respectively), and \(x\) is the distance along the flow front.

A model of the mold was first created by ABAQUS. The basic procedures of FEM modeling, such as creating parts, generating mesh, and assigning boundary conditions, were carried out by ABAQUS. The FEM model was then exported to IDEAS.
to apply the pressure load. IDEAS has a special function that can define the pressure load by using an equation as a function of $x$ and $y$. The pressure profile in Equation D.2 was applied to the mold cavity as shown in Figure D.2. The FEM model with the applied pressure load was then exported from IDEAS to ABAQUS in order to solve the problem and determine the deformation at different nodes along the mold cavity. The simulation of the mold deflection when the flow front reaches the mold end is shown in Figure D.3. The deflection of the mold cavity due to the filling pressure of the IMC material at different flow fronts is summarized in Figure D.4. It was found that the deflection of the mold cavity was relatively small compared to the coating thickness and therefore the mold deflection of the rigid mold such as steel mold can be neglected in the IMC process.
Figure D.1 The filling pressure applied to the mold cavity at different flow fronts.
Figure D.2 The pressure profile applied to the mold cavity when the flow front reaches the mold end.
Figure D.3 The simulation result of the mold deflection when the flow front reaches the mold end.
Figure D.4 The deflection of the mold cavity due to the filling pressure of the IMC material at different flow fronts.
BIBLIOGRAPHY


