# 1 Overview of Plastics Molding

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The context of plastics molding will be briefly introduced in this chapter using the most popular method of injection molding. Two major topics are included in this chapter:

1. Introduction to Injection Molding: The systems of injection molding and the defects of injection molded products are described.
2. Core Values of Molding Simulation: The core values of simulation in injection molding will be introduced at the end of this chapter.
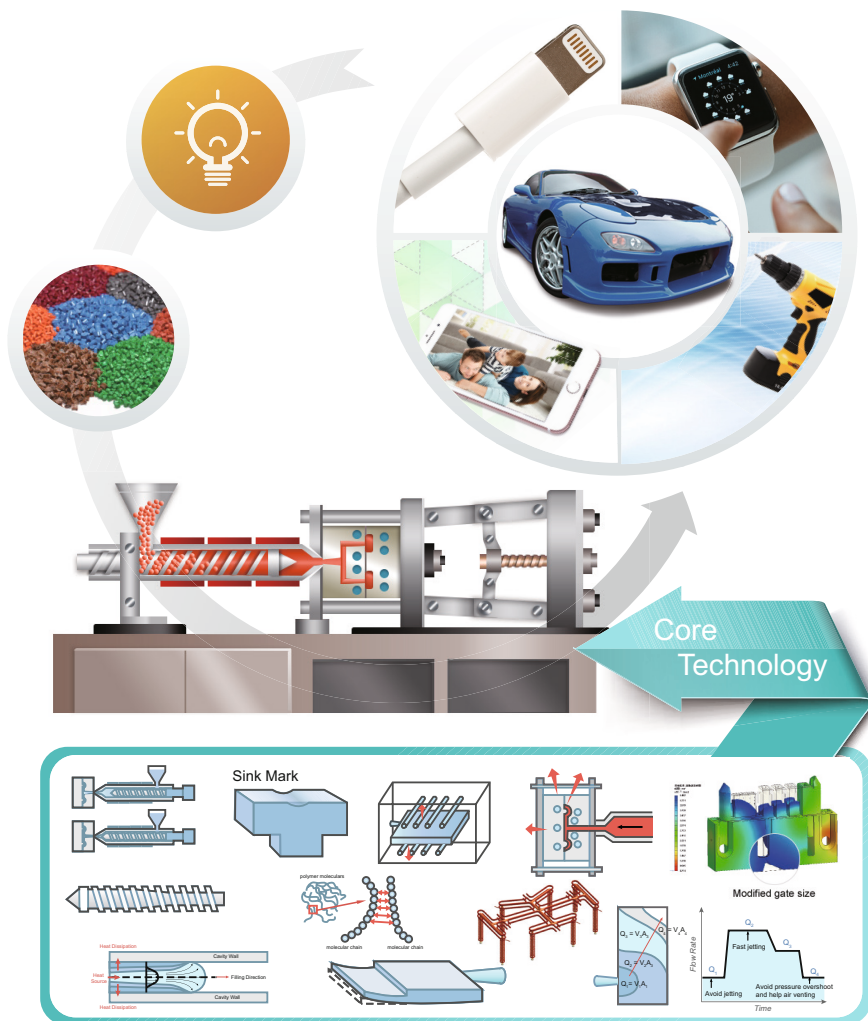
## ■ 1.1 Introduction to Injection Molding

Plastics can be shaped because of their ductility and plasticity. Therefore, plastics have been widely used in daily life and become a necessary part of the current world. The source of plastic products comes from customers' "needs", which are then developed to "design concepts". Such design concepts will be delivered to product designers for product design before being handed over to mold designers for mold design and development, as shown in Figure 1.1.

There are four stages from product development to mass production:

1. Design product drawings according to its functions, appearance, material, and processes, and hand over to mold factories for the design and manufacturing of molds.
2. Mold designers undertake discussion, drawing design, machining, mold-closing, and other procedures upon receiving product drawings, samples, or relevant specifications regarding material, weight, color, etc., which are used to manufacture the molds based on the conclusions made in the mold manufacturability meeting. The manufactured molds will be delivered to molding factories for mold test, modification, and detection.

3. Molding engineers execute tests to obtain better molding conditions for smooth production during the mold test stage, and provide feedback comments for mold modification regarding the difficult points for molding. The mold test will be executed repeatedly after the mold modification until the product quality achieves the specification of the mold test.

4. The production yield is improved via small-scale production and quality certification before the mass production stage begins. To obtain high-quality plastic products, one must first understand the relevant principles and mechanisms of the molding process. This section will briefly introduce the most common components of injection molding systems.



**Figure 1.1** Development of workflow of mold products

### 1.1.1 The Systems of Injection Molding

#### 1.1.1.1 The Cycle of Injection Molding

First, what is injection molding? Simply speaking, it is a process of making a product by injecting plastic material of liquid state into a mold cavity via the help of injection molding machines. When the plastic material enters the injection molding machine through a hopper, it is turned into a melted state after being squeezed by the screw from which a large amount of heat is generated through friction. The melted plastic accumulates in the front of the cylinder and is constantly heated in order to maintain the temperature for injection. The process mentioned above is called plastification, as shown in Figure 1.2.
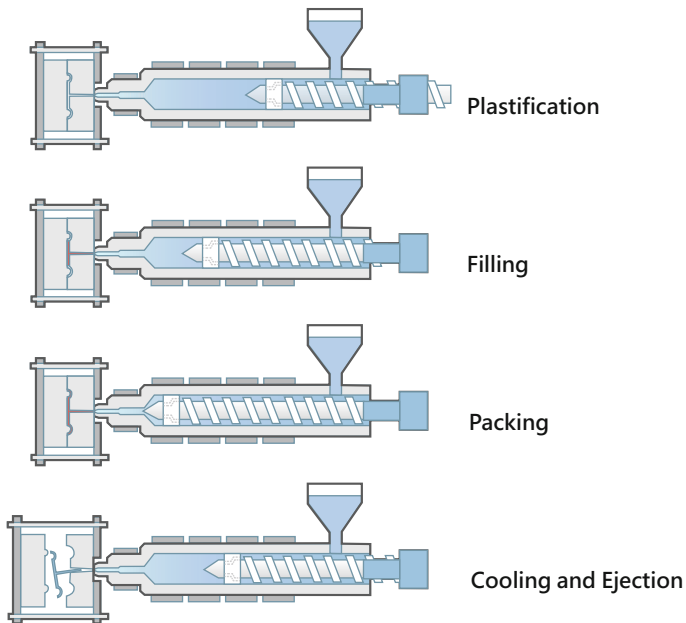


**Figure 1.2** Cycle of injection molding

Then, the melted plastic will be pushed forward into the closed mold cavity by the screw, a process that is called injection. After the initial injection is completed, when the high molecular weight melted plastic has fully filled the mold cavity, more melted plastic is injected under high pressure in order to compensate for the decrease in the volume of the plastic due to cooling as well as to make sure the mold cavity is perfectly filled until the sprue is solidified, a process that is called packing. Finally, the movable side moves back until the ejection pin reaches the rear platen to eject the molded product, runner system, and waste. This cycle is known as the molding cycle of injection molding.

### 1.1.1.2  Injection Machine

Figure 1.3 shows a basic injection molding machine (injection machine), which is suitable for manufacturing products of different shapes from thermoplastic or thermosetting plastics. There are two basic functions: 1) heating of the plastics to a melted state, and 2) application of high pressure to inject the melted plastic to fill the mold cavity completely.

Injection machine systems often have different components due to different types and uses, but generally comprise injection unit, clamping unit, mold unit, plastification unit, feed unit, and control unit.
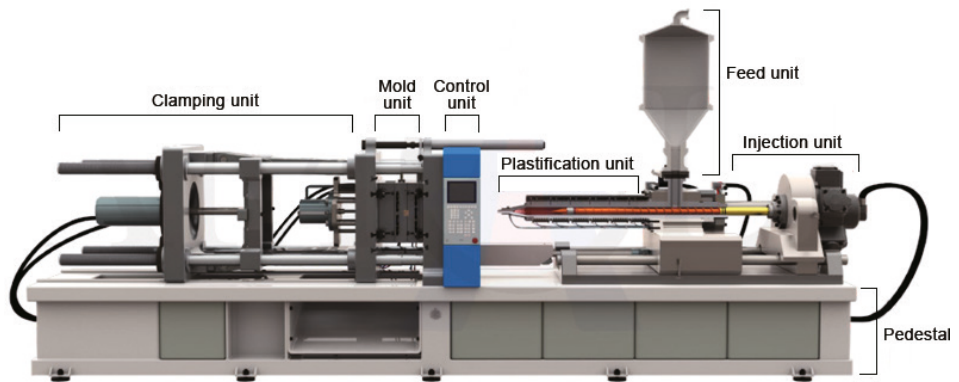


**Figure 1.3**  Injection machine

In industrial plastics processing methods, whether extrusion, injection, calendering, blow molding, film blowing, or spinning, a huge quantity of additional auxiliary equipment is always required to complete each processing step. The optimization, automation, and rationalization of auxiliary equipment for plastics processing play a role in determining product quality and the economic viability of the process.

Next, we will introduce the equipment required for injection molding in detail. This includes the feed, control, plastification, injection, and mold systems.

### 1.1.1.2.1  Feed System

Generally, there are two kinds of feed systems, namely independent and central. Independent feed equipment is usually set above the feeding port of the injection machine, i. e. the hopper with inverted cone structure, as shown in Figure 1.4(a). Some are supplemented by a heating or drying device, and also with a metering device to quantify the plastics, as shown in Figure 1.4(b).

The other kind of central feed system (also called automatic feed system or centralized feed system), including suction machine, central material loader, and conveying control system, has the advantages of continuous feeding, centralized automatic control, uniform mixing, and flexibility to change colors.
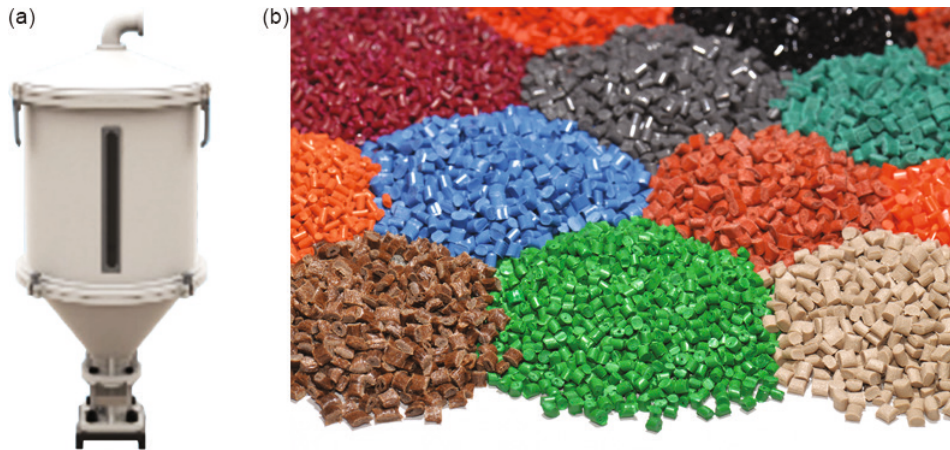


**Figure 1.4** (a) Hopper and (b) plastic pellets

### 1.1.1.2.2 Control System

The control system (Figure 1.5) can be said to be the brain and nerve center of the entire injection machine. The pressure, temperature, speed and time of the machine are controlled via the set values input by the operator that will directly affect the molding cycle and product quality.

The key physical parameters of injection molding processing are temperature, pressure, speed, time, and position, each of which includes the following:

1. Temperature includes resin drying temperature, barrel temperature, melt temperature, mold temperature, machine oil temperature, and working environment temperature.

2. Pressure includes filling pressure, holding pressure, back pressure, ejection pressure, mold opening pressure, and mold clamping pressure.

3. Speed includes injection speed, screw rotation speed, mold opening and closing speeds, and ejection speed.
   Time includes filling time, pressure holding time, cooling time, and resin drying time.

4. Position covers measuring position, VP switch position, eject position, and switch mode position.
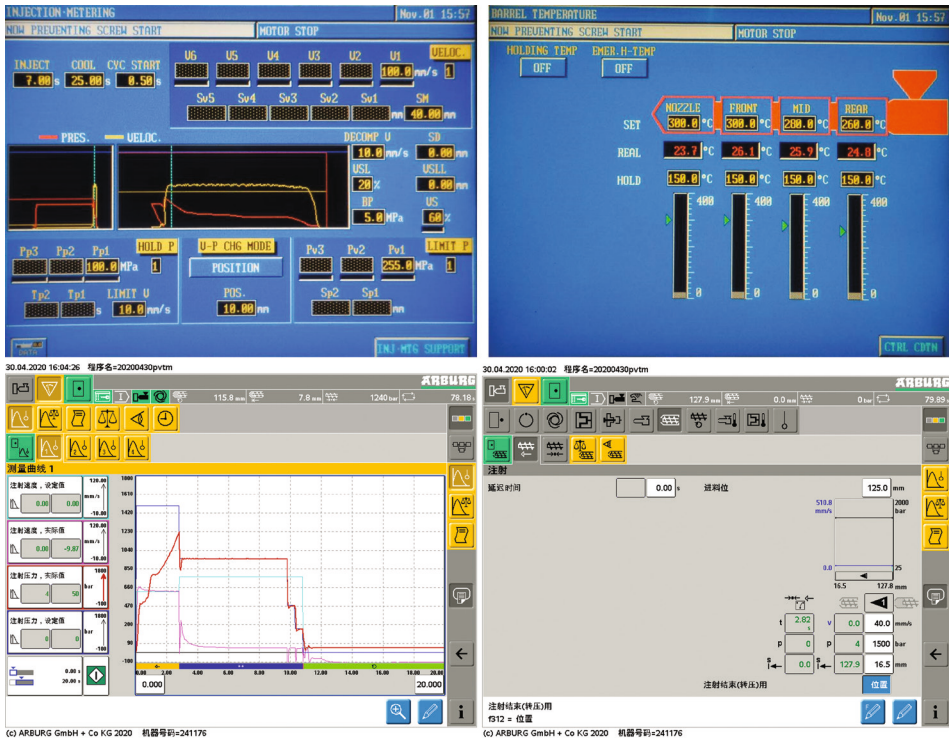
**Figure 1.5**  Control panels from Nissei and Arburg

One of the biggest problems encountered in common development and quality control of molded products during the production process is ineffective quality control due to using a one-way, indirect method for operating injection machines and system control devices. Therefore, it is important to analyze the characteristics of the machines so as to understand the different ways in which they can be used to exert good control over the process conditions.

### 1.1.1.2.3  Plastification System

Plastification is a process that uses the mechanical energy of the screw and the thermal energy of the heater to melt the incoming solid plastic, which is then applied with high pressure to be ready for injection. The plastic is turned into a melted state after being squeezed by the screw from which a large amount of heat is generated through friction. The melted plastic accumulates in the front of the cylinder and is constantly heated in order to maintain the temperature.

As shown in Figure 1.6 and Figure 1.7, the solid plastic enters the screw channel via the inlet hopper. With the high rotation speed of the screw that generates a shear stress effect with the barrel, the plastic is mixed and transferred along the screw channel. As the solid plastic is heated by the electric heaters outside the

barrel and due to the shear stress effect, it turns into a melted state as the temperature rises inside the barrel.
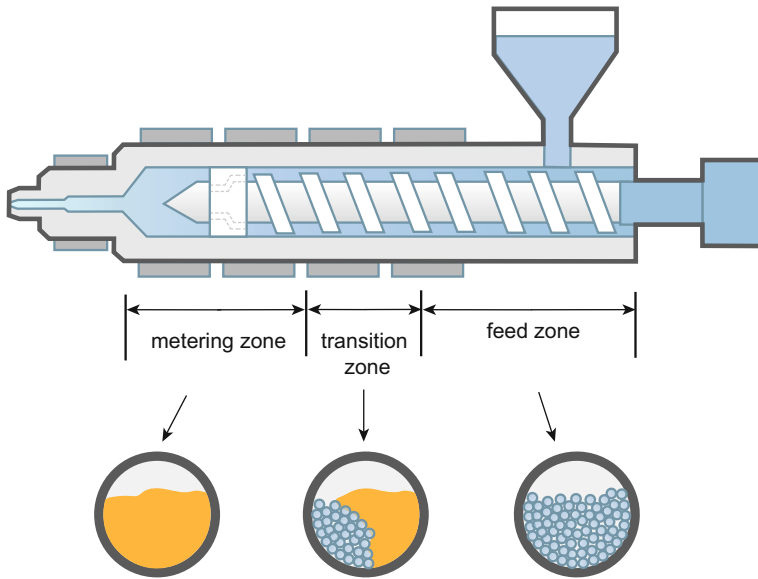


**Figure 1.6** Barrel and plastification
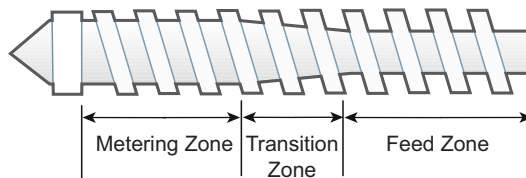


**Figure 1.7** Screw

The screw is divided into three zones (Figure 1.7):

1. Feed zone: The fixed feed depth of the screw channel is for pre-heating, transferring, and pushing the plastic granules, which start to melt at the end of the feed zone.

2. Transition zone: The thread depth is gradually decreased in the transition zone, the purpose of which is melting, mixing, shearing, and compressing of the plastic, and pressurized venting. The plastic must be completely melted in this zone. The volume of the melted plastic will be reduced and should be compressed accordingly to avoid incomplete compression and poor venting.

3. Metering zone: The fixed metering depth of the screw channel is for transfer and metering of the melted plastic, as well as providing sufficient pressure to

maintain a uniform temperature and stabilize the flow of the melted plastic. The length of this zone greatly affects the quality of the melt injected into the mold cavity. The longer the metering zone, the better is the chain mixing result. But a zone that is too long will cause a long dwell time of the melt in the barrel and will induce thermal decomposition. In contrast, a zone that is too short will lead to an uneven melt temperature.

The length and geometry of the zones in the screw directly affect the extent of plastification and the transport efficiency of the plastic. Judicious screw selection is very important for injection molding.

### 1.1.1.2.4  Injection System

The injection system is mainly responsible for filling and packing (Figure 1.8). For the filling stage, the screw moves forward to inject the melted plastics into the closed mold cavity through the nozzle to finish the filling process. When the melted plastic enters the cavity, the air is expelled from the ejection pin, parting line, and vent holes. Under-injection would occur if the liquidity is poor or the injection pressure is insufficient; in contrast, if the liquidity is too high, flash (see Section 1.1.2.3) would occur on the parting facet of the plastic part.
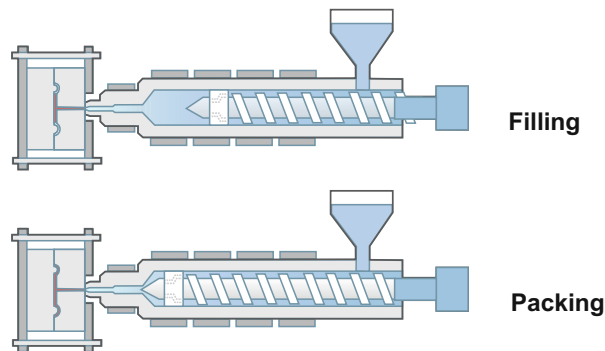


**Figure 1.8**  Injection system

After the mold cavity has been almost filled by the melt in the filling stage, the machine continues to apply high pressure to inject more melt into the mold cavity, to pre-compensate for the plastic volume shrinkage caused by cooling and to ensure that the melt completely fills the mold in the packing stage. Packing continues until the gate is sealed or the packing time ends.

### 1.1.1.2.5 Mold System

The mold system generally includes a fixed side and a movable side platen. The space inside the platens is the mold cavity, and is where the plastic is molded into shape. The mold also consists of ejection mechanisms such as ejector pins or ejector platens for ejecting the solidified product from the cavity. A typical structure is shown in Figure 1.9.



**Figure 1.9**  Open mold

Molds are important in injection molding. The basic structure of a mold is generally divided into three types: two-platen mold, three-platen mold, and hot runner. The decision for a particular mold structure is generally made by customers or according to products. A plastic mold consists of seven major systems: guiding, support, molding component, pouring, cooling, ejection, and venting systems. Using a sliding block is a way to handle undercuts, but normally the mechanism of mold opening and closing is sufficient for lateral parting, core extracting, and position reset.

A complete cycle time of plastics injection molding consists of filling, packing, cooling, and mold opening times, among which the cooling time has the highest proportion at about 70–80%. Therefore, the design of cooling system is a critical step which directly affects the length of cycle time, production efficiency, and cost. The following chapters will introduce the characteristics of plastic processing and the key points of mold design in detail.

## 1.1.2 Defects in Injection Molded Products

Product defects present another concern when plastic is turned into the final product through the foregoing processes. The plastic takes its shape gradually through the cooling during the process of injection molding, and usually it has the form of a near-finished product when it leaves the mold. If there are defects in the plastic product, it is necessary to analyze and understand the factors that are the cause.

The common injection molding defects are briefly described as follows:

### 1.1.2.1 Short Shot

The phenomenon called the "short shot", shown in Figure 1.10, gives a defective appearance to the final plastic product, and is caused by under-filling of the mold cavity. It is most apparent at in thinner zones or at the end of runners, and is mainly caused by insufficient plastic supply or poor liquidity of the plastic itself, so that the liquid state halts prematurely during the filling process. Therefore, any factor that affects the smooth flowing of the melted plastic is likely to cause short shot defects, such as insufficient amount of plastic injected, too high flow resistance, or insufficient liquidity.
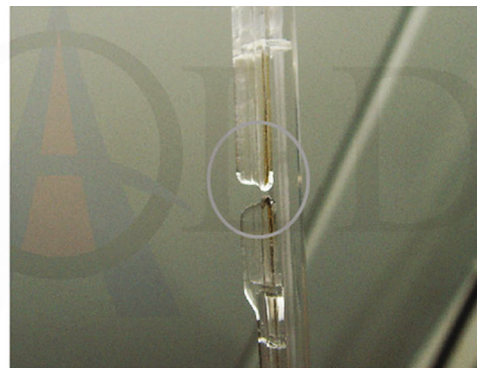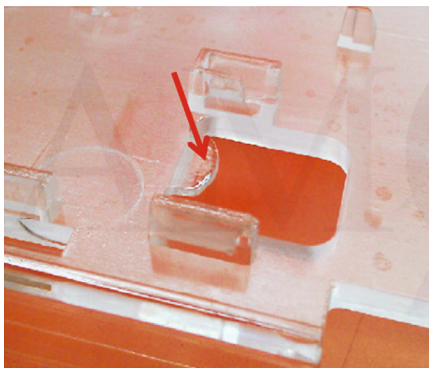


**Figure 1.10**  Short shot

In addition to a low temperature of melted plastic and mold wall, a thin part geometry or improper sprue location or length can also generate short shot defects as the mold cavity cannot be filled up. Improper configuration of the vent hole is also likely to cause a short shot.

It should be confirmed that the hopper has enough plastic if a short shot is observed. Then, the cylinder should be checked for blockage and the back-pressure valve checked for failure, which can result in a low injection pressure or material leakage. However, a long injection time can also cause a short shot.

### 1.1.2.2 Warp

Warp denotes the distortion or deformation of a product after injection molding. It is the defect type most commonly seen in injection molded products. Figure 1.11 shows a warped finished product which has two parts that cannot be assembled together. However, even if the product is not a combinative part but a single product, warp can also give rise to customer complaints and product returns. Therefore, product warp should be strictly controlled to within the tolerance.
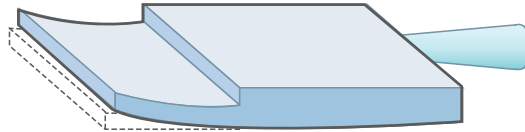


**Figure 1.11**  Warp resulting in a molded product that cannot be fitted

Thermal expansion and contraction are also seen in plastics. The melted plastic starts to cool down and solidify as it enters the mold cavity, and it contracts during the process of cooling and solidification. If the contraction rate is evenly distributed across the product, warp would not be seen and only shrinkage would result. However, with the interaction between the external factors, e.g. molding conditions, mold cooling design, product appearance design, and the plastics characteristics, e.g. molecular chain and fiber orientation, it is very difficult for plastic finished products to contract evenly or with low contraction rate.

It can be seen from the above that the causes of warp are various, complicated, and interdependent. Ways of reducing warp are a very important concern for producers.

### 1.1.2.3 Flash

Flash is generated as there is a gap existing at the split plane via which the melted plastics spills outside the mold cavity, as shown in Figure 1.12.
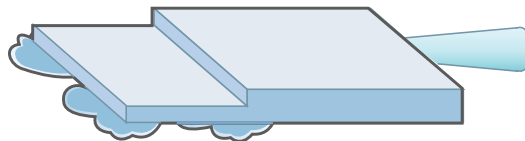


**Figure 1.12**  Flash

The main causes of such formation are as follows:

1.  Mold clamping force is too small: A pushing force is applied to the mold by the melted plastics during the injection molding process, especially if the central area of the mold cavity is subjected to excessive high pressure the mold will separate from the parting plane.

2.  Mold gap: The causes that the moving and stationary side of the mold cannot contact completely consist of a) a parting plane that is defective and not parallel between each side, and b) impurities on the parting plane that create gaps on the parting plane.

3.  Improper molding conditions: Wrong choice of molding machine, over-temperature of melted plastics, and excessive injection pressure are all causes of flash generation.

4.  Improper venting system: Flash will be generated if the venting is insufficient or the venting groove is too deep.

### 1.1.2.4  Sink Mark and Void

The formation of sink marks and voids is a phenomenon observed in thick areas where there is not enough plastic supplied during the cooling process, as shown in Figure 1.13.
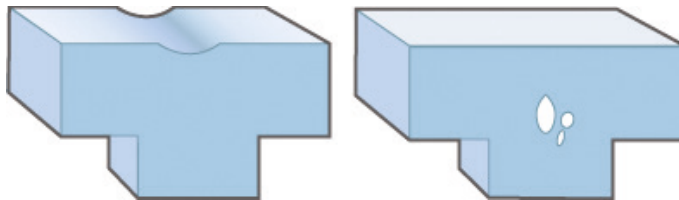
**Figure 1.13**  Sink mark / void

Sink marks are generated as the plastic contacting the mold walls cools and hardens before the inner plastic starts to cool down, and hence the surface is pulled inward by contraction. If the surface strength is sufficient, voids are generated instead of sink marks. Therefore, sink marks and voids are often seen at the rib parts or the backside of a convex surface. In conclusion, sink marks and voids are generated easily if the contraction is uneven between the inner and outer part in some areas.

### 1.1.2.5 Air Trap

Air trap denotes a condition in which the melt front of the melted plastic traps the air inside the mold cavity, so that the air cannot escape from the venting holes or the gaps in the mounting parts. A possible consequence is shown in Figure 1.14.
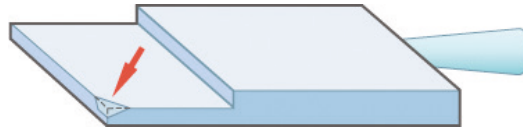


**Figure 1.14** Air trap

Generally speaking, air trap mostly occurs in the area filled last, where there is no venting hole or the venting holes are too small, with the result that bubbles, short shot, or surface defects are generated inside the plastic part. In addition, any large difference in the thickness of the parts will lead the melt flows toward the thicker area instead of the thinner area, giving rise to the race-tracking effect, which is also one of the reasons for air trap.

### 1.1.2.6 Burn Mark

The causes of burn marks are very similar to those of air traps. The major cause is that the air trapped inside the mold cavity is overheated by compression and creates dark marks on the plastic surface as shown in Figure 1.15. When the air inside the mold cavity is compressed, the pressure and temperature rise so rapidly that the surface of the plastic part at the end of the flowing path is decomposed and thereby burn marks are generated. Generally, burn marks usually occur in tandem with air traps.
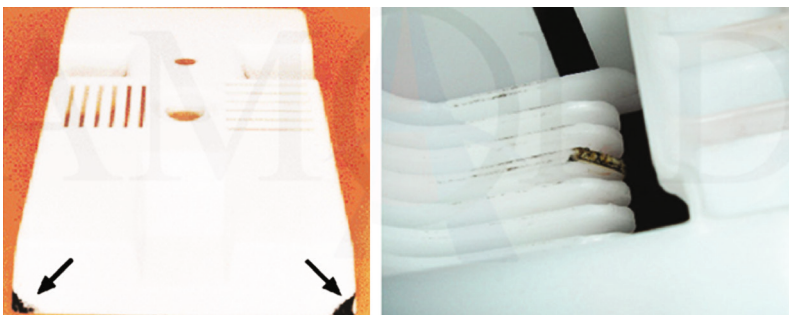


**Figure 1.15** Burn mark

### 1.1.2.7  Delamination

The main cause for delamination (layer separation) is due to the mixing of two incompatible materials or material types used in the molding process that are too dissimilar, as shown in Figure 1.16. In addition, delamination is also possible to occur if the temperature of the melted plastic is too low, the humidity of the material is too high, or the runner and sprue are not smooth.
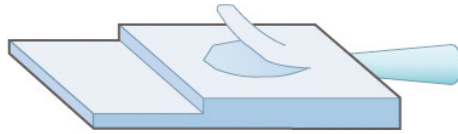


**Figure 1.16**  Delamination

### 1.1.2.8  Fish Eye

Fish eyes, as shown in Figure 1.17, are usually caused by unmelted plastic because of insufficient cylinder temperature and screw rotating speed, and low backside pressure. The phenomenon can also result from using too much recycled material or contaminated plastic. Therefore, if the above-mentioned situation can be avoided, the probability of fish-eye occurrence can be effectively reduced.
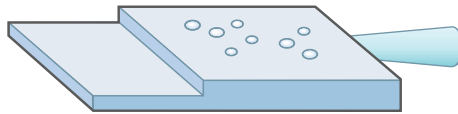


**Figure 1.17**  Fish eye

### 1.1.2.9  Flow Mark

Flow marks, as shown in Figure 1.18, are generated mainly if the temperature of the melted plastic is not evenly distributed or the viscosity of the melted plastic is excessively high.
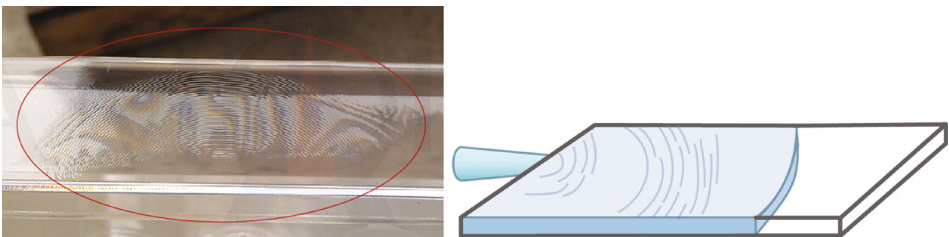


**Figure 1.18**  Flow mark

An excessively low temperature causes friction and pushing between the plastic and the mold cavity, and results in the plastic's hardening too quickly and leaving a flow mark, as shown in Figure 1.19. In addition, flow marks may occur if the melt near the gate solidifies due to unexpected cooling, or the melt is unable to provide compensation in the packing stage.



(a)                                             (b)
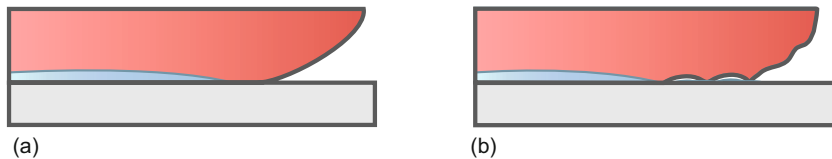
**Figure 1.19** (a) General fountain flow and (b) over-rapid cooling conditions that give rise to uneven local temperatures will readily cause flow marks

### 1.1.2.10  Stress Mark

On the surface of the injection molded part, a shiny white mark occasionally appears and is called a stress mark. Generally speaking, a stress mark is induced by internal stress. If the thickness of a plastic part varies a lot, the cooling speed at a thinner area differs significantly from that of other areas. Then, the uncooled melted plastic will apply stress on the cooled plastics, which generates a stress mark due to inner stress, as shown in Figure 1.20.
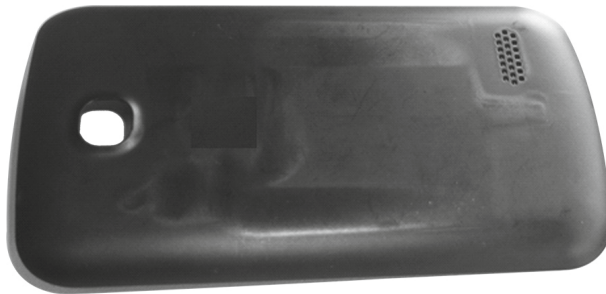


**Figure 1.20** Stress mark

### 1.1.2.11  Hesitation

When the mold cavity is being filled, the melted plastic tends to move to a thicker and low-flow-resistance area, which it fills up first before filling the thinner area. Therefore, the melted plastic usually hardens at a stagnation point as the flow stops at the thinner area. It is highly possible for the solidified plastic to be pushed to the surface of the plastic part and create a hesitation mark when the following melted plastic starts to move to such a thinner area, as shown in Figure 1.21. In addition, hesitation often leads to short shots because the plastic usually completely solidifies at the stagnation point.
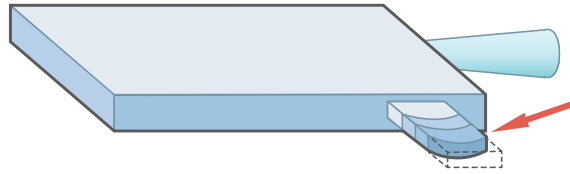
**Figure 1.21**  Hesitation

### 1.1.2.12  Jetting

Jetting is usually generated when the melted plastic passes through a narrow sprue or runner into the mold cavity with a high speed, as shown in Figure 1.22. Jetting normally causes contact between cold materials as the temperature of the plastic strips injected into the mold cavity drops and the strips make contact with each other afterward. The strength of the plastic part will be reduced when jetting happens, which is more likely to cause surface and internal defects at the same time. Thus, jetting should be avoided as much as possible in order to assure production quality.
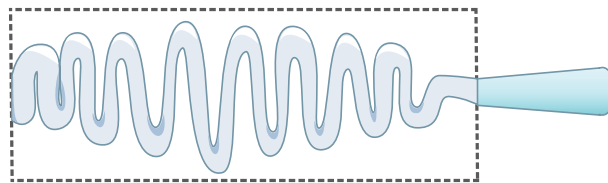


**Figure 1.22**  Jetting

### 1.1.2.13  Splay

Splays, as shown in Figure 1.23, are caused by the incomplete release of humidity or other volatile gases mixed in the plastic melt during the plastification stage, or by gases generated from slight decomposition of the plastic due to an excessively high pre-heating temperature.

If the plastic is not properly dried before manufacturing, the moisture inside will evaporate into steam during injection filling, which causes bubbles to flow along with the melted plastics inside the mold cavity and thus silver stripes (splays) will occur along the flowing direction. If the bubbles cannot be expelled entirely upon completion of filling, splays will also occur on the surface of the plastic part.

**Figure 1.23** Splay

### 1.1.2.14  Weld Line

When two or more plastic flow fronts merge together during the injection process, incomplete fusion can occur as the melt front is of lower temperature and hardens first. Hence, weld lines, as shown in Figure 1.24, are generated. Such defects are usually seen around the holes or the merging boundaries of the finished products. Therefore, when race-tracking effects take place, they are usually accompanied by weld lines. To avoid the generation of weld lines, extreme care should be taken regarding conditions such as significant thickness changes or multiple sprues in the mold.
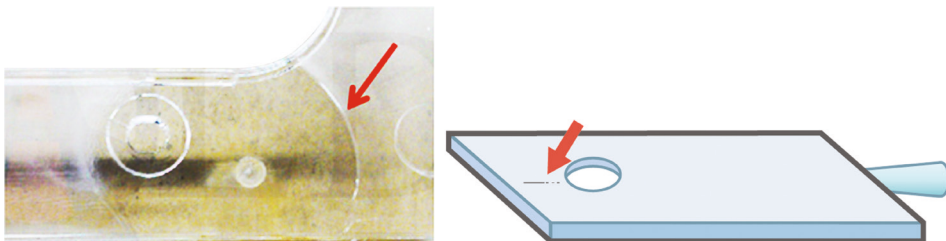


**Figure 1.24** Weld line

The plastic melts cannot be completely fused at the weld line, as a result of which the strength of the plastic part is lowered. Therefore, if weld lines cannot be avoided, the position and size of the gate should be adjusted to make the weld lines occur in as inconspicuous a low-stress area as possible. Generally, melt fronts converging from two directions at less than 135° will give rise to weld lines, as shown in Figure 1.25.
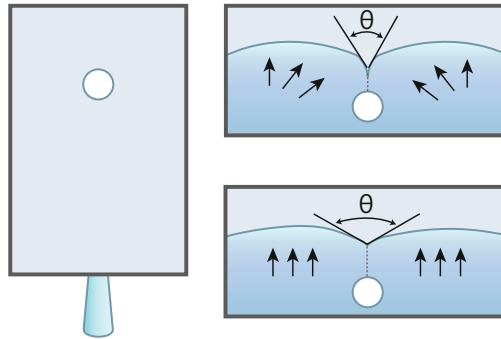
**Figure 1.25**  The converging of melt fronts

# ■ 1.2  Core Values of Molding Simulation

From the foregoing introduction to plastics injection molding, it can be seen that the types of defects are of various kinds, which can be categorized as appearance or dimensional issues, as shown in Figure 1.26.

Concept    CAD design    Mold fabrication    Production



Many defects happened !   Why?

Burnings    Weld line    Warp    Flash
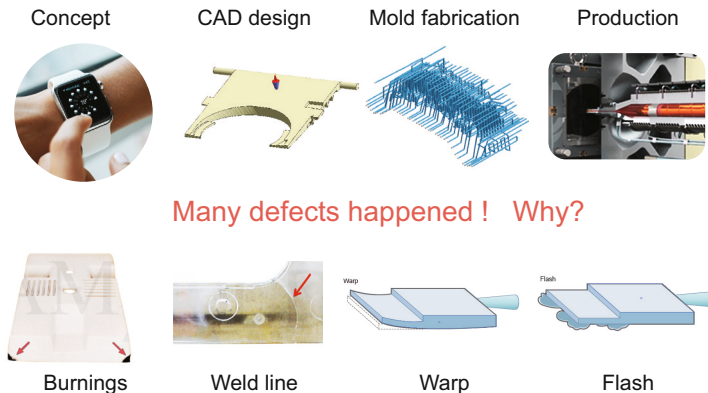
**Figure 1.26**  Molding challenges: design quality

When facing these defect issues, the traditional solution is the trial-and-error method, i.e. to repeat mold test and mold modification until the product specifications are met, which usually takes gigantic amount of time, labor, and other costs. However, with the assistance of CAE (Computer Aided Engineering) tools, the production process becomes more efficient and the product quality gets better, while waste is further reduced, with environmental benefits. An introduction to CAE, including its application possibilities in injection molding, is given below.

## 1.2.1 Application of CAE Technology in Injection Molding

CAE is a kind of computer aided engineering software and technology that uses computer simulation and analysis to assist the diagnosis and development of complicated injection molding processes. CAE is able to integrate the complicated rheological, thermal, and mechanical properties of a material, and enables designers and developers to do qualitative and quantitative analysis and diagnosis for mold design as well as analysis and diagnosis for existing molds and operating conditions.

From the CAE analysis result, developers can explore the causes of problems that occur and test different design changes to find out the most appropriate solution, which is not achievable by the traditional trial-and-error method. Furthermore, if the design change involves modifications of products or molds, the cost of time, labor, machine, material, and energy by repeated mold tests and modifications is even beyond estimation. Hence, it is common to implement CAE for design verification during the development process.

We know that the injection process is a major factor that determines product quality. Going through solid, melted, and back to solid states in a short time involves rearrangement of plastic molecules. If we can effectively control the transition of plastic properties in the process, the structural strength of the product can be assured.

Where is CAE used?

CAE is not always suitable to provide assistance for injection molding, as shown in Figure 1.27.
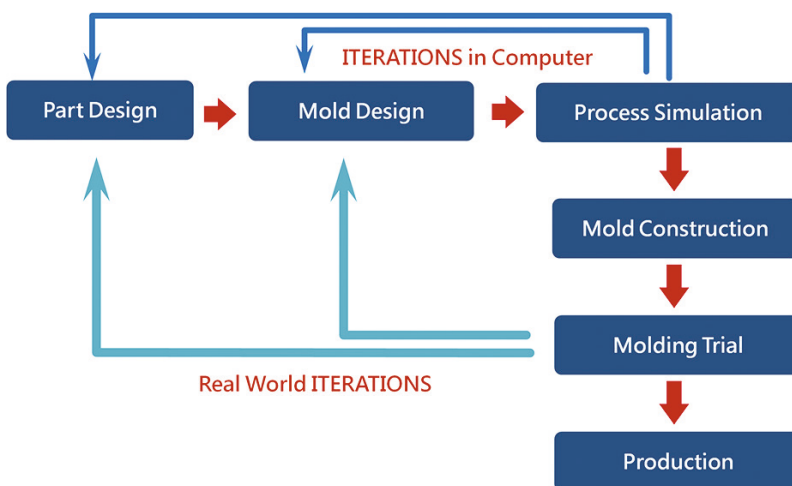


**Figure 1.27**  New concepts in product development of injection molding processes

The best opportunities for using CAE in the injection molding process are:

1.  At the product design stage and before mold construction: Predict and amend possible defects in product design and reduce the cost for mold opening.

2.  After mold construction but before mass production: If the product is defective, but the causes are difficult to solve via onsite mold tests, this can be analyzed to determine the causes for defect generation through regenerating the actual defects and issues via simulation.

3.  After mold construction and during mass production: Find out any possibility for yield improvement and molding cycle time shortening via simulation to further increase the productivity.

4.  Create an in-house database: Summarize the problem-solving knowledge and create problem-determination SOPs (standard operation procedures) by constantly accumulating project counts.

Hereunder is an example of a cap for spraying deodorant in mass production. How do we utilize CAE to help the manufacture? This situation meets the above-mentioned CAE application opportunity item 3. For the product in mass production, using trial-and-error to further improve productivity or yield is time- and labor-consuming, which makes CAE a pretty good choice in this application.

As shown in Figure 1.28(a), with CAE analysis we can see that the temperature difference between inside and outside of the cap is 45 °C in EOC (end of cooling), which leads to thermal stress and causes quality issues. The high product temperature also affects the ejection time (problem discovery).
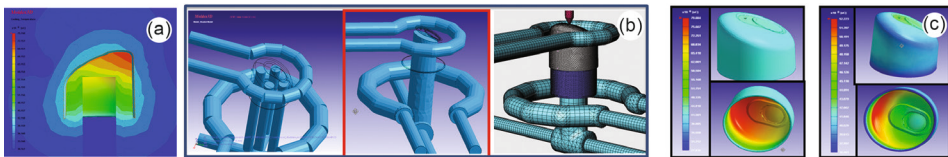


**Figure 1.28**  CAE example: spray deodorant cap

As shown in Figure 1.28(b), originally, the cooling channel design was a big pipe; however, by considering abnormal cooling channel design and comparing three different models, the one in the middle shows the best result. This is a good example of using CAE to save time and labor without redesigning the mold.

As shown in Figure 1.28(c), the new design reduces the temperature difference by 15 °C.

Final result: The productivity is increased by 25% as the cycle time is shortened. For an annual production of 4 million pieces, 4 million seconds (46 days) are saved therefrom. In addition, the quality is improved simultaneously as the temperature difference is reduced.

This example clearly tells us that, with proper use of CAE tools, we can improve existing processes without affecting current production lines and with only little cost.

The following chapters will introduce the principles, models, and usage of CAE in detail, from theory to practice, as well as its applications in various industries and molding technologies, so that readers can better understand and learn how to use CAE to solve problems.

# 2 Material Properties of Plastics

Chen-Chieh (Jye) Wang

Generally, the plastic material for injection molding is in a pellet form, which is heated and melted during the molding process, and is given shape and function before cooling down to become solid again. Therefore, an understanding of different materials regarding their rheological, thermal, thermodynamic, kinetic, chemical, and mechanical properties is essential to obtain the desired application characteristics, functions, molding parameters, product quality, and precision of CAE simulation. Material properties are explored individually in the following sections.

## ■ 2.1 Overview

Polymer materials are everywhere, from our daily lives to high-tech fields (such as electro-optical, biomedical, and high performance applications). Polymers consist of many chemical units (monomers) after polymerization, such as polyethylene (PE), whose monomer is ethylene. Polymers have tremendous molecular weights (MW) ranging from tens of thousands to millions and thus are called "macromolecules".

Figure 2.1(a) shows that the bonding of monomers can be linear or branched. For example, in branched PE, the molecules cannot pack closely together due to steric hindrance of the branches, and so its density is lower; it is therefore called low-density polyethylene (LDPE). In contrast, linear PE is more regular and the polymer chains can pack together more closely and crystallize efficiently; it is therefore called high-density polyethylene (HDPE).
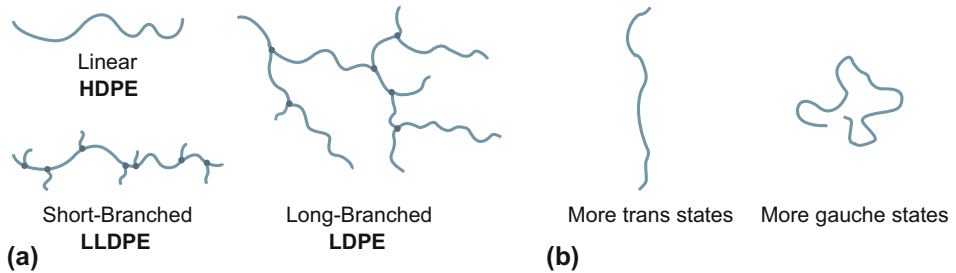
**Figure 2.1** (a) Molecular configurations of polyethylene and (b) conformations of polymer chains

In the polymer chain, the atoms are connected by covalent bonding forces. The bond energy of the C-C covalent bond is around 80 kcal/mol. The rotation of a single covalent bond gives rise to the bond "conformation", i.e., cis, trans, and gauche states. Since there are many bonds in a polymer chain, a single polymer chain can have tremendously accessible chain conformations. The different chain conformations have different shapes, a fact which also implies a different volume of occupied space, as shown in Figure 2.1(b). Additionally, intermolecular interaction (van der Waals forces) occurs among molecular chains, inducing atoms to pack more closely together, preventing atoms from chain crossover and leading to chain entanglement, as shown in Figure 2.2(a). The entanglement of chains plays an important role in the viscoelastic behavior of materials.
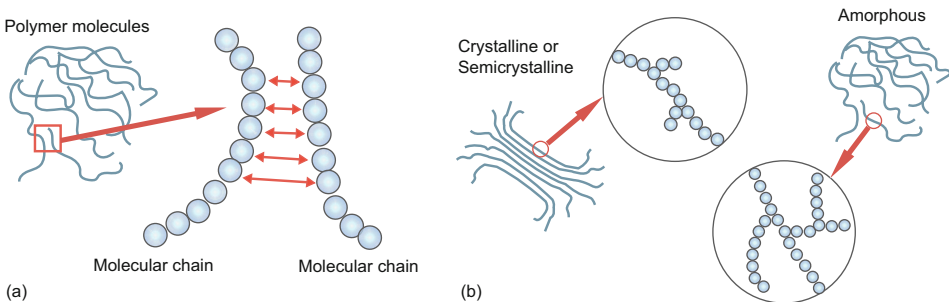


**Figure 2.2** (a) Interactions among macromolecules and (b) classification of thermoplastic polymers

When the polymer material is heated, the thermal energy imparted to the atoms is sufficient to overcome the energy for performing large-scale molecular movements, and the material softens. When the temperature is high enough for the polymer chain to move freely, the material flows like a liquid. A plastic that can be melted by heat and reverts to the solid state after cooling is generally called "thermoplastic". If the temperature is further increased, the thermal energy may be high

enough to break the covalent bonds. The molecular chain may then break into fragments in a process called "degradation". In summary, the polymer behaves like a solid when the temperature is lower than the glass transition temperature at which the molecules freeze. The material behaves like a rubber when molecules are able to perform large-scale movements and like a liquid when it can move freely.

In accordance with their molecular morphology in the solid state, thermoplastic polymers can be classified into two categories: crystalline and amorphous. The amorphous morphology has no long-range order structure. In other words, the chains pack randomly throughout the material, e. g. as in PMMA, a-PS, and ABS. In contrast, crystalline polymers (such as i-PP, PE, nylon) can form orderly stacks of folded chains called lamellae, which are like crystals with an orderly arrangement of atoms.

In contrast to thermoplastics, thermoset polymers cure irreversibly. After heating, they cannot return to the original state, which means that they cannot be processed again. Examples are phenolic resins, melamine, UP, PU, and epoxy.

When a thermoset material is heated, its molecular chains will cross-link with each other to form a three-dimensional network structure due to chemical reaction. After the cross-linking reaction, the material cannot flow or be re-formed under the constraint of the cross-linked structure, and exhibits solid behavior, as shown in Figure 2.3. The higher the cross-linking density, the more constrained it becomes and therefore the material becomes harder.
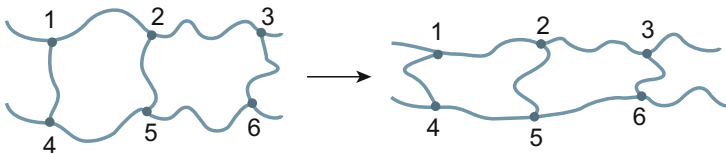


**Figure 2.3** Network structure of thermoset materials

# ■ 2.2 Rheological Properties

The flow behavior of polymers is within the realm of rheology, which is the study of the deformation and flow of materials. Polymer rheology covers experimental research on the measurement of fluid viscosity, the relationship between molecular structure, pressure, and temperature, and the effect on rheological properties of solvents and plasticizers, as well as Newtonian and non-Newtonian fluid mechanics, and other theoretical research such as molecular rheology, which has become

a popular field in recent years. The reason why the rheological behavior of polymeric fluid is different from that of simple molecules is that a polymer's molecular weight is often as high as $10^5$ to $10^8$ g/mol, consisting of long-chain molecules, sometimes with branched structure. The rheological behavior of polymers therefore plays an important role in injection molding. When melted plastic is injected into the mold cavity, the flow resistance and behavior are related to its rheological properties with regard to how the mold cavity is filled, how much injection pressure is required to inject the melted plastic through sprues and runners, what the temperatures of the melt and mold should be, etc. It is also instrumental in designing the runner and sprue locations so as to avoid unnecessary packing and weld lines. The shrinkage, warp, and deformation of the product are affected by the molecular orientation, crystallinity, and residual stress after filling and cooling of the melted plastic. In summary, an understanding of rheology is beneficial to product and mold design, which can also help to solve injection molding issues, and derive the greatest benefits from CAE.

## 2.2.1 Viscosity

Consider an incompressible fluid located in the space between two parallel plates, as shown in Figure 2.4.
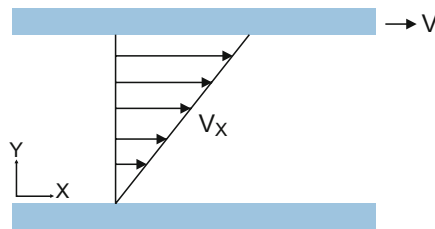


**Figure 2.4**  Flow between two parallel plates

Assume the areas of top and bottom plate are both $A$, and the two plates maintain a small distance $Y$ between each other. If an external force $F$ is applied to the top plate, the top plate can move at a constant velocity $V$, while the bottom plate remains stationary. Such flow is called simple shear flow. It was found by experiment that when a steady state is reached, $(F/A)$ is in proportion to $(V/Y)$, where the proportional constant $\eta$ denotes the viscosity of the fluid (Equation 2.1). $(F/A)$ is called the shear stress, $\tau_{xy}$, and $(V/Y)$ is called the shear rate, $\dot{\gamma}$, giving Equation 2.2, which is known as Newton's Law of Viscosity:

$$\frac{F}{A} = \eta \frac{V}{Y} \qquad\qquad (2.1)$$

$$\tau_{xy} = \eta\dot{\gamma} \tag{2.2}$$

Shear rate denotes the difference in velocity of each point in the flow field, reflecting the velocity gradient in a flow.

### 2.2.1.1  Effects of Non-Newtonian and Molecular Conformation

A fluid is defined as being Newtonian only if the stress and shear rate are related by a constant viscosity (Equation 2.2) that does not depend on the stress or shear rate of the flow. The viscosity can be regarded as the resistance to flow and deformation. The resistance results from the collision of and friction among the molecules during flow. It can be influenced by material compositions, temperature, and pressure.

The flow resistance (viscosity) of a polymer depends on the orientation and conformation of molecular chains. Since orientation and conformation vary with the flow fields, the viscosity may change with shear rate, as shown in Figure 2.5.



**Polymer Molecules**

e.g.,PE,PP...

**Non-Newtonian Viscosity**

*Shear Viscosity*

Lower temperature

Higher temperature

*Shear Rate*

Viscosity = ∫ ( composition, T,P )
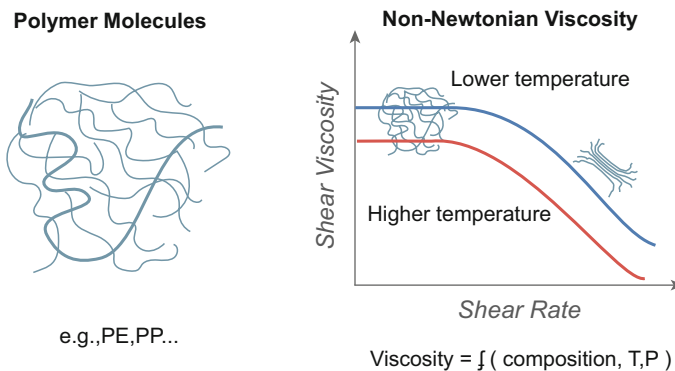
**Figure 2.5**  Molecular structure and viscosity of polymer molecules

For a polymer of low molecular weight, the flow resistance and viscosity are lower because its molecules are shorter, whereas a polymer with longer molecules has a higher viscosity due to the molecular size and the number of entanglements among the molecular chains. The relationship between viscosity and molecular weight is shown in Figure 2.6, where a larger slope is observed once the molecular weight exceeds a critical value, owing to the effect of entanglement.
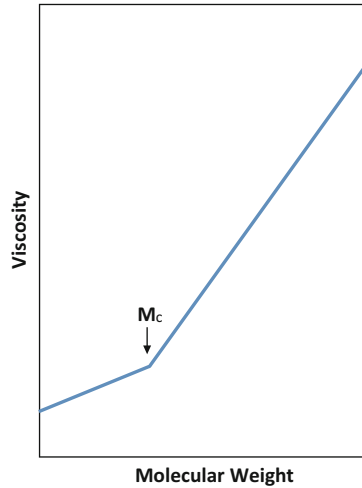
**Figure 2.6**  Viscosity at various molecular weights

In macromolecules, entanglements act as obstacles to the movement of a polymer chain, creating a restricted tube with surrounding chains in such a way that the chain can only wriggle along the tube, while the lateral motions of the chain are restricted. Such motion is called "reptation". Based on this model, Doi and Edwards [1] proposed a mathematical derivation that links microscopic molecular topology to macroscopic rheological properties. The results also show that the viscosity increases with about a 3.4 power of the molecular weight [2]. This conclusion is in agreement with experimental measurement for many polymers [3].

### 2.2.1.2  Effects of Shear Rate

Fluids that obey Newton's Law of Viscosity (Equation 2.2) are called Newtonian fluids, and can be observed in many gases, or liquids and solutions of low molecular weight. Since the viscosity of a Newtonian fluid is irrelevant to shear rate at a constant temperature, the graph showing the relationship between them is just a horizontal line (Figure 2.7(a)). There is a linear relationship between shear stress and shear rate which takes the form of a straight line passing through the origin on the graph (Figure 2.7(b)).

For polymeric fluids, the viscosity usually exhibits shear-rate-dependent properties. A fluid whose viscosity decreases with increase in shear rate (Figure 2.7(a)) is called a shear thinning fluid or pseudoplastic fluid. In contrast, a fluid whose viscosity increases with increase in shear rate is called a dilatant fluid, also known as a shear-thickening fluid.
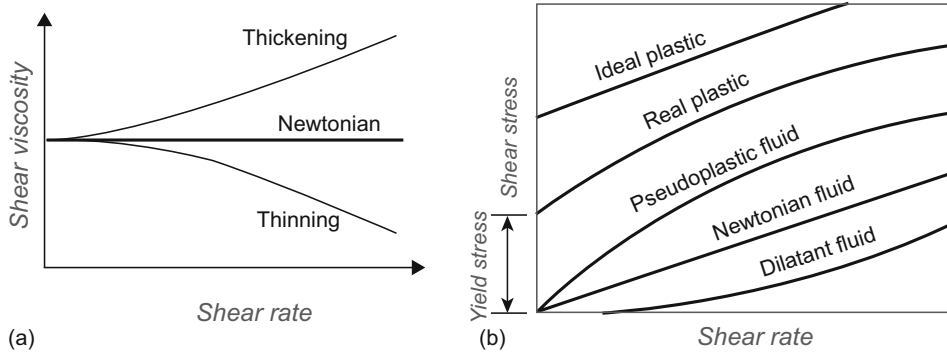
**Figure 2.7** (a) Shear viscosity vs. shear rate and (b) shear stress vs. shear rate

Some fluids, such as suspensions or slurry solutions, usually do not flow under small shear stress. The flow starts when the external force is larger than the yield stress; such a fluid is called a viscoplastic fluid, also known as a Bingham fluid.

Most polymeric fluids can be classified as pseudoplastic fluids. Figure 2.8 shows the dependence of shear rate on shear stress and viscosity for a typical polymeric fluid under shear flow. With increase in shear rate, the polymer chains start to disentangle and align along the direction of flow. The alignment reduces the molecular interactions, as a result of which the viscosity continues decreasing as the shear rate increases, i.e. shear-thinning behavior occurs. When the shear rate gets extremely high, the oriented molecules do not have sufficient time to revert to the coiled state and are completely aligned under the shear stress of the fluid. The flow resistance and viscosity reach the minimum ($\eta_\infty$) theoretically. However, this phenomenon is usually difficult to measure in polymer melts, because the degradation will be very acute under such high shear rates and stress.
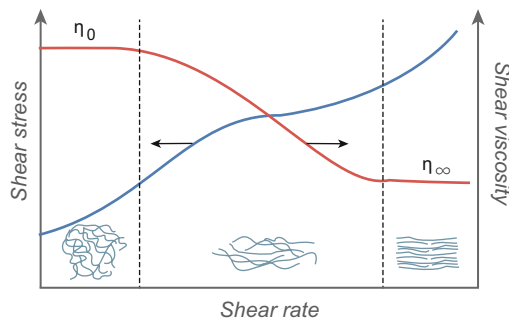


**Figure 2.8** Shear viscosity and shear stress vs. shear rate

### 2.2.1.3 Effects of Temperature

The viscosity of polymeric fluids not only is sensitive to the shear rate, but also changes with temperature. This phenomenon of viscosity changing with temperature is also observed in common Newtonian fluids. As shown in Figure 2.9, the curve of viscosity moves toward the bottom left of the graph as the temperature rises. At higher temperatures, the polymer chains have a larger free volume and mobility and so find it much easier to overcome the interaction energy of molecules. Therefore, raising the processing temperature is commonly used to increase the flowability of polymer melts.
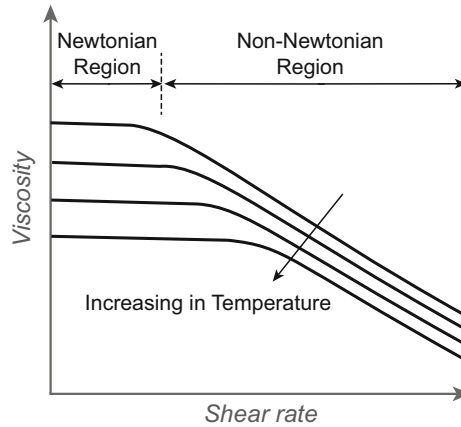


**Figure 2.9** Shear viscosity of various temperatures

To describe the temperature effect on viscosity, the shift factor, $a_T$ is defined as:

$$a_T \equiv \frac{\eta_0(T)}{\eta_0(T_0)} \tag{2.3}$$

where $\eta_0$ is the zero shear rate viscosity under temperature $T$ and $T_0$, respectively.

The viscosity under various temperatures and shear rates can be expressed as the viscosity at reference temperature:

$$\eta(T,\dot{\gamma}) = a_T \eta(T_0, \dot{\gamma} \cdot a_T) \tag{2.4}$$

Commonly, there are two models to describe the relationship between $a_T$ and temperature:

1. Arrhenius-type equation:

$$a_T = \exp\left(\frac{\Delta H}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right) \tag{2.5}$$

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