DESIGN OF DISPERSIVE MIXING DEVICES

Chris Rauwendaal, Rauwendaal Extrusion Engineering, Inc.
Tim Osswald, University of Wisconsin, Madison
Paul Gramann and Bruce Davis, The Madison Group

ABSTRACT

Mixing is one of the main functions of screw extruders. In the analysis of mixing, there are two mixing mechanisms that need to be considered: distributive and dispersive mixing. It is well known that single screw extruders generally have poor dispersive mixing capability, even when dispersive mixing elements are incorporated into the screw design. This paper will discuss the requirements for dispersive mixing, current dispersive mixing elements used in single screw extruders will be analyzed, and the lack of efficient dispersive mixing will be explained. A new generation of dispersive mixing elements will be introduced for use in both single and twin screw extruders and internal mixers. A two and three dimensional flow simulation will be used to analyze the mixing performance of these new mixers. Experimental work on the new mixing elements will be also be presented; the results demonstrate that it is possible to achieve dispersive mixing on single screw extruders that is as good as what can be achieved on twin screw extruders. The implications of these results on the compounding industry will be briefly discussed.

INTRODUCTION

Single screw extruders with simple conveying screws have poor mixing capability (1, 2). To improve the mixing capability, mixing sections are often incorporated in the screw design. The most commonly used distributive mixing elements are pin mixers, slotted flight mixers, and cavity mixers. Commonly used dispersive mixing elements are blister rings and fluted mixing sections. Even though various dispersive mixing elements have been available since the 1960s, the dispersive mixing ability of single screw extruders is rather poor compared to that of twin screw compounding extruders. In this paper, we will examine the limitations of current dispersive mixers and introduce a new generation of dispersive mixers that will allow single screw extruders to match or better the dispersive mixing ability of twin screw extruders.

LIMITATIONS OF CURRENT DISPERSIVE MIXERS

Important requirements for dispersive mixing elements were formulated by Rauwendaal (1, 8); they are:

A. The mixing section should have a high stress region, HSR, where the material is subjected to high, preferably elongational, stresses to break down agglomerates and droplets.
B. The HSR should be designed such that the exposure to high shear stresses occurs only for a short time to avoid excessive power consumption and melt temperature rise.
C. All fluid elements should experience the same high stress level multiple times to achieve uniform and efficient mixing.

If we analyze current dispersive mixers based on these requirements, we find that most current dispersive mixers only meet these requirements partially.

The most commonly used dispersive mixer in single screw extruders is the LeRoy mixer (3), popularized by Maddock. There are several versions of the fluted mixing section (1) commercially available, with the helical LeRoy being a popular mixing section because of its low pressure drop and good streamlining. Like the LeRoy mixer, most current dispersive mixers rely on shear stresses to achieve breakdown of the agglomerates. However, since elongational flow has open streamlines and generates higher stresses, it is more effective in breaking down agglomerates and droplets (4). Therefore, elongational stresses are preferred in a dispersive mixer. A new dispersive mixer based on the generation of elongational flow was developed at the NRC in Montreal, Canada (5). This extensional flow mixer (EFM) is placed at the discharge end of an extruder and the flow through the mixer is pressure driven.

In most current, shear flow, dispersive mixers the material passes through the HSR only once; thus, severely limiting the level of dispersion that can be achieved. To achieve a fine level of dispersion it is generally necessary for the agglomerates or droplets to be broken down several times. Therefore, a single pass through a high stress region is not sufficient in most cases and multiple passes through a high stress region are critical. If the agglomerate is of the order of 1000 μm and needs to be reduced to the 1 μm level, it will take about 10 rupture events if we assume that each rupture event reduces the agglomerate size by 50 percent. It should be noted that drop breakup does not always reduce the drop size by 50 percent. The most efficient mechanism for dispersing liquids is to deform droplets into extended threads at high Capillarity number at let them disintegrate into smaller droplets. The droplets that form can be much smaller than the initial droplet size – formation of over 10,000 droplets from a single drop has been reported.

If each pass through a high stress region produces one rupture, then it becomes clear that a dispersive mixer that exposes the polymer melt to only one high stress exposure is not likely to achieve a fine level of dispersion. This is an important reason why current dispersive mixers in single screw extruders generally do not work well. The lack of strong elongational flow and multiple passes through the HSRs explains why current dispersive mixers for single screw extruders have limited dispersive mixing capability.

NEW DISPERSIVE MIXERS FOR SINGLE SCREW EXTRUDERS

With the requirements formulated above, new geometries have been developed that substantially improve dispersive mixing; a patent application for this new dispersive mixing technology is pending. These mixers, called CRD mixers, can be incorporated along the extruder screw. As stated earlier, the key to the enhanced mixing efficiency is the generation of elongational flow in the high stress regions and achieving multiple passes of all fluid elements through the HSRs.

Elongational flow is not easily achieved in screw extruders. It is generated most efficiently by modifying the leading flight flanks of a mixing section such that the space between the flank and the barrel becomes wedge shaped. Such geometries create lobal mixing and have been used in twin screw extruders (6). This can be done by either slanting the leading flight flank or by using a curved flight flank geometry as shown in figure 1. Multiple passes through the HSRs can be achieved by using a multi-flighted geometry combined with a generous flight clearance. A possible geometry is shown in figure 2.

In order to achieve multiple passes through the HSRs, they should be designed such that significant flow takes place through them. This issue was studied by Tadmor and Manas-Zloczower (2). Substantial flow through the HSR can be achieved by increasing the flight clearance. However, this is only part of the story because without randomization of the polymer melt, increasing the flight clearance will only result in mixing of the outer recirculating region (1). Another problem with a large flight clearance is that it leaves a thick stagnant layer of polymer melt on the barrel surface. Using at least one wiping flight in addition to the mixing flights can circumvent this problem. An early version of the CRD mixer is shown in figure 3. Instead of incorporating separate wiping and conveying flights, it is possible to use one or more flights that incorporate wiping and mixing segments along their length. A possible geometry is shown in figure 4. Complete barrel wiping can be achieved by making sure that at least one wiping flight segment is present at every axial position along the mixer.

By intentionally incorporating distributive mixing in the dispersive mixer, randomization of the fluid elements can be achieved. This gives each fluid element equal chance to experience the dispersive lobal mixing action. Without this, only fluid elements in the outer recirculating region (shell) would participate in the dispersive mixing process (1, 7). The slotted geometry shown in figures 2-4 has proven to be quite effective for distributive mixing (8). The helix angle of the mixing flights can be positive, negative, and even zero. It is possible to use elements with 90° helix angle and stagger the elements to achieve forward or rearward conveying, similar to kneading blocks in co-rotating twin screw extruders. The difference is that the dispersion disks can be designed to achieve maximum dispersion without the geometric constraints associated with self-wiping action (1). An example of a collection of staggered dispersion disks is shown in figure 5.

The mixer should be designed such that all fluid elements are exposed to a minimum number of passes through the high stress region. This requires a high enough flow rate through the high stress regions and efficient distributive mixing. Determination of the appropriate clearance of the mixing flights is discussed in the next section.

DETERMINING THE PROPER CLEARANCE VALUE WITH RESPECT TO FLOW RATE

According to Tadmor and Manas-Zloczower (2) the passage distribution function can be written as:

$$G_k = \frac{\lambda^k e^{-\lambda}}{k!} \qquad (1)$$

where k is the number of passes through the clearance, the dimensionless time $\lambda = t_r / \bar{t}$ is the ratio of the residence time t_r and the mean residence time $\bar{t}$ of the controlled volume. The residence time for a Newtonian fluid can be approximated as follows:

$$t_r = \frac{2z}{v_{bz}(1-r)} \qquad (2)$$

where z is the helical length of the screw section considered, v_{bz} the down-channel barrel velocity, and r the throttle ratio (pressure flow rate divided by drag flow rate). The mean residence time is the ratio of the controlled volume $WH\Delta z$ to the volumetric leakage flow rate over the flight; it can be determined from:

$$\bar{t} = \frac{2WH}{\delta v_{bx}\left(1 + \frac{W}{w_f}\frac{\delta^2}{H^2}\right)} \tag{3}$$

where W is the channel width, H the channel depth, δ the radial flight clearance, v_{bx} the cross-channel barrel velocity, and w_f the flight width. The dimensionless time can be written as:

$$\lambda = \frac{L\delta\left(1 + \frac{W}{w_f}\frac{\delta^2}{H^2}\right)}{WH(1-r)\cos\phi} \tag{4}$$

where L is the axial length corresponding to down-channel distance z. The fraction of the fluid experiencing zero passes through the clearance is:

$$G_0 = e^{-\lambda} \tag{5}$$

The G_0 fraction should be low to ensure that most of the fluid experiences at least one or more passes through the clearance. In single screw extruders with a simple conveying screw the λ value is typically about 0.1. This corresponds to a G_0 fraction of around 0.9. In this case, most of the fluid passes through the extruder without ever passing through the clearance. The passage distribution function for this case is shown in figure 6.

We can use the expressions above to determine the minimum λ value that will yield a G_0 less than 0.01, meaning that less than one percent of the fluid will not pass through the clearance at all. This is achieved when the dimensionless time $\lambda > 4.6$. For certain values of L, H, W, r, φ, w_f we can then determine how large the flight clearance δ has to be to make $\lambda > 4.6$ or $G_0 < 0.01$. The passage distribution function for $\lambda = 4.6$ is shown in figure 7. The distribution at $\lambda = 4.6$ is quite different from that at $\lambda = 0.1$. With $\lambda = 4.6$, the G_0 fraction is quite low and most of the fluid experiences 4 passes through the HSR. The value G_4 is about 0.19; this means that about 19 percent of the fluid passes through the HSR 4 times.

When L=3W, r=0, and $\phi = 17.67°$, the ratio of δ/H has to be about 0.8 to achieve a $G_0 < 0.01$. Clearly, with such a high ratio of δ/H it will be almost impossible to create large stresses in the clearance and to accomplish effective dispersive mixing. From equation 4 it is clear what geometric variables we have to change to achieve a low G_0 fraction at a small clearance. We can do this by 1) increasing L, the length of the mixing section, 2) increasing φ, the helix angle, 3) reducing w_f, the width of the flight, and 4) increasing the number of flights. Increasing the number of flights reduces the channel width, W.

If we increase the helix angle from 17.67 to 60 degrees with the other values being the same, the δ/H ratio has to be about 0.35 or greater for the G_0 fraction to be less than 0.01. This value is still rather large, but substantially better than 0.8. The δ/H ratio can be further reduced by increasing the length of the mixing section or reducing the flight width or by increasing the helix angle even more. The point is that this procedure allows a first order determination of the design variables. Further refinement of the initial values can be obtained from computer simulation.

DETERMINING THE PROPER CLEARANCE VALUE WITH RESPECT TO STRESS LEVEL

Another important requirement for dispersive mixing is that the stresses generated in the HSR are high enough to achieve rupture of the agglomerate or droplet. The highest shear stresses occur in the region where the mixing flight has the smallest flight clearance. The shear rate at this point can be expressed as:

$$\dot{\gamma} = \frac{\pi D N}{\delta} \tag{6}$$

If the shear viscosity of the polymer melt is η_s, the maximum shear stress can be written as:

$$\tau_{max} = \frac{\pi \eta_s D N}{\delta} \tag{7}$$

If the critical shear stress required for rupture is τ_{crit}, the maximum flight clearance that can achieve dispersion can be expressed as:

$$\delta_{max} = \frac{\pi \eta_s D N}{\tau_{crit}} \tag{8}$$

If the viscosity is η_s=500 Pa-sec, the screw diameter D=120 mm, the screw speed N=1.5 rev/sec, and the critical shear stress τ_{crit}=140,000 Pa, then the maximum clearance of the mixing flight is δ_{max}=2 mm.

DETERMINING THE PROPER FLIGHT FLANK GEOMETRY

As explained earlier, for efficient dispersion it is more important to achieve elongational stresses than shear stresses. Elongational stresses are generated in the wedge-shaped region between the pushing flight flank and the barrel. The elongation rate in the wedge can be obtained by using a procedure suggested by Cogswell (9) and further developed by Tadmor (10). The average stretch rate close to the entrance of the flight clearance can thus be written as:

$$\dot{\varepsilon} \approx \frac{(1+r_d)\pi D N \delta \tan\alpha}{H^2} \tag{9}$$

where α is the wedge angle between the pushing flight flank and the barrel surface and r_d the throttle ratio (pressure flow rate divided by drag flow rate)

The elongational stress can thus be expressed as:

$$\sigma \approx \frac{(1+r_d)\pi DN\delta\eta_e \tan\alpha}{H^2} \tag{10}$$

where η_e is the elongational viscosity

If the critical elongational stress required for rupture is σ_{crit}, the following inequality must be satisfied for dispersion to occur:

$$\frac{(1+r_d)\pi DN\delta\eta_e \tan\alpha}{H^2} \geq \sigma_{crit} \tag{11}$$

From this expression the critical parameters for the flight flank geometry can be determined. Unfortunately, expressions 9-11 are valid only for small values of the wedge angle α. As a result, these expressions have limited usefulness. If we assume that the drag flow in the channel is forced through the flight clearance, the average stretch rate can be approximated by:

$$\dot{\varepsilon} \approx \frac{\pi DN \tan\alpha}{2\delta} \tag{12}$$

With this expression, we can determine a maximum flight clearance for dispersive mixing based on the requirement that the elongational stress must be greater than the critical elongational stress. This leads to the following expression:

$$\delta_{max} = \frac{\pi DN\eta_e \tan\alpha}{2\sigma_{crit}} \tag{13}$$

If the diameter D=120 mm, the screw speed N=1.5 rev/sec, the elongational viscosity η_e=1,500 Pa-sec, α=30 degrees, and the critical elongational stress σ_{crit}=100,000 Pa, then the maximum flight clearance is δ_{max}=2.45 mm. The expressions above can be used for a first order approximation of the critical geometrical parameters of the mixer. For accurate determination, numerical techniques are necessary to capture the complexity of actual flow.

SLOT GEOMETRY

The slots in the mixing section can be used to achieve efficient distributive mixing, similar to mixing in a Saxton (11) mixing section. The slot geometry typically used in distributive mixers is a straight slot. For dispersive mixing, however, it is better to use a tapered slot because this will create additional elongational flow as material passes through the slot. The geometry of the slot can be made such that the flight maintains full wiping capability. The geometry of the slotted flight is shown in figure 8.

The flight maintains complete wiping capability when the axial component of the pushing slot flank, L_{f2}, is greater than the axial slot width, L_s. This is the case when:

$$\sin^2 f_f \cot f_{s2} + \sin f_f \cos f_s \leq \frac{w_f}{w_s} \quad (14)$$

When the flight helix angle f_f=45 degrees, the inequality simplifies to:

$$\cot f_{s2} + 1 \leq 2 w_f / w_s \quad (15)$$

Figure 9 shows the smallest values of the slot flank angle for which the inequality above is satisfied. As figure 9 indicates, the slot flank angle must be increased as the ratio of flight width to slot width ratio decreases. When the slot width is twice the flight width, the slot flank angle has to be 90 degrees to maintain full wiping. As a result, this will be the smallest value of the width ratio that will be practical. The preferred range of the flight to slot width ratio is from 1:1 to 3:1.

COMPUTER SIMULATION

The analytical approach to mixer design has some severe limitations because of the difficulties in analyzing flow in a complicated mixer geometry. A better approach to analyze complicated mixers is to use mathematical modeling and computer simulation. One simulation tool that lends itself well to the analysis of complicated mixer geometries is the boundary element method (BEM). This method allows a determination of the optimum value of the flight clearance, flight flank geometry, and spacing of the slots to achieve the proper combination of dispersive and distributive mixing action. Recently, a three dimensional BEM package was developed at the University of Wisconsin in Madison (12) and commercialized by The Madison Group (13).

To help determine the flight flank geometry and clearance, a two-dimensional BEM analysis was initially performed. To evaluate the strength of the elongational flow vs. the shear flow, the flow number (14) was analyzed. The flow number is the ratio of the magnitude of the rate of deformation tensor $\dot{g}$ to the sum of $\dot{g} + w$, where w is the magnitude of the vorticity tensor.

$$c = \frac{\dot{g}}{\dot{g} + w} \quad (16)$$

When c=1.0 the flow is pure elongational flow, c=0.5 simple shear flow, and c=0.0 pure rotational flow.

To determine the mixing capability of a system the forces that the mixer can apply are of extreme importance. In simple shear flow, the maximum hydrodynamic force acting on a dumbbell shaped cluster is given by (15):

$$F_{shear} = 3\pi\eta_s\dot{\gamma}r_p^{\;2} \qquad (17)$$

and for pure elongational flow:

$$F_{elongation} = 6\pi\eta_e\dot{\gamma}r_p^{\;2} \qquad (18)$$

where η_s is shear viscosity of the carrier fluid, η_e the elongational viscosity, and r_p the radii of particles making up the cluster. Considering that the elongational viscosity is usually three times the shear viscosity, the equations above indicate that elongational flow can generate substantially higher stresses than shear flow.

Using the BEM simulation, the flow number and forces at any point in the mixer can be computed. Moreover, particles can be tracked through the mixer to determine streamlines and detect possible stagnant regions. Figure 10 shows the calculated streamlines in the proposed mixing section. Here, at every time step, the strain rates and flow numbers are calculated. Figure 11 shows the flow number of a particle as it flows through the system. Flow numbers are achieved as high a 0.95, indicating that strong elongational flow can be generated in the new mixers. Similarly, figure 12 shows the magnitude of the rate of deformation tensor of the particle as it flows through the system. As the particle approaches the flight, it “feels” an increase in the elongational flow. While passing over the top of the flight, the elongational flow switches to shear flow, but at the same time the magnitude of the rate of deformation tensor increases. This effect will increase the mixing capability of the system.

One of the goals of this mixing section is to provide improved distributive mixing as well as dispersive mixing. Introducing grooves in the modified flight will increase the distributive mixing and at the same time allow the recirculation areas shown in figure 10 to be broken up. To calculate the splitting of the material (distributive mixing effect) as it flows through the mixer, a 3-dimensional BEM analysis was performed. Figure 13 shows how a grouping of particles flow through a region of the mixer. As expected, some particles flow over the modified flight while others flow through the groove. Again, this effect will increase the distributive and dispersive mixing capability of the mixer.

One of the findings of the BEM simulations was that the number of passes through the mixing clearance reduces as the pressure gradient along the mixer reduces. This effect was also observed in mixing experiments when tests were performed at low discharge pressure. In extrusion experiments (16), it was found that the mixing quality reduces when the discharge pressure is low, less than 5 MPa. Obviously, this problem is inherent in any open mixer design. It can be avoided by adopting a closed mixer design, such as the fluted mixer. Figure 14 shows the geometry of a new fluted mixer that achieves 4 passes through the mixing clearance. The advantage of this geometry is that all fluid elements will be exposed to 4 passages of the mixing clearance regardless of the discharge pressure. The disadvantage is that the distributive mixing capability is reduced relative to the open mixer and extruder output will tend to be lower.

CONCLUSIONS

The new CRD mixer technology allows single screw extruders to achieve dispersive mixing as good as that of intermeshing twin screw extruders; this was confirmed by mixing experiments (16). This finding contradicts traditional thinking about mixing in single screw extruders (17). The new mixer technology will allow single screw extruders to be used in applications where thus far only twin screw extruders could be considered. Thus, the use of single screw extruders can potentially be broadened significantly. The CRD mixers can be incorporated into existing or new extruder screws, making implementation simple and inexpensive. Mixers that are mounted downstream of extruders are more difficult to install and more expensive.

The new mixer geometries can improve mixing not only in single screw extruders, but also in non-intermeshing twin screw extruders. Current tangential extruders have limited dispersive mixing capability. Using the new mixer technology may allow these extruders to compete effectively with intermeshing twin screw extruders in applications where dispersive mixing is required; again, expanding the potential uses of these machines. Some aspects of the mixing technology can even be applied to intermeshing twin screw extruders to improve dispersive mixing. Also, internal mixers can benefit from this new mixer technology; this applies to both batch and continuous internal mixers. In internal mixers the empirical sigma type mixing rotor can be replaced with a more efficient CRD type rotor designed from sound engineering principles.

The boundary element method is a useful tool in the development and design of mixing sections with complex geometry. The BEM results of the new mixers indicate that strong elongational flow can indeed be generated by the wedge shaped geometry of the mixing flights. Also, multiple passes through the HSRs can be achieved, provided that the mixing flight clearance is properly dimensioned.

NOMENCLATURE

Lower case Roman characters

k = number of passes through the clearance
r = throttle ratio (pressure flow divided by drag flow)
r_p = particle radius
t_r = residence time
v_{bz} = down-channel barrel velocity
w_f = flight width
z = down-channel distance along the screw

Upper case Roman characters

D = diameter
F = force
G = passage distribution function
H = channel depth
L = axial length of the screw
N = screw rotational speed
W = width of the screw channel

Greek characters

α = taper angle
δ = flight clearance
$\dot{e}$ = rate of elongation
λ = dimensionless time
ϕ = flight helix angle
η = viscosity
$\dot{g}$ = rate of deformation tensor
τ = shear stress
σ = elongational stress
ω = vorticity tensor

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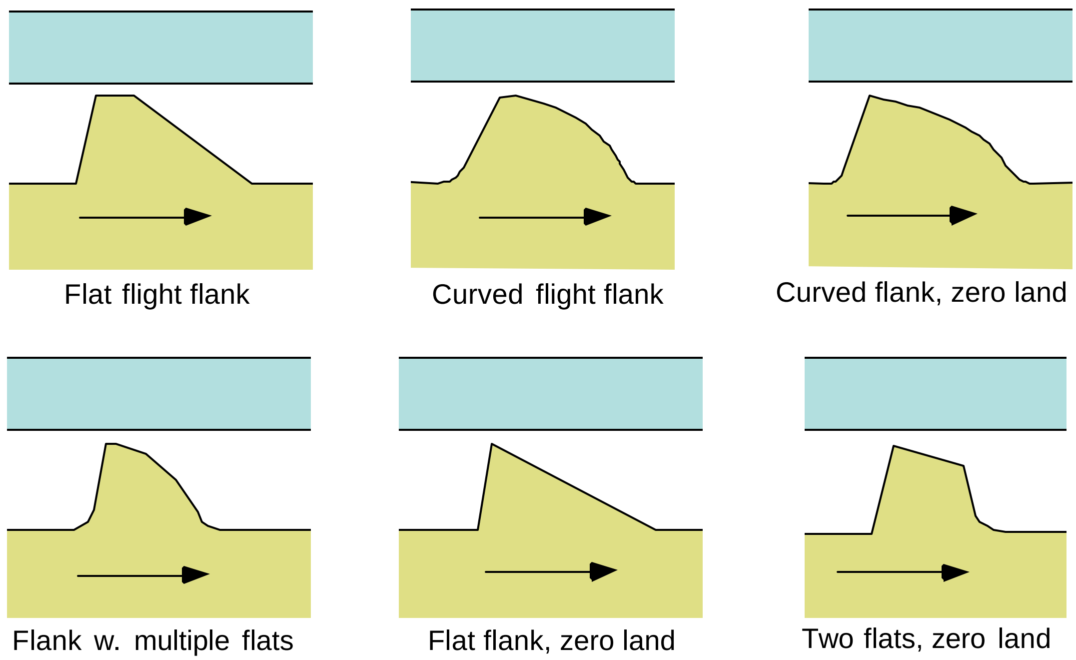

Figure 1, Flight geometries to create elongational flow; the arrows indicate the movement of the screw flight relative to the barrel

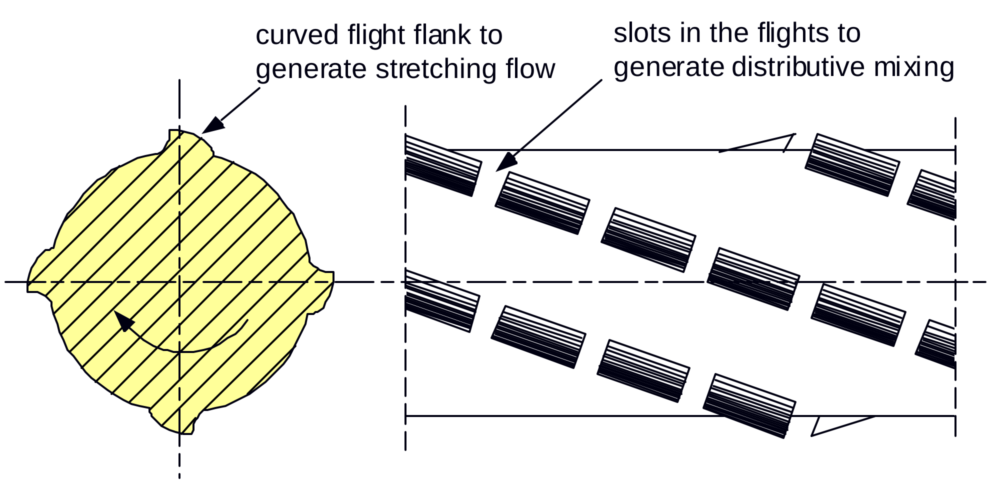

Figure 2, A helical, multi-flighted, dispersive/distributive mixer; the curved arrow indicates the direction of rotation of the mixing element

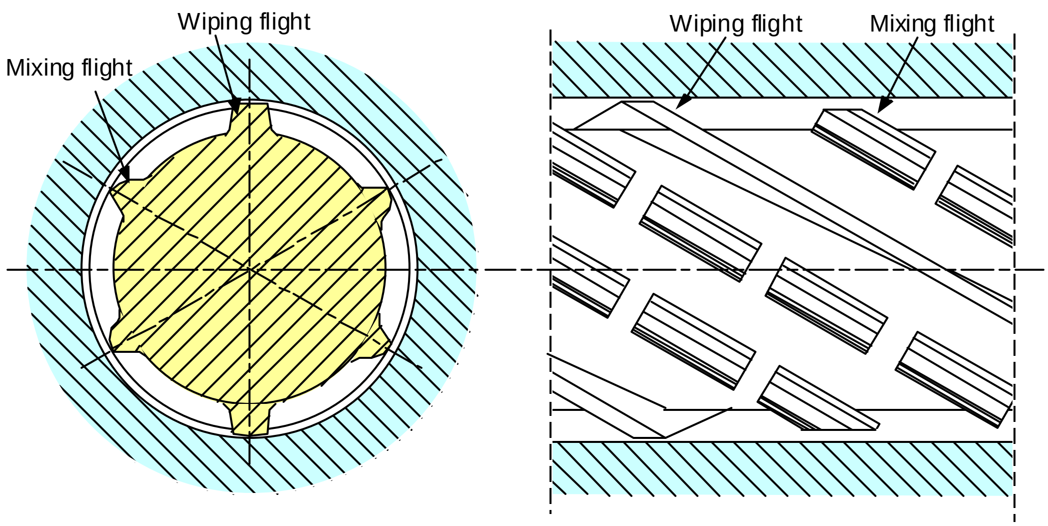

Figure 3, A multi-flighted mixer with mixing and wiping flights

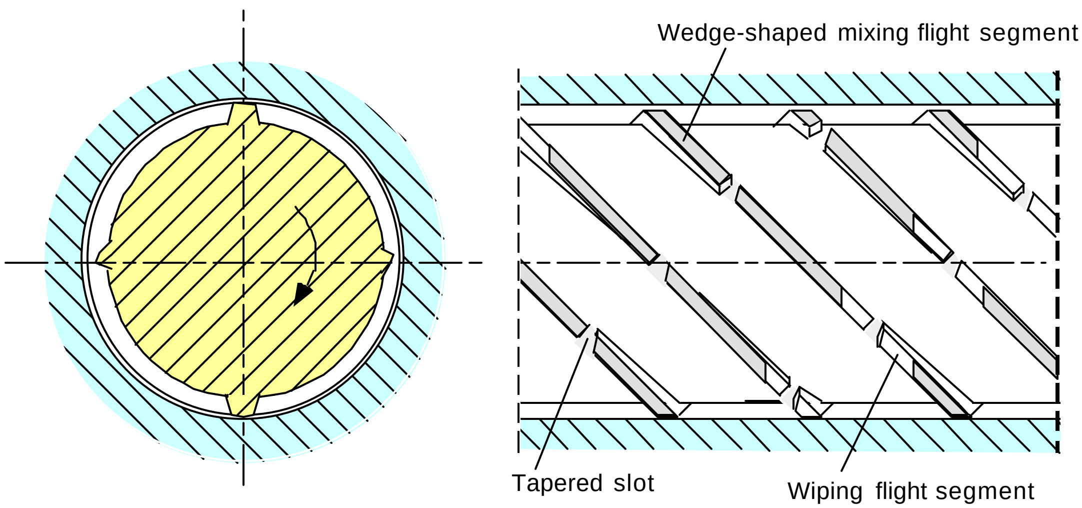

Figure 4, A multi-flighted mixer with multi-function flights

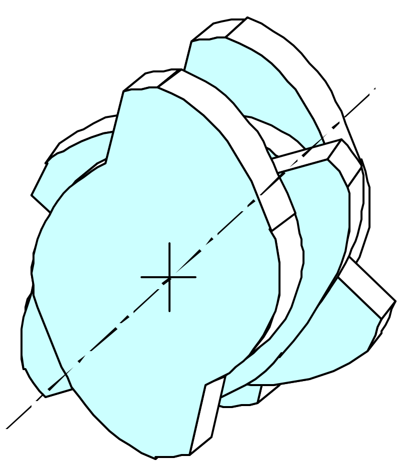

Figure 5, Staggered dispersion disks

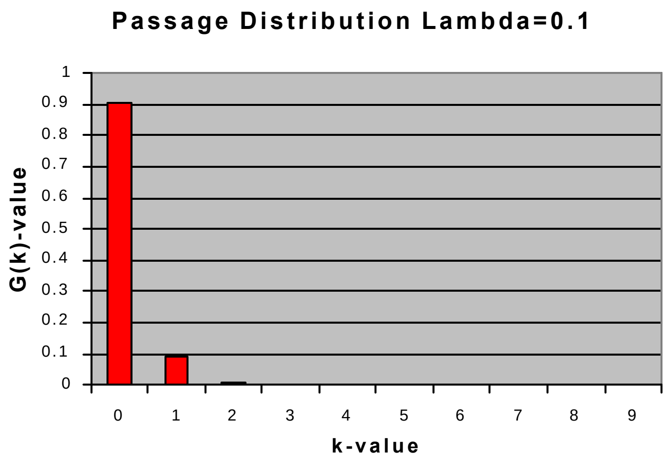

Figure 6, The passage distribution function for $\lambda=0.1$

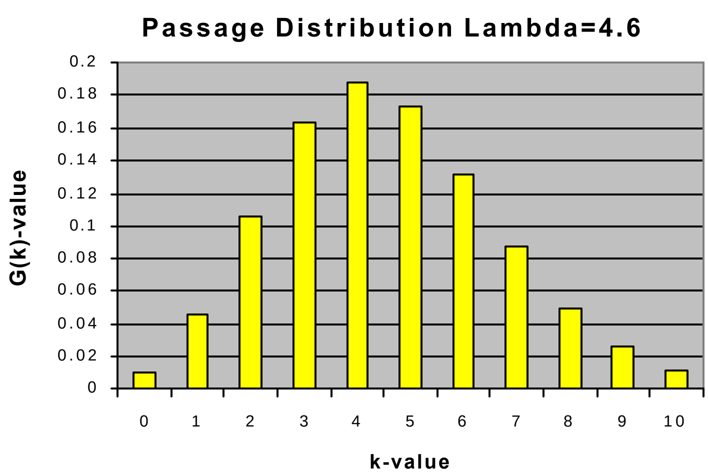

Figure 7, The passage distribution function for $\lambda=4.6$

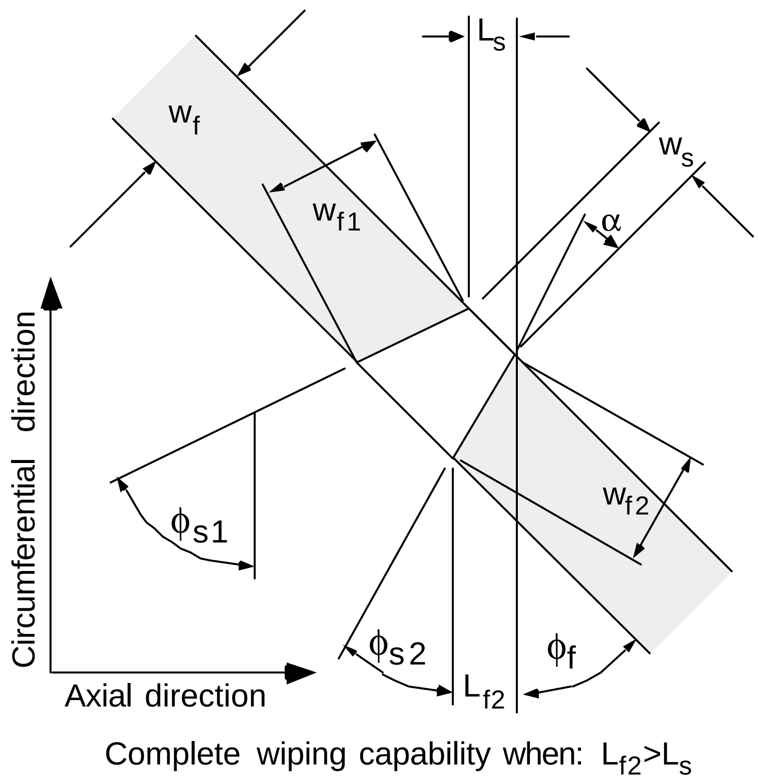

Figure 8, Flight geometry with tapered slot

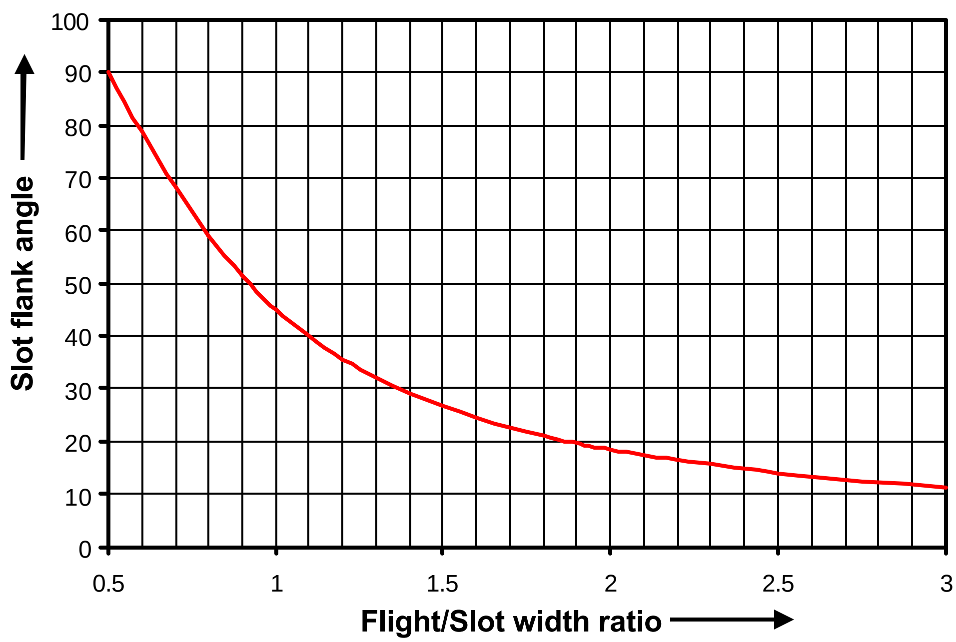

Figure 9, Minimum slot flank angle for flight helix angle of 45 degrees

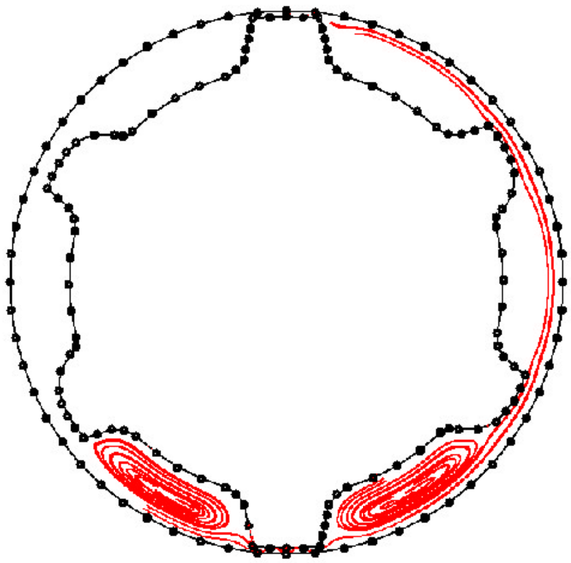

Figure 10, Predicted streamlines in mixer shown in figure 3

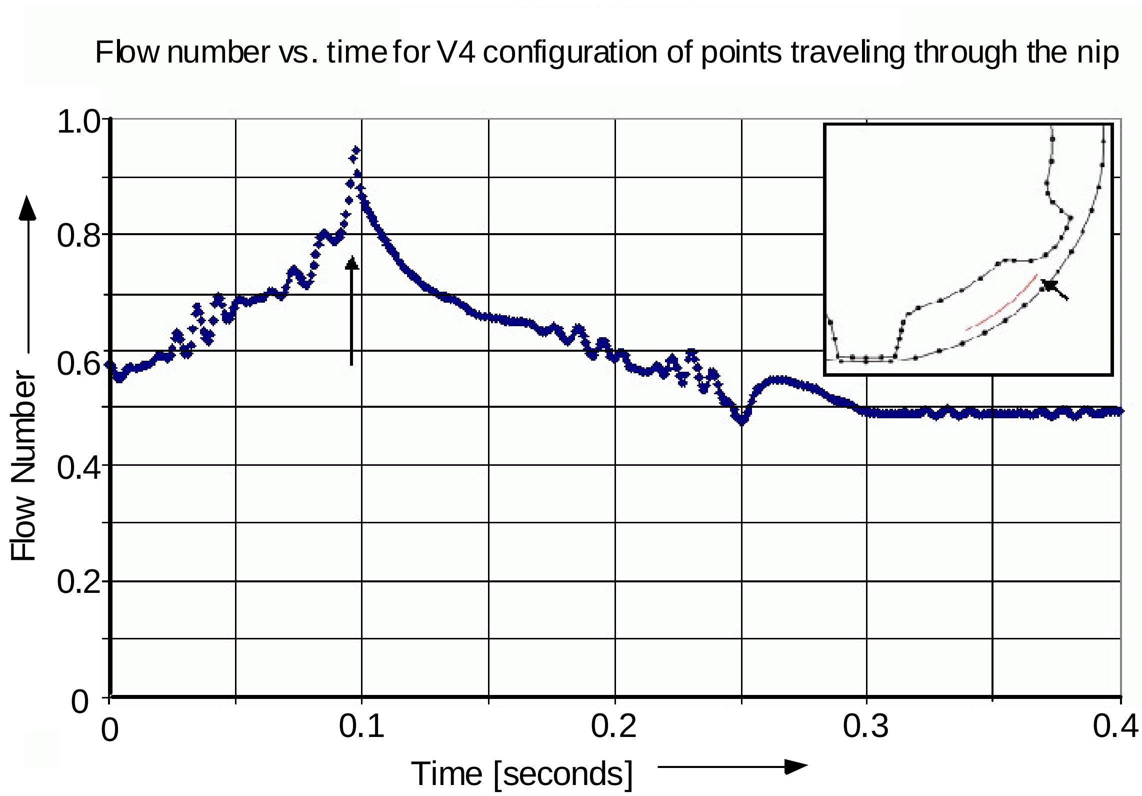

Figure 11, Flow number versus time for a point traveling through the nip region of the mixer shown in figure 3

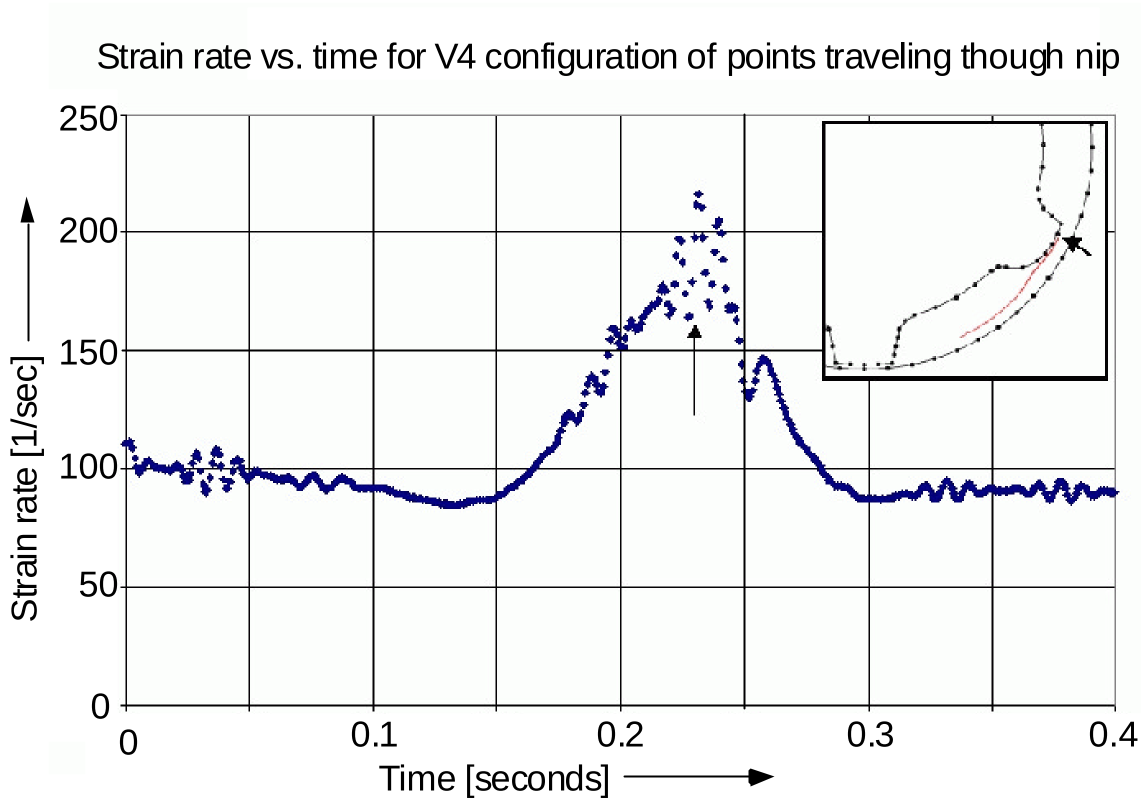

Figure 12, Strain rate versus time for points traveling through the nip

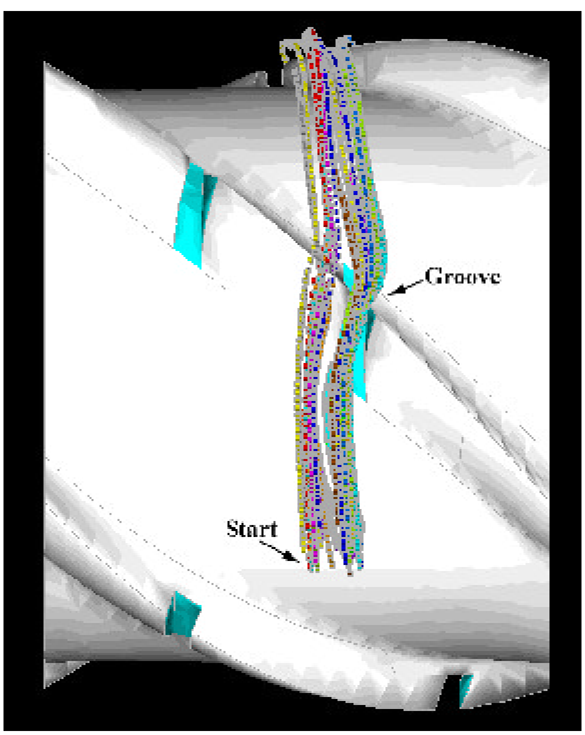

Figure 13, Tracking of multiple points in 3D simulation

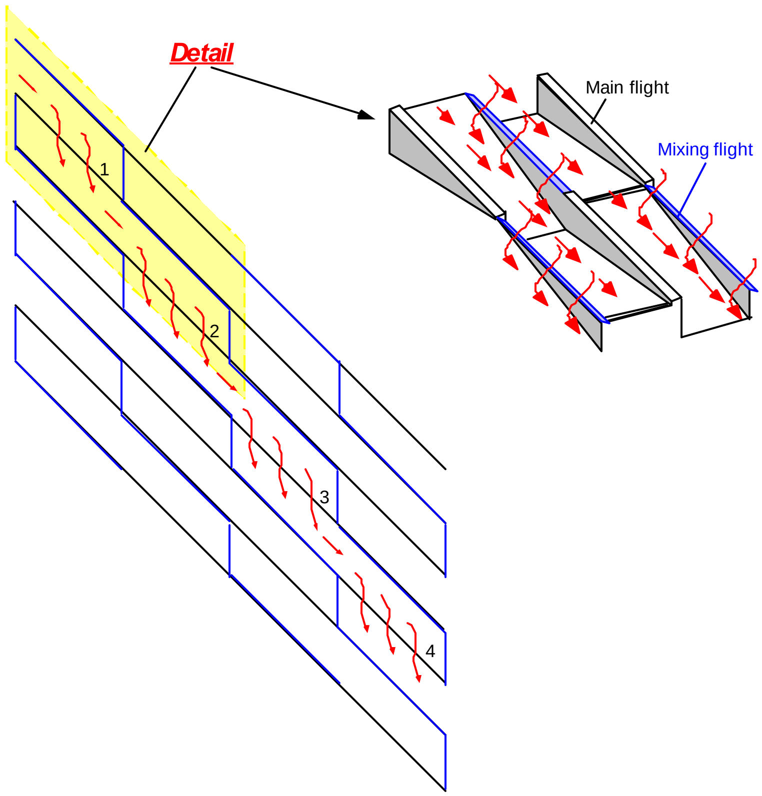

Figure 14, A fluted CRD mixing section with helical flutes