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## Single-screw Extrusion: Principles

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### 1.1 Introduction

Until recently, single-screw extruders (SSE) have little changed in principle since their invention around 1897. They are mechanically simple devices. A one-piece screw, continuously rotated within a barrel, develops a good quality melt and generates high stable pressures for consistent output. These inherent characteristics, combined with low cost and low maintenance, make it the machine of choice for the production of virtually all extruded products.

Historically, the polymers and particulate they carry (including active pharmaceutical ingredients or API) are subjected to compressive shear-dominated deformation. Compression of particulates, such as API, forces the particulate together into agglomerations under very high pressure *before and during melting*. When this happens, shear deformation is insufficient to break the agglomerations into their constituent parts. Agglomerations within a polymer matrix define a poorly mixed product.

Many ingenious schemes are known to improve the basic screw. Since the 1950s, a variety of mixers have been available. Some of these force material into small spaces for additional shearing. Some divide the flow into many streams so that smaller masses are sheared more effectively. Some make use of pins embedded in the root of the screw and some cut the screw flights. They have one thing in common that limits their effectiveness, however: they are placed after the screw melts the material, and most of a screw is necessarily dedicated to producing a melted polymer. Typically, these mixers are less than four screw diameters long.

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Since around the 1970s, various barrier or melt separation screws became widely available. These force material over a barrier flight of reduced dimension (compared to the main flight), preventing unmelted material from moving downstream. As the material moves over the barrier flight, it receives additional shearing and is therefore mixed a little bit better. Some screws force material back and forth across barriers which also slightly improves the SSE mixing.

To some degree, all of these inventions are incrementally successful. However, they do not change the fundamentals of compression and shear dominance in the SSE. Until recently, the SSE was therefore an agglomerating machine.

Meanwhile, the twin-screw extruder (TSE), and in particular the parallel intermeshing co-rotating TSE<sup>1</sup>, became the dominant continuous compounding mixer for polymers and particulate. This is because it works on a fundamentally different and better principle: *It melts prior to the final compression of the melt*. This means that it prevents agglomeration of the ingredients and has no need to then break up agglomerates formed by compression. Fundamentally, it is not shear dominated. Instead, material moving through the intersection of the screws is extended. Such deformation is elongational. Elongation, instead of pushing API particles together, *pulls them apart*. Unlike the SSEs discussed above, the TSE mixers do not start mixing near the end of the screw. They do not dedicate just a few length-over-diameter or  $L/D$  ratios to mixing; instead, they combine elongational melting and mixing early in the extruder in a first set of kneaders and then repeat the elongational melt-mixing process with additional kneaders. In this way, a substantial part of the TSE length is dedicated to elongational melt-mixing.

However, the TSE has flaws. Not all the material moves through the intermesh region; some material escapes down the channels without moving through the extensional fields. In addition, some material will see the intermesh many times. The key elongational history of the polymer and API will therefore be uneven. Compared to single screws, the TSE is less pressure stable; compared to singles, the TSE does not generate high pressures. (When a gear pump is used to generate high stable pressures they require a sophisticated algorithm that is sensitive to small changes, especially in the starve feeding system.)

Very recently, significant advances in fundamental SSE technology have changed the landscape. Costeux et al. proved in 2011 [1] that the SSE could have dominant elongational flow where melting occurred before compression. There is therefore no need to break up agglomerates. Unlike the TSE, all the material can consistently pass through the elongational mixers. Melting and mixing are started very near the hopper so that a significant part of the total length of the SSE becomes a mixer. These new SSEs retain their advantages of simplicity and low cost. They can still generate high and stable pressures most suitable for hot-melt extrusion (HME) production, even when starve fed without a complex control system.

### 1.2 Ideal Compounding

In order to understand the SSE for HME, we must understand compounding as we will necessarily have at least an API and a polymer. It is undesirable to have local concentrations

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<sup>1</sup> Since this particular TSE dominates the market, the use of TSE throughout this chapter should be understood to mean the parallel intermeshing type.

of API or polymer in the product. Compounding is defined as combining two or more ingredients, but really good compounding has additional requirements. The melt-mixing process should treat the material equally. It should not be overly mixed in one region and under-mixed in another. Mixing should apply the least amount of energy to limit degradation of the components.

Compounding is accomplished by taking local concentrations and reducing them to a satisfactory size where satisfaction depends on the use. This is accomplished by dispersion (breaking solids or globules into smaller concentrations) or distribution (rearrangement of solids or melt).

Local concentrations will occur when polymer pellets are dry-mixed with API. Each pellet is a local concentration that must be distributed to incorporate the API. The API can also be thought of as a local concentration that must be distributed within the polymer pellets. Local concentrations are immediately reduced when working with a powder/powder blend (compared to pellet/powder). The better the mixture, the easier it is for an extruder to further reduce the local concentrations. Nevertheless, no matter how well mixed two powders are, there will be local concentrations at some scale. The job of the extruder is to further reduce these concentrations. This cannot be accomplished through a purely compressive screw since that takes the mixture and, at best, maintains the dry-mix quality<sup>2</sup>. Instead, elongation is required to draw the concentrated regions apart.

An ideal HME mixer would maintain ingredient quality during the compounding process. Both plastics and API degrade due to thermal and mechanical stress. To mix well, there should be an orderly progression through the mixing process that maintains the quality of the ingredients.

Thermally, a single heat history of the shortest possible duration at the lowest temperature is preferred.

Mechanically, an elongationally dominated system, *where all the material has the same elongational history*, is preferred. This will minimize unnecessary mechanical degradation and decrease the thermal processing time to achieve the same result. Since the shear component of the mechanical system builds excessive heat (compared to the elongational component), it should be minimized.

### 1.3 Basics of the Single-screw Extruder

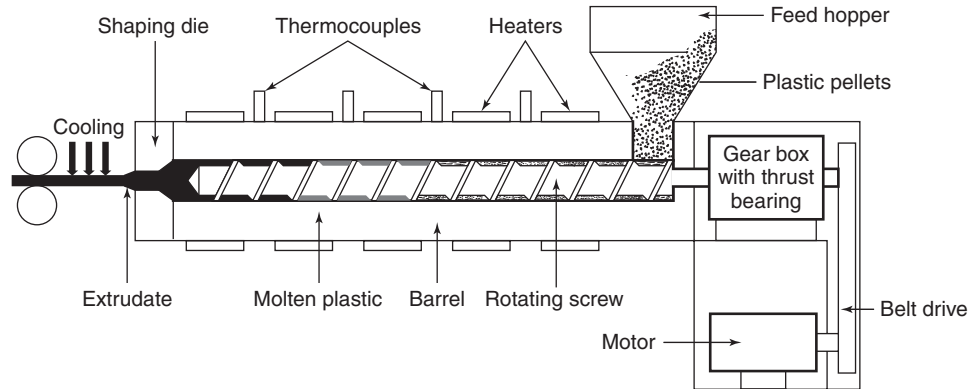
Low bulk density polymer solids, often mixed with various forms of particulate (such as API), most commonly fall from a hopper into a long, continuously rotated extruder screw within a temperature controlled barrel, as depicted in Figure 1.1.

The screw forces the solid material into a decreasing space along the screw at higher temperatures. There the compressed material is pushed up against the heated container (the barrel). The compression both forces the air out of the hopper and melts the material by pushing the material against the hot metal barrel. The dense/molten material is continuously pumped forward through a shaping die. The material exits the die where it is drawn down in a free molten state through a cooling medium until solid while continually pulled.

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<sup>2</sup>Compressive screws, in some circumstances, can take an orderly mix and agglomerate the ingredients. This will occur when the act of squeezing the mixture separates the ingredients. This is more common than is generally realized.

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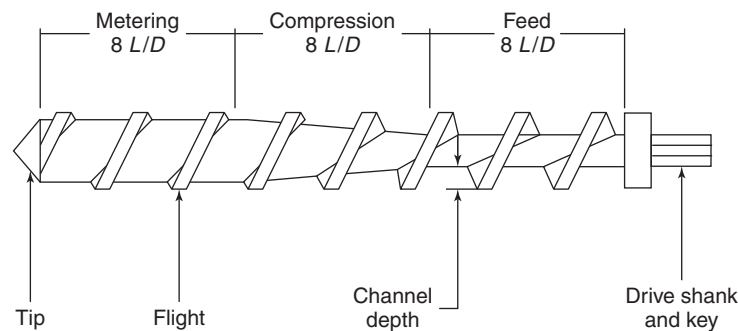
**Figure 1.1** Horizontal SSE driven at feed end.

The key to the process is the extruder screw. While many variations can be considered, the classic screw has a constant diameter. The modern screw length is usually 24–50 times its diameter. This is expressed as the length-over-diameter ratio or  $L/D$  ratio. Screws are, most commonly, made from a solid piece of steel leaving a screw root that is polished. The flights are ground and fit closely within the barrel. Figure 1.2 depicts a general-purpose polymer 24/1  $L/D$  screw.

Typically, the one-piece screw is driven from the right through a simple key on a shaft that fits into the gear reducer of the extruder. The general-purpose screw has a flight pitch equal to the screw diameter. A classic general-purpose screw has three parts (the feed, the compression and the metering section), all of equal length.

Most HME extruders are small and many are used for research and development. Sometimes, the very high API cost prohibits use by any but the smallest SSEs.

Plastic pellets for HME extruders are made in bulk. They are the same size for all extruders, often in the range 0.13–0.19 inch. This means that the channel depth must be sufficiently large for pellets to fit. Otherwise, the pellets will jam when entering the screw and such jamming can break the screw. Screws with a 0.18-inch feed channel depth are



**Figure 1.2** A 24/1  $L/D$  general-purpose screw.

recommended. Extruders for the drive system above are available in sizes as small as 1 inch diameter. Smaller screws with a feed-driven drive system become so weak that even a small upset (such as a single oversized pellet) can cause the screw to break.

For many HME applications, 1 inch extruders are too large because of the cost of formulation in the research and development phase. Smaller screws are available with the recommended 0.18-inch feed channel depth in combination with a second type of drive system.

In Figure 1.2, note that the root diameter of the metering section is much larger than the root of the feed section. The strength of the root increases with the cube of diameter. If the screw is driven through the metering section, the screw itself becomes much stronger since the highest torque is transmitted through the biggest root diameter (as depicted in Figure 1.3). This allows screws as small as 0.625 inch diameter. Since the output of an extruder screw decreases with the square of the diameter, a 0.625 inch extruder will only have one-quarter of the output of a 1-inch diameter extruder, a good thing when ingredients are scarce or expensive.

To prevent material from leaking into the gearbox, a special seal is used (see Figure 1.3). This seal has a reverse flight compared to the main part of the screw. By making the pitch and channel depth small, it becomes much more powerful than the main screw and the HME material itself becomes the seal. The seal is best with two channels, one deep channel and one shallow. Material moves from the deep channel (the fill length is longer for a deep channel) and into the shallow channel and back into the main flow, preventing stagnation.

Such seals are particularly useful for pressure stability. Since they act as an accumulator, they suppress small surges or variations in pressure and output. Once the small surges are dampened, it is then possible to use an automatic pressure controller to maintain the pressure as fine as  $\pm 10$  psi in the barrel [2].

The discharge-driven design is commonly made as a vertical machine. This exposes the screw to the feedstock for easy entry into the screw.

Below the 0.625-inch diameter, screws usually become too weak for the most common pellet sizes. However, smaller extruders are made including 0.5, 0.375 and even 0.25 inch screws. These are built for free-flowing powders or ground pellets. This puts the general lower limits for HME at about 10 grams per hour.

### 1.3.1 Screw Feed Section

Referring to Figure 1.2, the ‘feed’ channel depth (and so the root diameter) is constant and is associated with solids conveying. Temperatures in the feed section are therefore usually set below the melting temperature of the plastic<sup>3</sup>. If the temperatures are set too high, then the material will melt and conveyance (feeding) will stop as material will stick to the screw rather than be conveyed by it.

Pressure in the feed is usually very low and often zero as the screw is acting as a conveyor. Solids conveying needs little torque so accounts for a small percentage of the total motor load.

<sup>3</sup>It is important to realize that the temperature is not directly controlled along the entire length of the screw; only the barrel surrounding the screw is directly temperature controlled.

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**Feed Sections<sup>1</sup>:** Select the feed section that is right for your feed stock, output and pressure stability:

- Standard (smooth bore)
- Classic (smooth bore)
- Aggressive (smooth bore)
- Grooved Bore Series<sup>1</sup>
- Roller Feed (for soft strips)
- Melt Feed (for reactors)

**Screw:** Working L/D 24.1 in standard and custom designs including mixing sections.

**Barrel:** Nitrided stainless steel or bi-metallic lined for corrosion or wear resistance.

**Heated Clamping Plate:** Heaters provide thermal control to prevent freeze-off. Screws secure transfer tube for leak free operation.

**Die:** Available dies include strand, film, monofilament, coextrusion, tubing, and sheet.

**Transfer Tube:** Heated by the barrel and the clamping plate to eliminate cold spots, the transfer tube holds the breaker plate.

**Breaker Plate:** Holds the screen pack in streamlined stainless steel construction.

**Gear Reducer:** Double enveloping, low backlash gearing with high performance integral thrust bearings.

**DC Motor:** Includes tach feedback for uniform speed control.

**Hopper:** Stainless steel (s.s.), optionally sealed for nitrogen purge or powdered feed stocks.

**Feed Section Cooling:** Hardened s.s. features (3) L/D's of directed cooling for positive temperature control of solids conveying.

**Stainless Steel Cover:** Cooling fans are optional for precision temperature control.

**Barrel Heaters:** Standard mica or high temperature mineral filled.

**Type "J" Thermocouple Ports**

**Pressure Port & Rupture Dics<sup>2</sup>:** Pressure measurement before the breaker plate is a recommended option.

**Surge Suppressor<sup>1</sup>:** Automatic surge reduction in every screw.

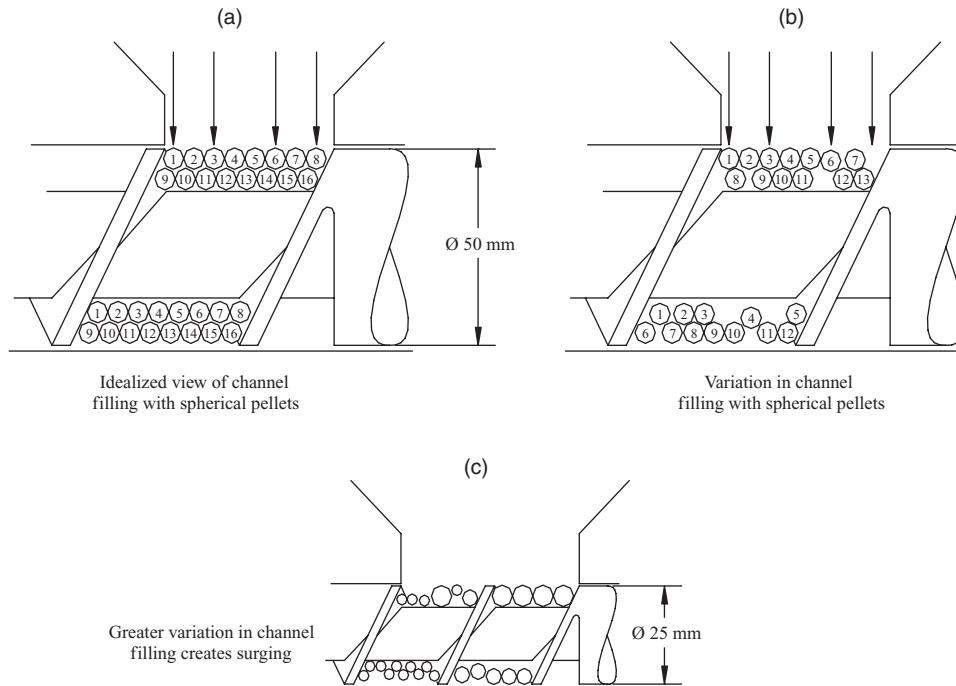
**Barrel Flange:** Change the extruder's output direction<sup>3</sup> by rotating the flange on the gearbox. Flange cooling keeps the gearbox oil cool. Assembly is shown for standard right to left operation.

**Adjust Height and Level:** change the center line of the output as needed on swivel brass pads. Optional mounting system available<sup>3</sup>.

**Figure 1.3** Discharge-driven vertical extruder.

Temperature changes to the feed can cause complex changes in extrusion behavior; they can change the barrel friction, which is the driving force for material transport along the screw which is resistive to flow. Feed temperature is therefore usually optimized to control the solids conveying. This provides the most uniform pressure stability, typically measured at the barrel discharge. When the pressure is unstable, the extruder is said to 'surge' because changes in barrel pressure cause changes in output.

Changes in the feed section temperature of the screw change the amount of preheating of the solids. Higher preheat temperatures (especially in smaller extruders) can mean easier



**Figure 1.4** Idealized feeding in small screws.

material deformation within the decreasing channel of the melting zone, and lower torque which we see as a reduction in motor load. Uniform feeding should not be assumed.

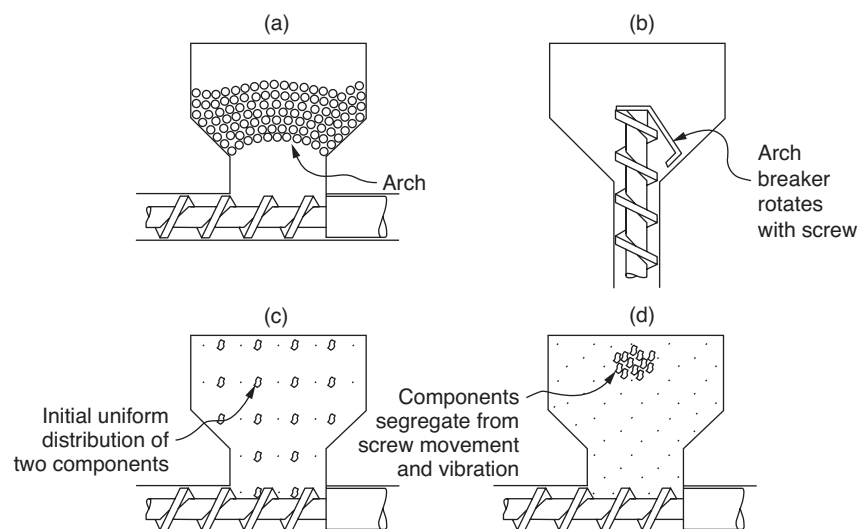
In Figure 1.4a, an idealized (but completely unrealistic) view is shown with each of the perfectly spherical pellets falling perfectly into the screw channel. Figure 1.4b takes a step in an more likely direction, showing gaps between pellets and a small difference in the number of pellets top and bottom of 12–13 (which is not insignificant). Whatever variation exists in the first part of the screw is transferred downstream to some degree.

Figure 1.4c shows a more realistic variation in pellet size. One need only look at a handful of typical pellets to see significant variations in diameter; often the largest is twice the diameter of the smallest. If the pellets were spheres, the mass of the largest pellets would be eight times greater than the smallest pellets. Figure 1.4c shows a large difference (not atypical) in mass in the two flights, as will occur over time. In a large extruder, the average mass is not greatly affected by relative size of the pellets. In smaller extruders, it will cause wide variations in mass transfer and make surging more likely.

Other problems include arching or bridging over the opening, as depicted in Figure 1.5a, and where feeding will cease. This problem can be lessened by adding a stirrer as in Figure 1.5b. It is not only pellets that can arch over the opening but also powders. Ideally, HME materials should be free flowing so that they can easily move into the screw channel. When poured onto a flat plate, they should have an angle of repose of less than 45° [3]. If



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**Figure 1.5** Feedstock arching and material separation.

the angle is much greater, there will be a tendency to compact within the feed section of the barrel or the hopper.

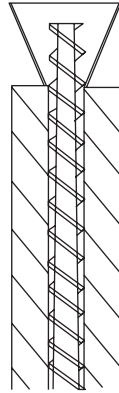
It should not be assumed that a uniform mixture in the hopper will reach the screw channel in the same uniform mixture. Preferential feeding (because of ingredient size or geometry), the motion of the screw or vibration can change a perfectly uniform mixture (Figure 1.5c) and de-mix it before it can reach the screw channel. This can be solved by starve feeding, that is, reducing the input to the screw to less than the maximum it can take by gravity, with multiple feeders. This will reduce the quality of input mixture, which puts greater demands on the extruder compounding.

Once the material reaches the channel, we can consider solids transportation (Figure 1.6). Once the material has moved into the screw channel, it is propelled down the screw by friction. However, it is not the friction of the screw that drives the material forward but the friction of the barrel. Consider the purely theoretical situation depicted in Figure 1.6, where the screw is stationary and the barrel revolves around the screw. It is clear that the friction of the barrel contacts the mixture and would drag it in a circle but, since the screw flights are pitched, the material is dragged forward against the screw.

This is not a very positive system when compared to positive displacement pumps, and is easily defeated. Since higher barrel than screw friction is required, anything that reduces barrel friction will change or even defeat transport. For example, the addition of a small amount of a slippery liquid to a pellet/API mixture will lubricate the barrel. The resistance of the screw can then be higher than the barrel friction and forward motion will stop.

Another important consideration for HME extrusion is the density of the feedstock. Pellets are the most common feedstock for extrusion. For HME extrusion however, there is a natural desire to work with ground or powdered polymers so that the input mixture is better mixed. This almost always reduces the bulk density of the feedstock as ground





Conveyance occurs when barrel friction on the material mixture is higher than the screw's resistance.

**Figure 1.6** Consider friction when visualizing a stationary screw and rotating barrel.

material is irregular and does not stack neatly into a dense form like a pellet. If we imagine a lowered bulk density mixture entering the screw channel as in Figure 1.6, the barrel friction is again reduced until it becomes so low that there will be insufficient friction to overcome the resistance of the screw. Flow will stop when barrel slippage is complete.

While the feed section is particularly sensitive to changes in friction, material is driven forward by friction in all parts of the extruder. It should be recognized that friction is poorly understood and that within the HME extruder friction is very complex, changing with temperature and local conditions.

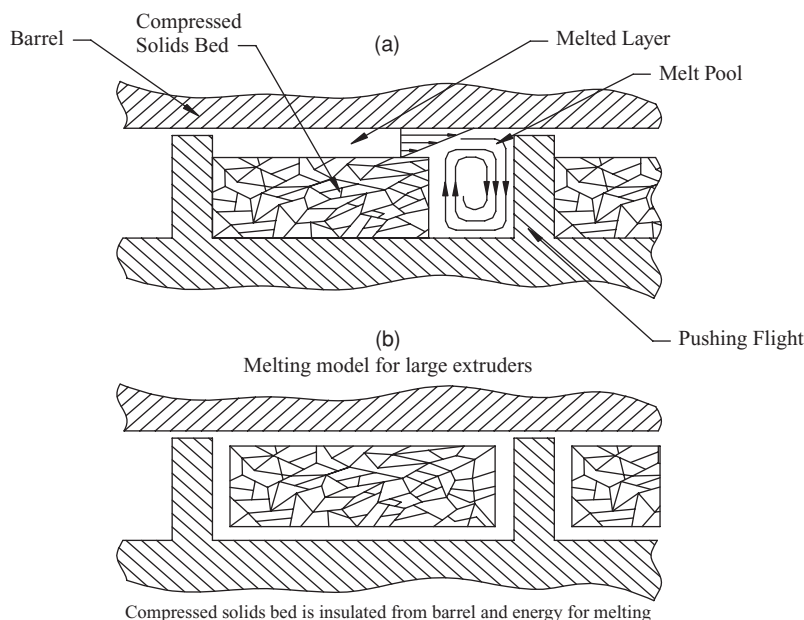
### 1.3.2 Screw Compressor Section

The second third of the general-purpose screw, also called the transition section, has a channel depth that diminishes over its length to one-third of the feed depth. It is then said to have a 3:1 apparent compression ratio (ACR). This part of the screw is associated with melting and removal of air which is pushed out the hopper. Temperatures are typically set to allow ready deformation of the material. This is necessary because the space along the channel is decreasing and, if temperatures are too low, material will jam in the screw. Most such jams are temporary but this stopping and starting is largely responsible for surging. The jamming is reflected in higher screw torque, which we see as higher motor load.

The ACR must be high enough to squeeze out the air from the feedstock, but not so high that it prevents material from flowing to the next section.

The lower bulk density of some HME mixtures also requires a change to the screw. Since there is a lower bulk density in the feed flights, there is also less mass. A 3:1 ACR is general-purpose only because pellets are the most common feedstock. These dense pellets will generally fill the screw once the air is removed during compression and create a stable flow. However, once the bulk density is reduced as described, the 3:1 screw will no longer deliver sufficient material to fill the screw in a stable fashion and the output is likely to surge. For reduced bulk density powder/powder mixtures, a 4:1 ACR is typical.

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**Figure 1.7** Melting model in SSE.

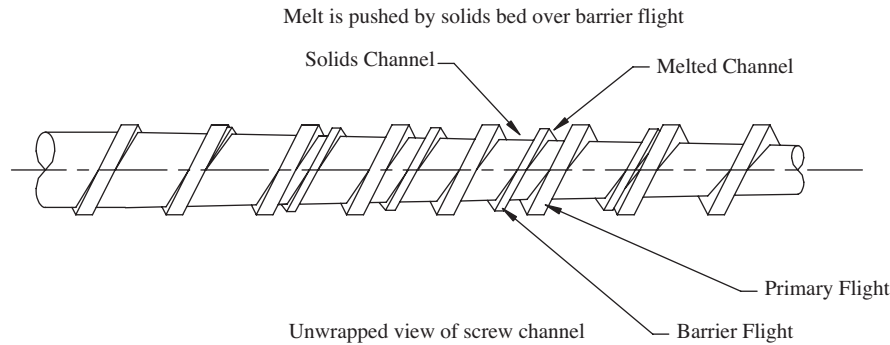
As material is compressed, it is pushed up against the metal barrel and forms a solids bed. It is easy to see that API particulate would be compressed into agglomerates between parts of the solids bed. The portion of the solids bed that is pushed up against the heated metal quickly transfers its energy to the polymer-API mixture and a melted layer forms. Since the polymer beneath this layer is insulated by the melted material itself, heat transfer to the rest of the mass in the channel is slowed. Before it can melt, it is scraped by the advancing flight as depicted in Figure 1.7a.

As screws become larger, the heat transfer from the screw root and flights also transfers energy to the outside of the solids bed (Figure 1.7b), resulting in a cold compressed solids bed that ‘floats’ within melted material. The solids bed is now isolated from metal contact; developing a good-quality melt is now unlikely if this solids bed simply proceeds down-channel.

The solution to the problem is to drain the melt as quickly as it occurs, as shown in Figure 1.8. These screws are called melt-separation screws.<sup>4</sup> The oldest design (the Uniroyal) is depicted in the figure, but a variety of designs are available.

A common problem with barrier screws is compaction of the solids bed such that the solids bed stops moving. This prevents the continual flow of material movement through the screw. This compaction can occur anywhere along the barrier, but is most likely at the beginning and end of the barrier. This can cause surging, gel showers, carbon specs and loss

<sup>4</sup>It is common to refer to these as ‘barrier screws’. However, barrier screws can have other purposes besides separating the melt from the solids bed and for mixing in particular.



**Figure 1.8** The Uniroyal screw design.

of output. Han et al. [4] showed that the removal of part of the first barrier could prevent these problems in some circumstances. Nevertheless, it should be noted that barrier screws increase the compressive force on API with a greater tendency towards agglomerations.

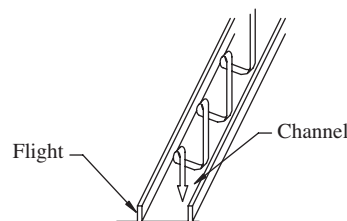
### 1.3.3 Screw Metering Section

Once the materials are melted, they flow through the metering section in molten form. Flow is a combination of the barrel drag flow and pressure flow. The flow is visualized by the straightening of the meter's spiral channel and the barrel is considered as a plane moving across the stationary channel, as in Figure 1.9.

The barrel drags material towards the pushing side of the flight. Since there is only a very small gap between the barrel and screw, material is then driven against the pushing side of the flight, across the screw root and back up the trailing side of the screw. When this is combined with pressure flow in the channel, spiraling occurs. Just as in any tube (in this case a spiraling tube), the centermost material moves forwards more quickly than material at the outside of the tube. The combination of drag flow and pressure flow therefore create, in a very limited way, axial mixing in the metering section.

### 1.3.4 Mixers

A wide variety of mixers can be added before, during or after the metering section either in general-purpose screws or melt-separation screws. Most of these are distributive mixers with little claim to dispersive capability, and are described in the following sections.

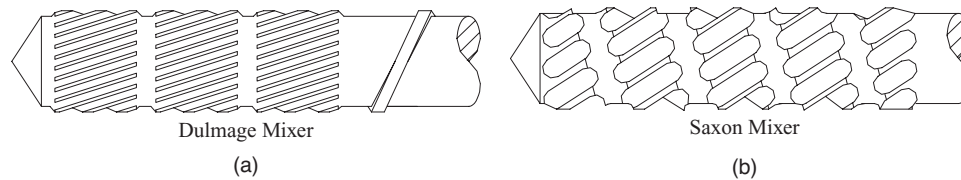


**Figure 1.9** Spiral flow in straightened metering section.

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**Figure 1.10** Pin mixers break up spiral flow.



**Figure 1.11** Slotted mixers for energy exchange.

### 1.3.4.1 Mixing Pins

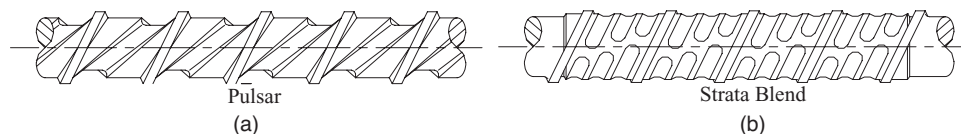
Pins can be placed between flights (most commonly round or diamond-shaped) or in lieu of flights, as shown in Figure 1.10. Pins are often made small in diameter because the greater the number of pins, the more the flow is combined and recombined. However, small pins will bend and can fatigue over time and eventually break. Round pins tend to have an area behind them where materials can stagnate, hence other shapes such as diamonds are used. It should be noted that, unless the diamond-shaped pins are properly oriented in the flow and very close together, they too will have stagnant zones.

### 1.3.4.2 Slotted Mixers

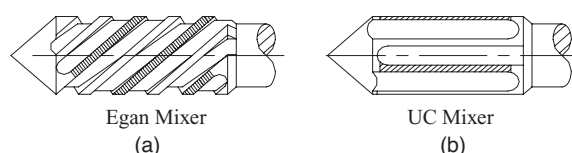
Figures 1.11a and 1.11b show common slotted mixers. The flowing materials are separated into many streams to reduce their large mass into smaller portions. Each small portion rotates in its channel and allows for some heat exchange at the barrel for better thermal mixing before the flows recombine.

### 1.3.4.3 Variable-depth Mixers

Figures 1.12a and 1.12b depict variable-channel-depth mixers. Presumably, these could influence axial mixing by changing the drag flow and pressure flow components referred to in Figure 1.9.



**Figure 1.12** Shifting material by changing root diameter.



**Figure 1.13** Fluted shearing mixers.

#### 1.3.4.4 Shear Mixers

Figures 1.13a and 1.13b depict two long-established mixers where materials are forced through narrow slots for additional shearing, and thought to have mild distributive capability.

### 1.3.5 Limitations of Conventional Single-screw Mixers

Invariably, the question of which of these mixers is the best mixer and under what circumstances arises. The most consistent testing has been by Dow Chemical using the same procedure to compare various screws and mixers. ABS (acrylonitrile, butadiene, styrene) resin is compounded with about 12% white pigment to form an opaque background and pelletized. Then, black color concentrate pellets are added at 0.5–3.0% to the compounded pellets and a strand is made. When the strand is sectioned, black spirals (from the rotation of the screw) appear. Screws with the least distinct spirals are judged best.

At Antec 2010, the author reported [5]

“Very consistent mixer studies include the Maddock [...], Stratablend (trademark New Castle) [...], Energy Transfer [...], Variable Barrier Energy Transfer [...], and the DM2 with Eagle Mixing Tip [...]—generally referred to as high performance screws. One study even includes the more complex Twente mixing ring, the Barr sleeve mixer and a Barr ring mixer [...]. These papers describe a spiraling pattern in the extrudate.”

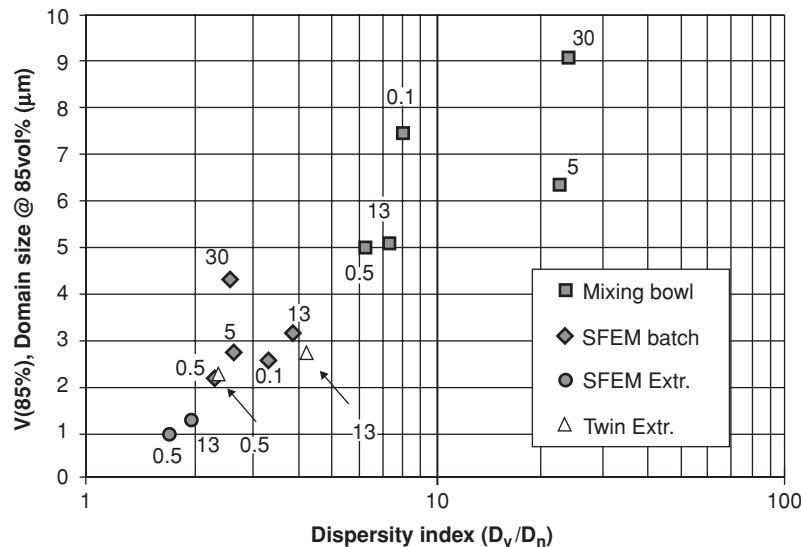
All the screws and mixers lessened the distinct spiral pattern of the control Screw somewhat. However, spiraling patterns were still easy to see in all screws. The conventional SSE, while good at melting and pumping, has therefore not approached the mixing performance of the TSE.

## 1.4 SSE Elongational Mixers

It was generally believed that the SSE could not create substantial elongational flow. By means of its two screws, the TSE readily draws material apart (just as two hands readily draw on the ends of a rubber band to stretch it). The SSE was thought permanently handicapped and therefore incapable of significant stretching flow.

Imagine two counter-rotating metal rolls with a small gap between them. Material (such as rubber, molten polymer or a man’s tie) will be drawn into the inlet and expelled on the other. If only one roll is driven, material is still pulled in and expelled; only one surface therefore needs to move to form a pump. A single screw has a moving surface so it is possible to create a pump.

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**Figure 1.14** Quantified mixing (courtesy of Dow Chemical, Antec 2011).

Such pumps can be defeated by pushing more material into the roll gap above than it can remove. The same moving surfaces become resistive to flow. The greater the force applied to push material through the ex-pump, the greater the resistance and the higher the temperature rise. Similarly, the most popular screw designs (the barrier screws, Egan and UC mixers) are intended to work by pushing material through a small gap.

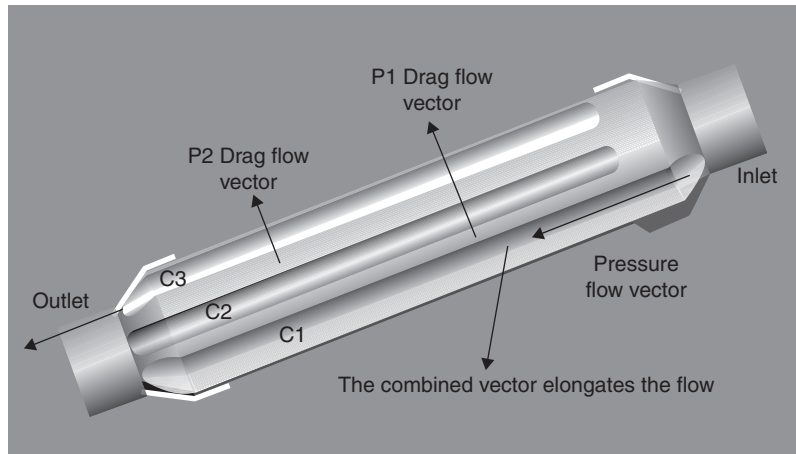
A member of the newer class of elongationally dominant screws was tested using a similar procedure of testing black color concentrates against a pigmented background. This screw has a series of three spiral flow elongational mixers (SFEM) on the screw and is called an Elongator. Even at 200 times magnification, no spiral patterns were found.

This is not surprising. Work had been presented showing a much finer scale of mixing than spirals in rod seen by eye. For example, in 2007 [6] polystyrene was mixed with polyethylene and shown to disperse to 1  $\mu m$  scale, carbon nano-tubes and ceramic particulate were distributed to the 500 nm scale.

While pictures at very high magnification are helpful, quantitative mixing comparisons have remained elusive. However, at Antec 2011, Costeux et al. [1] presented a paper that quantified mixtures from four different processing tools. It shows that the SFEM Elongator is elongationally dominant because it breaks down blends of high viscosity ratios that cannot be dispersed by shear alone.

Figure 1.14 is a plot of mixtures processed on four different mixers: two batch and two continuous. The numbers indicate the MI (melt index) of the PE component in the 70% PP (polypropylene) 30% PE (polyethylene) blend.

The vertical axis shows the distribution of the minor phase domains. Domains are actually like spheres: the lower the number, the smaller the diameter and the better the mixing. The horizontal axis shows the domain volume divided by the number of domains. The lower the dispersity index, the more uniform the domains.



**Figure 1.15** Flow vectors in AFEM Recirculator.

An atomic force microscope (AFM) was used to examine the samples and the minor phase domains were then digitized. Mixing was quantified by digitizing the domains of the minor phase and applying image analysis to extract 3D domain distributions.

The plot shows that the SFEM batch mixer mixed better than the mixing bowl batch mixer. For the continuous devices, the SFEM single screw was superior to the twin.

It is important to remember that these domains are spherical. The volume of a sphere decreases rapidly with diameter. If the diameter of a sphere is reduced by half, its volume is reduced by an eighth. If the mixing bowl makes spheres with a diameter of  $5\text{ }\mu\text{m}$  (as in the 0.5 MI material), they will have volume of  $65.5\text{ }\mu\text{m}^3$ . Both the twin-screw and the SFEM batch mixer made  $2\text{ }\mu\text{m}$  diameter spheres of the same material with a volume of  $4.2\text{ }\mu\text{m}^3$ , making 15 times as many smaller spheres than the bowl mixer. The twin-screw and SFEM batch mixer therefore disperse 15 times better than the mixing bowl.

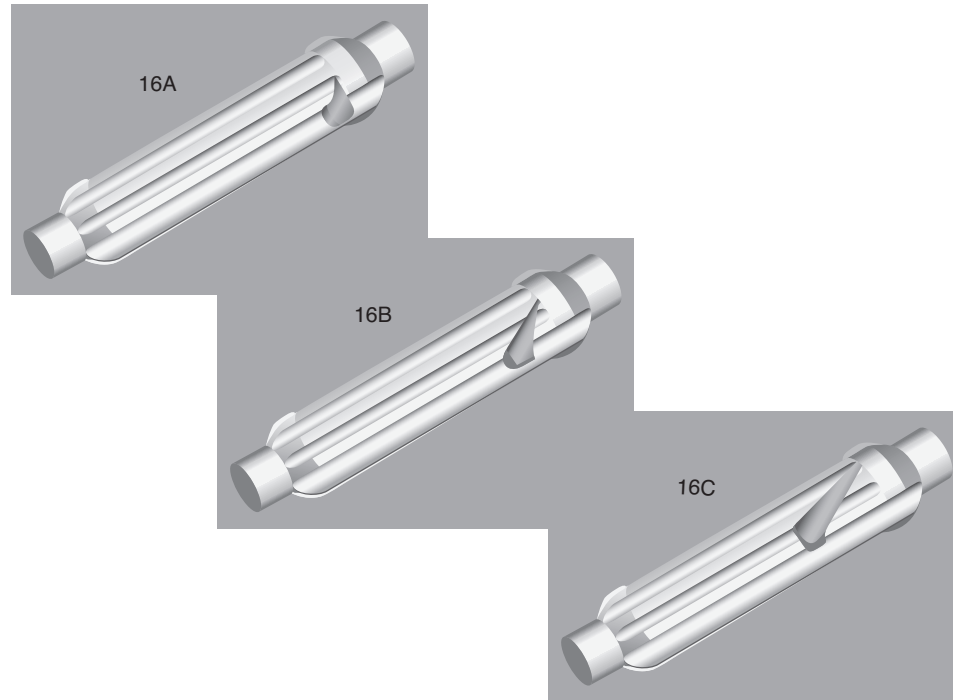
Likewise, since the SFEM Elongator screw mixer made  $1\text{ }\mu\text{m}$  domains (a volume of  $0.5\text{ }\mu\text{m}^3$ ) for the same material, the SFEM Elongator mixed 8 times better than the twin-screw. This new class of mixers can therefore mix particulate and polymers in ways that have not been possible previously.

There are two types of elongational mixers: the SFEM Elongator and the AFEM (axial fluted elongation mixer) Recirculator (Figure 1.15). The AFEM Elongator has a first axial channel (C1) next to a first pump (P1). Although P1 has the same geometry as a barrier, it has a different behavior than a barrier. A barrier screw forces material over the barrier in an attempt to shear the material, which requires a great deal of pressure. However, if the pressure is low in the channel, then the same barrier geometry becomes a pump which pulls on viscous materials.

Elongational flow is created as the material moves down the first channel (pushed down the channel by pressure flow) and is pulled by the pump by drag flow at an angle. The pressure flow moves in the direction of the inlet vector down the C1 channel (parallel to the screw axis) while the drag flow moves the material at  $90^\circ$  (a right angle to the screw



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**Figure 1.16** The length of the plane (compared to its width) increases as the C1 channel is increasingly starved. The width can increase to the limit of the P1 pumping capacity.

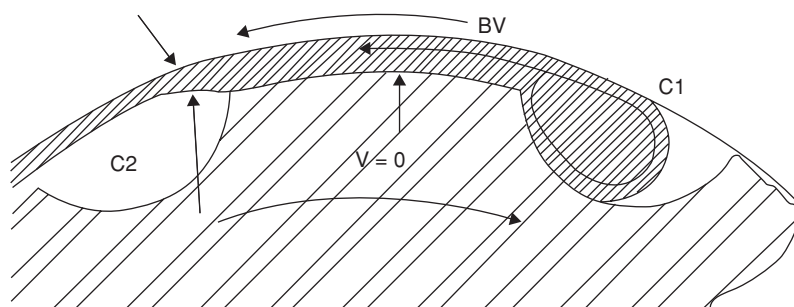
axis) as shown by the drag flow vector. The combined vector is  $45^\circ$  when the vectors are of equal length; this becomes stretched.

When the P1 pumping capacity is higher than the input to the channel, 100% of the material is stretched as it moves to the pump. The drag flow pumping capacity is easily kept higher than the input to the channel by starve feeding. The fill length of C1 depends on the amount of starve feeding. If the pump's capacity is exceeded, some material can flow out the end of C1 and not be stretched.

A colored section of material (representing a local concentration of API), surrounded by clear material entering C1, will be drawn by P1 at the entry as shown in Figure 1.16. This section will start to deform into a plane as shown in Figure 1.16a. As the local concentration moves down the channel, the mass in the channel is reduced and the plane becomes larger as in Figure 1.16a. Eventually, the entire local concentration of API is converted into a plane. This can be thought of as the short local cylinder becoming a wider and longer flat surface.

While Figure 1.16 is representative, the actual plane created in the transverse direction is much more elongated than shown.

The process begins with shear as shown in Figure 1.17. Because the pressure is near zero in C1, the flow over P1 is nearly pure shear. This is very unlike the flow over a barrier flight which is primarily pressure flow, necessary to force material over the barrier. Pressure flow



**Figure 1.17** Film stretches again over C2.

does not contribute much to mixing. Instead this ‘pure’ shear flow reorients the material as the material sticks to the barrel and the screw. This reorganizes the flow and further distributes the API.

After the shear flow, material reaches a second channel C2 which lowers the resistance of the screw drastically on the material near the screw. However, it does not change the adhesion to the barrel. This creates a powerful 2D stretching and converts the material into a thin film at the two arrows in Figure 1.17.

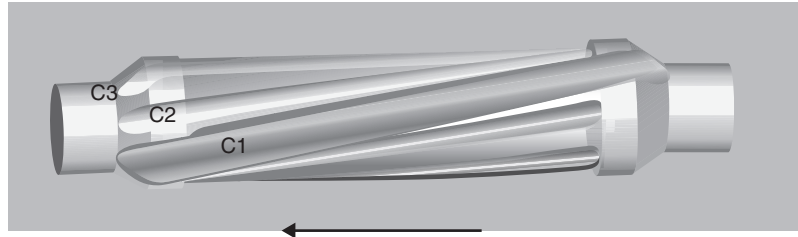
The thin film at zero pressure is useful for degassing when a volatile is present. A hole can be placed in the barrel and the gas extracted from the thin film by pressure flow towards the downstream flight. The pressure may also push material into the empty end (the end away from the hopper) of the C2 and C3 channels. In this case, some material can move upstream in the C2 and C3 channels and recirculate. The amount of recirculation depends on the distance from the AFEM Recirculator to the downstream flight and the amount of C1 fill. If the C1 channel is very starved, there can be more recirculatory flow than input flow. This is usually only advantageous for extremely difficult mixing problems (such as nano-compounding) rather than HME applications. If the C1 fill is greater than the capacity of P1, then there will be no recirculation and material can exit C1.

There is another useful feature of the AFEM Recirculator. During an upward surge in pressure, the fill length of C1 will lengthen and will shorten during the trough of the surge. The mixer will therefore act as an accumulator and will dampen pressure and flow instabilities. Each additional mixer increases the dampening to make the final flow surprisingly stable, even when the screw is starve fed.

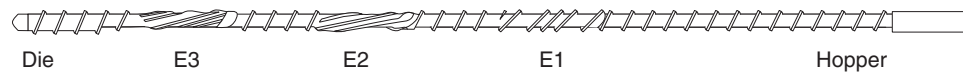
The second type of screw in this class is the SFEM Elongator, as shown in Figure 1.18. The design is very similar to the AFEM Recirculator, but has a pitched design and flights connected to the mixer. The pitch increases the forwarding ability of the screw, which minimizes the residence time within the screw. The connected flights mean that the output of any channel flows immediately onto a flight and then moves downstream. Recirculation therefore does not occur, which makes the SFEM Elongator better for most HME applications. Figure 1.18 has two sets of C1, P1, C2, P2, C3 surrounded by a flight clearance.

Most of the same principles outlined for the AFEM Recirculator apply to the SFEM Elongator. That is, the first channel has 3D elongation, the first pump has shear undiminished by pressure flow to reorganize the material top to bottom and it has 2D stretching as the

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**Figure 1.18** The SFEM Elongator stretches but does not recirculate.



**Figure 1.19**

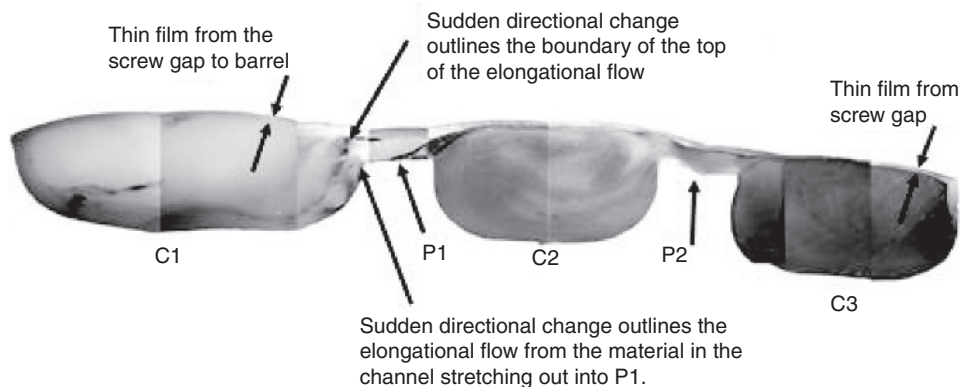
material moves from P1 to P2 over the second channel. When the material is pumped from C3, the material moves immediately onto the connected downstream flight and is forwarded so that recirculation does not occur, keeping the residence time short.

The stretching flows in the channels have been observed. This is done by mixing color concentrate into the polymer, stopping the screw and cooling the material as quickly as possible on the screw. The stretching flows are preserved by the color within the cooled pullouts. This is more easily observed for flood-fed conditions where the C2 channel is filled. This makes extraction of the cold screw and subsequent sectioning easier. Figure 1.19 depicts the schematic of the SFEM Elongator screw.

The thick frozen section shown in Figure 1.20 is from the second of three Elongators (E2) where 2% blue color concentrate was mixed with polypropylene [1]. The arrows point to the material's movement downstream within the channels. Traces of color on the root of the screw show the angle of rotation within the C2 and C3 channel.



**Figure 1.20** A thick frozen section that was cooled and then removed from the screw. For a better understanding of the figure, please refer to the color section.



**Figure 1.21** A composite of nine pictures shows the elongational mixing flows. For a better understanding of the figure, please refer to the color section.

Figure 1.21 is the same cross-section as shown in Figure 1.20, but thin-sectioned and magnified for additional detail by stitching together 8 separate pictures. A dramatic difference in the quality of the mixture is seen as the material moves from C1 to C2 and from C2 to C3.

Flights of the screw are located to the far left and far right of the cold pull-out in Figure 1.21. These flights have a clearance to the barrel of about 0.004 inch. Material ‘leaks’ through the gap and is seen as a thin film. This film is dragged along by the barrel through the mixer until finally disappearing in C3.

In C1, the individual pellets are not visible as they are in a typical compressed solids bed of material. Instead, having flowed through E1 and the following channels, the material arrives in C1 as a highly viscous melt.

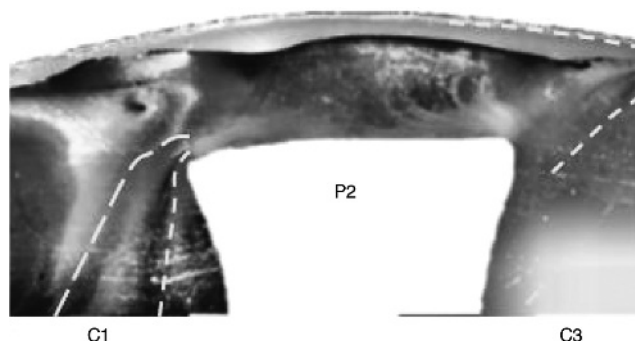
Material in C1 is then dragged to the right towards P1. The two arrows within C1 outline the boundaries of the elongational flow as the material approaches P1. Within P1, shear flow occurs. Immediately after P1, the exiting material is dragged into a very thin layer just beneath the leakage flow material. This is the stretching flow that is primarily 2D and greatly extends the material because of the high barrel velocity. The thickness of this stretched material appears much less than the leakage flow thickness.

A similar process occurs as material moves from C2 and approaches P2, as depicted in Figure 1.22. Material over P2 must now contain the material in C3 so it is not sheared in the same way as P1, as can be seen by the flow lines in P2 and the change in the leakage flow dimensions. The material near the output of P2 elongates and converges, as shown by the dotted lines. This is similar to the flow immediately after P1.

In an HME extruder, starve feeding is preferred to flood feeding. Flood feeding fills the screw to its maximum capacity from the hopper. Flood feeding can allow compression of the API before the first SFEM Elongator and can cause agglomeration.

Starve feeding uses various volumetric feeders or a gravimetric feeder to limit the flow into the screw. Because the flow in the solids channel is less than the capacity of the screw, the partially empty channel has no pressure on the API. This prevents compression and

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**Figure 1.22** Dotted lines show the converging (extensional) mixing flows at P2. For a better understanding of the figure, please refer to the color section.

agglomeration before the material enters C1. By feeding at a rate less than the P1 capacity, C1 will empty, C2 will not fill as in the flood-fed example above and all the processed material will move into C3. It will then have the same thermal and mechanical processing history. Since the system is elongationally dominant (rather than shear dominant) it will have the lowest energy input to accomplish the mixing.

### 1.5 Summary

To compound well means to mix all the ingredients with the same thermal and mechanical heat history using the least amount of energy. A bell curve showing the number of mixing cycles does not describe an orderly mixing process. The TSE by adding more mixers to increase the amount of material moving through a brief extensional field, creates a the greater the disparity between the over-mixed and the non-mixed ingredients. A good compounder requires a mixer that treats all the input in a predictable, orderly fashion.

The AFEM Recirculator is best used for mixtures where the API is extremely small or of low concentration and where the ingredients are thermally stable and can withstand a longer residence time.

The SFEM Elongator SSE is a most orderly compounder and is best for thermally sensitive materials and where venting is necessary. It accepts a disorderly mixture with local concentrations and methodically organizes it by elongating all of the input in the same way. The modern elongational SSE limits the amount of mixing to what is needed to achieve a certain goal. Because of its ability to exert elongational forces from the beginning of the cycle, the proper amount of mixing can be applied which limits the thermal and mechanical processing history.

The SSE is a low-cost processor that can compound and develop sufficiently high and stable pressures to make an HME product from a single heat history. When fitted with elongational screw technology, the SSE mixes as well as and better than any of the other technologies.

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