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ON THE MATHEMATICAL MODELLING OF THE INJECTION MOULDING PROCESS

C.W.M. SITTERS^{*} and J.F. DIJKSMAN[†]^{*}Eindhoven University of Technology, Eindhoven (The Netherlands)[†]Philips' Research Laboratories, Eindhoven (The Netherlands)

SYNOPSIS

A numerical method will be presented for the computation of the behaviour of a molten thermoplastic material during the filling of a narrow cavity. The viscosity of the molten polymer is temperature, pressure and shear rate dependent. Effects such as convection, conduction and viscous heating as well as solidification at the cooled walls will be taken into account.

1 INTRODUCTION AND STATEMENT OF THE PROBLEM

Injection moulding is a widely used process for the manufacturing of small or thin walled products. The raw granulated material is melted and homogenized in a reciprocating screw extruder. As soon as the material is sufficiently deformable it is injected into the mould at high speed. Thermoplastic materials are poor heat conductors. To keep the cycle time short, the walls of the cavity have to be cooled far below the glass transition temperature. The temperature distribution development in the flowing melt is rather complex. In the middle of the flow domain heat is transported mainly by convection. Close to the walls heat flow by conduction dominates. Because of the high viscosity η and shear rate $\dot{\gamma}$, viscous heating will be important. During solidification at the walls the transition heat has to be removed by conduction through the solidified layer. In this paper we confine ourselves to the analysis of the non-isothermal flow of an incompressible generalized Newtonian liquid in a narrow cavity with a viscosity function of the Carreau type, depending on temperature T , pressure p and shear rate $\dot{\gamma}$ (ref. 1):

$$\eta = e^{\frac{p}{p_0}} \eta^* ; \quad \eta^* = B_1 e^{\frac{A_1/T}{[1 + (B_2 e^{\frac{A_2/T}{\dot{\gamma}}})^2]^{(n-1)/2}}} \quad (1)$$

where A_1, A_2, B_1, B_2, p_0 and n are constants. We only regard amorphous polymers with a glass transition temperature T_m and a constant density ρ in both the solid and liquid phase.

The geometry of the cavity can be composed of a series connection of rather simple flow elements describing plane, radial and conical flow (Fig. 1). We assume that the channel is symmetric with respect to the local coordinate $z=0$. Essential is that the height is much smaller than the length of the cavity. The leading terms of the equations governing the problem become (ref. 1):

$$\frac{\partial p}{\partial x} = \frac{\partial}{\partial z} \left(\eta \frac{\partial v_x}{\partial z} \right) ; \quad \frac{\partial p}{\partial z} = 0 \quad \text{momentum equations} \quad (2)$$

$$\rho c_{pl} \dot{T} = \lambda_1 \frac{\partial^2 T}{\partial z^2} + \eta \dot{\gamma}^2 ; \quad \dot{\gamma} = \frac{\partial v_x}{\partial z} \quad \text{energy equation in fluid} \quad (3)$$

$$\rho c_{ps} \dot{T} = \lambda_s \frac{\partial^2 T}{\partial z^2} \quad \text{energy equation in solid} \quad (4)$$

with $\dot{T}$ the material derivative of the temperature. The continuity equation $\vec{\nabla} \cdot \vec{v} = 0$ will be discussed later. These equations are subjected to the following boundary conditions. At the flow front the atmospheric pressure is prescribed. At $z=0$ we have the symmetry conditions. At the gate ($x=0$) the injection temperature T_i and either the volume flux or the pressure are prescribed. At $z=\pm h(x)$, i.e. at the walls, the transport of heat depends on the temperature gradient in the wall. Assuming that this gradient is constant we have (ref. 2,3):

$$\lambda_s \frac{\partial T}{\partial z}(x, h) + H(T_w - T_c) = 0 \quad (5)$$

The subscripts s, w and c refer to solid, wall and coolant, respectively. H is the heat transfer coefficient. In most cases H is very large, so $T_w \approx T_c$. At the solid-liquid interfaces $z=\pm d(x)$, the glass transition temperature and the no-slip condition are imposed.

The velocity $(\vec{v}_x, \vec{v}_z)$ at which the solid-liquid interface penetrates the flowing material, depends on the temperature gradients in the liquid and solid phase according to (ref. 4):

$$\vec{v}_z \approx \frac{1}{K\phi} \left(\lambda_s \frac{\partial T_s}{\partial z} - \lambda_l \frac{\partial T_l}{\partial z} \right) ; \quad \vec{v}_x \approx 0 \quad (6)$$

Integration of the momentum equation into the z -direction yields:

$$\frac{\partial}{\partial x} \left(p_0 e^{-p/p_0} \right) = Q / (2L \int_0^{\frac{d}{\eta}} \frac{z}{\eta} dz) \quad (7)$$

$$v_x = \frac{Q}{2L} \left(\int \frac{z}{\eta} dz \right) / \left(\int_0^{\frac{d}{\eta}} \frac{z}{\eta} dz \right) \quad (8)$$

where Q is the total volume flux and L the length of the flow front. The viscosity η^* depends on the temperature and the shear rate, and therefore these relations have to be solved iteratively.

2 NUMERICAL APPROXIMATION

The mould is filled in a number of time steps. After each time step the position of the flow front is calculated and a new grid line is added there. All the other grid lines remain fixed. Suppose that at a certain time all equations and boundary conditions are satisfied. After a time step the whole domain is calculated line by line starting with the first line at the gate, using the following iterative computational scheme.

- 1) The equation governing the velocity of the solid-liquid interface. The velocity of this interface can be calculated with two different methods. One method uses the present position and the position at the previous time (backward difference), the other utilizes eq. 6 in an implicit manner using the present temperature distribution. The difference of these two velocities has to converge to zero during the iteration process.
- 2) The continuity equation. On the first grid line we define a number of grid points. On this line it is rather easy to calculate the velocity profile because the temperature is constant (T_i). When the velocity distribution has been approximated on any other grid line, we arrange the grid points on that line in such a way that the flux through two adjacent grid points equals the flux through the two corresponding points on the first grid line. After convergence the continuity equation will be satisfied automatically.
- 3) The energy equation. The temperature equations are solved by a finite difference technique. The material derivative of the temperature can be

Fig. 3. Built-up of solidified layer

Fig. 4. Temperature distribution

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SYMBOLS FOR PHYSICAL PROPERTIES

λ_l, λ_s	thermal conductivity in liquid and solid respectively
c_{pl}, c_{ps}	heat capacity in liquid and solid respectively
ρ	density
K	transition heat
T_m	glass transition temperature

MIXING PROCESSES IN POLYMER PROCESSING

Z. TADMOR

Department of Chemical Engineering, Stevens Institute of Technology, N.J.

SYNOPSIS

Pure polymers and copolymers are made processable and useful by compounding and mixing them with a broad variety of solid, liquid and gaseous additives. Moreover, as the number of chemically new, and commercially viable polymers diminish, increasing efforts are being made to meet new demands with existing polymers, by their mixing compounding and alloying with new additives in novel ways. In this paper, following a brief review of mixing technology and machinery, recent views on mixing mechanisms are discussed and a theoretical formulation of mixing processes is presented.

1. INTRODUCTION

Synthetic polymers, comprising of plastics, elastomers, fibers and coatings, are the exclusive products of the 20th century. They have a profound influence on our lives and technologies. Space technology would be inconceivable without them, as would be the electronic and computer technologies. The scale of the polymer industry can be well appreciated by recalling that world production of polymers (by volume) seems to have surpassed that of metals. Indeed the 20th century can well be coined the "polymer age." The phenomenal success of polymers is due perhaps as much to the relative ease and diversity of their processing into useful products, as to their unique combination of properties they possess.

The scientific understanding of polymers started with Herman Staudinger's macromolecular hypothesis in 1920. His work was followed by that of many other brilliant scientists to establish the polymer sciences as

accepted and respected branches of chemistry and physics. The "engineering" of polymers, on the other hand, that is their conversion into useful products, though preceding the scientific understanding of polymers (a phenomenon not uncharacteristic in the history of technology), is evolving into a well defined engineering discipline only in recent years. This evolutionary process of polymer engineering could only follow that of the polymer sciences as well as that of the science of rheology.

The structural breakdown of polymer processing (1) comprises of five elementary steps (solids handling, melting, mixing, pumping and stripping) and of five shaping steps (die forming, casting & molding, coating & calendering, mold coating, and secondary shaping). The elementary steps prepare the raw materials for shaping. Among the elementary steps, devolatilization (stripping) and mixing have been recently enjoying a great deal of attention. The interest in the former is driven by increasingly stringent health and environmental regulations as well as by the desire to improve properties by removing low molecular weight components; whereas, the interest in the latter stems from the realization that new property demands can no longer be economically met by chemically new polymers, but they can be frequently met by compounding, blending, alloying, foaming, reinforcing and reaction. Not only do these primarily mixing operations meet the new demands, but they also provide the best route for commercial competitiveness.

2. MIXING PROCESSES

Mixing is an ancient human activity, and consequently we have developed a great deal of intuition into its nature. Yet mixing processes of polymers are so varied (2) and demanding that they can tax the best designers. They include mixing of solids into a viscous liquid matrix, mixing of two viscoelastic melts which may be rheologically homogeneous or nonhomogeneous as well as thermodynamically compatible or non compatible, mixing of low viscosity liquids into high viscosity melts, and finally mixing of gases into viscous polymeric melts. All these operations are designed to ensure that the very many chemical components of a commercial polymer are sufficiently comingled. The additives convert a pure polymer into a useful one. Such mixing operations are generally called 'compounding,' which is a somewhat loosely defined term denoting in addition to mixing also a melting some-times devolatilizing as well as pelletizing.

The mixing process are not only varied in nature but highly constrained by the sensitivity of polymers to high temperature, oxidation and shearing. Thus, the desire for a thorough mixing must always be tempered by the need for the gentle handling of the polymer, and therefore, temperature, time and shear histories must be closely controlled. Yet in spite of all precaution the proper-ties of polymer do change each time they go through a processing machine. A crude measure of this change is the Melt Index shift, which is always followed up by a battery of physical and mechanical property tests.

Mixing processes of polymers can be divided into two categories involving different physical phenomena. One category is associated with the reduction in size of a segregated component which has a cohesive nature such as cohesive granular solids, liquid regions with surface tension as well as vapor or gas bubbles. This type of mixing is called dispersive or intensive mixing. It is dominated by the stress level within the deforming liquid matrix. A critical stress level must be exceeded to break up cohesive agglomerated solids (3). For breaking up a visco-elastic 'blob' or droplets in addition to stress the stress history becomes important (4). This type of mixing is relevant to blending and alloying of noncompatible polymeric melts, where both viscous and elastic properties of the melt play key roles (5). Vapor and gas bubble mechanics in viscoelastic liquids is important not only in classical foaming processes, but also in melt devolatilization where vapor and gas bubble deformation, breakup, and coalescence within the sheared liquid and bubble rupture at the liquid gas interface, determine to a large extent the outcome of the process (6).

In the absence of cohesive barriers, as in the mixing of thermodynamically compatible melts, or the mixing of melt regions at different temperatures or composition (e.g. containing non dispersive pigment or other additive which do not affect significantly rheological properties), the mixing is determined by the strain history imparted to the liquid. This type of mixing is called extensive or laminar mixing or simply blending. The primary mechanism of this mixing process is convection associated to the deformation of the liquid. The deformation is mostly by shear with some elongation. Thus, terms such as 'kneading' denoting squeezing type flow (shear and elongation) followed by folding, and 'milling' denoting smearing and wiping (combined shear and elongation with some dispersion), are frequently used to describe the nature of the mixing in the machine.

Mixing of polymers, in particular dispersive mixing is energy intensive.

For example preparing a LDPE color masterbatch requires a specific energy input of the order of 1.5 MJ/Kg (2). For comparison, heating the polymer from room temperature to 200°C requires only 0.6 MJ/Kg. Specific energy inputs for rubbers range up to 10 MJ/Kg. Clearly, the high energy inputs in the mixing processes, focuses attention on the need for effective heat removal to avoid polymer damage. In dispersive mixing, excessive temperature rise will not only damage the polymer, but due to decreasing viscosity may bring the dispersion process to a complete halt.

The quantitative analysis of the mixing processes must deal with the characterization of the mixture and that of the mixing process. Mixture characterization was reviewed elsewhere (1,7) and will not be discussed here. The quantitative analysis of the mixing processes involves the mathematical modeling and formulation of the associated physical mechanisms, and that of the processing machines. Certain aspects of these for both laminar and dispersive mixing will be discussed, subsequent to a brief review of mixing machinery.

3. MIXING MACHINERY

Mixing machinery and technologies have been recently reviewed in detail by Matthews (2). There is a broad variety of batch mixing machines mainly for low and medium range viscosities. For melt mixing, however, and primarily for dispersion the heated roll-mill and the Banbury type internal mixer (fig. 1) are the most important ones. Both were developed for rubber mixing and adopted by the plastics industry. The fundamentally different continuous mixers and compounders are schematically shown in fig. 1. Most common among these is the single screw extruder, with dozens of specialized 'mixing' screws (e.g. barrier type screws) and mixing sections (e.g. pins, torpedos, planetary gears, reverse flights, interrupted flights etc.). Motionless mixers are attached sometimes at the discharge end of single screw extruders. The single screw extruder with all these modification becomes a good extensive mixer and mild compounder, but cannot perform as an intensive mixer. The reciprocating single screw variation which provides for fully wiped surfaces and improved compounding capability, is a very imaginative extension of the single screw concept. Twin screw extruders-compounders are subdivided into four groups. The continuous mixer has two non-intermeshing rotors, much like those of the internal mixer, extended with short screw like elements to feed the rotors. It is, in fact, a conversion of the batch internal machine to a continuous one. It is considered a medium intensity compounder capable of high production rates, but it has no

Fig. 1 Schematic view of batch and continuous mixers

devolatilization or pumping capabilities. In order to resolve the latter deficiency a screw extruder or more recently even a gear pump is added to the machine. The non intermeshing tangential twin screw type machine are basically similar to the single screw machine, with improved extensive mixing (8) and good devolatilization capabilities. The fully intermeshing counter rotating twin screw machines are basically positive displacement pumps. The intermeshing corotating screw machine come with a variety of mixing and kneading elements tailored to provide extensive and intensive mixing as well as devolatilization capabilities. Gear pumps are sometimes connected in tandem for energy savings and lowering of extrudate temperatures. Finally, fig. 1 schematizes three disk type compounders. The spiral disk which is tantamount to a flat screw extruder, the normal stress extruder, which utilizes the elastic properties of the polymer for pressurization, and the more recent corotating disk compounder (9), which like the corotating twin screw compounder, can be designed to provide extensive and intensive mixing, as well as devolatilization capabilities.

4. EXTENSIVE MIXING

4.1 Rheologically Homogeneous Liquids

When two viscous liquids are mixed the interfacial area between them increases. The ratio of final to initial area A/A_0 , is a quantitative measure of laminar mixing and for homogeneous deformation is given by (1,10):

$$\frac{A}{A_0} = \left[\frac{\cos^2 \alpha'}{\lambda_x^2} + \frac{\cos^2 \beta'}{\lambda_y^2} + \frac{\cos^2 \gamma'}{\lambda_z^2} \right]^{1/2} \quad (1)$$

where $\cos \alpha'$, $\cos \beta'$ and $\cos \gamma'$ are the directional cosines of the initial orientation of the interfacial area and λ_x , λ_y , and λ_z are the principal elongational ratios. For randomly oriented initial area elements in simple shear flow, eq. 1 shows that the area ratio is one half the shear strain. Eq. 1 was generalized for an arbitrary flow by Ottino et al (12) who also reviewed recently laminar mixing (13). Simple shearing, though easily attainable in polymer mixers, tends to align the interfacial area in a uniquely unfavorable direction (11,12). Erwin (14) showed that if N periodic randomizing steps are introduced, the interfacial area ratio becomes

$$\frac{A}{A_0} = \frac{1}{2} \left(\frac{\gamma}{N} \right)^N \quad (2)$$

which explains the very positive effect of even the simplest mixing section in screw extruders. If optimal orientation of 45° to the direction of shear is maintained at all times, that is the deformation becomes pure shear or planar extension, the inter-facial area will increase exponentially with deformation (1,15).

The first attempt to deal with a realistic mixer is McKelvey's (16) derivation of an average shear strain in single screw extruders, modified by Tadmor et al. (17), who also defined a strain distribution function $f(\gamma)d\gamma$, derived it for the screw extruder(1) and suggested the mean strain as a quantitative measure of continuous mixers. However, if significant reorientation occurs along the mixer, the total strain by itself cannot be a useful measure of mixing anymore, and the exact flow path has to be followed (12,13). But, calculating mixing performance from basic principles is limited to relatively simple configurations such as helical annular mixer, certain motionless mixers and constant depth single screw mixer with numerous approximations. The computational effort for real mixers is enormous and experimental techniques using tracer studies (7) are being applied to elucidate laminar mixing mechanism. Such techniques were used very effectively by Erwin et al in studying single screw, twin screw and motionless mixers as well as by David (18) for studying laminar mixing in co-rotating disk processor. The complexity of the flow pattern induced in real mixers, reflects the necessity to randomize orientation and to distribute composition and interfacial area elements throughout the volume.

4.2 RHEOLOGICALLY NON-HOMOGENEOUS LIQUIDS

In mixing rheologically nonhomogeneous systems, viscosity ratio, elasticity and surface tension are of interest. Mixing is no longer measured just by interfacial area and its distribution throughout the volume, but also by the morphology of the blend. Van Oene (19) reviewed many of the phenomena associated with both dispersed and stratified flows of two liquids. It is generally asserted that it is more difficult to mix a low viscosity liquid into high viscosity one, than the other way around. Simple layered analysis, (1,20) shows that the more viscous the liquid the less will it tend to deform.

But, such analysis is oversimplified. For example, the low viscosity liquid tends to encapsulate the other liquid (19), and the interface between two viscoelastic liquids will be distorted in complex ways (21). Big and Middleman (22) investigated the effect of viscosity ratio on interface evolution in cross channel drag flow, and though it appears that equal viscosity are to be preferred results cannot be generalized. Arimond and Erwin (23) explored the mixing of a randomly distributed molten pellets in realistic shear flows. They claim that, in systems of viscous pellets in less viscous continuous phase, wall effects and pellet-pellet interaction play a key role in the mixing process.

One of the most important areas of mixing of different polymer melts is alloying (19,24,25). The morphology of the 'blend,' hence its physical properties, depends to a great extent on the mixing process (25). Van Oene (5) derived a thermodynamic criterion based on the primary normal stress function of the components and the interfacial tension, to predict the basic morphology of the blend, that is which will be the dispersed phase and which will be the continuous one. However, much further work is needed in this important area of mixing, both in analyzing realistic systems as well as devising design criteria for mixer design.

5. DISPERSIVE MIXING

5.1 Dispersive Mechanisms

Dispersive mixing is perhaps the most demanding type of mixing. The mixing of carbon black into rubber is a prime example, and the most carefully investigated one. Carbon black aggregate of a typical size of 150 nm, cluster into large agglomerates of sizes up to 100,000 nm. They are held together by Van-der-Waals forces, and the objective of dispersive mixing is to rupture the agglomerate into its constituents, and distribute them throughout the volume. Rumpf (26) modelled a randomly packed cohesive agglomerate and derived an expression for the tensile strength σ ,

$$\sigma = \frac{9}{8} \left(\frac{1-\epsilon}{\epsilon} \right) \frac{F}{d^2} \quad (3)$$

where ϵ is the porosity, d is the diameter of the particles forming the

agglomerate and F is the cohesive force between two individual particles which can be obtained from the Bradley-Hamaker theory. Thus, for equal sized particles $F = C_0 d$, and for carbon in polystyrene environment C_0 is of the order $4.0 - 4.8 \times 10^{-911}$ N/nm (27). Rumpf's model is an approximate one, and perhaps the approach developed recently by Thornton (28), of micromechanical examination of particulate matter using numerical simulation, may yield a much more realistic method to deal with agglomerates in dispersive mixing.

Mixing of carbon black into rubber, mostly a batch operation carried out in internal mixers, has four stages: incorporation, dispersion, distribution and plasticization (29). During incorporation encapsulation and wetting of the solids takes place, and it is probably during this stage that the nature, strength, and initial size distribution of agglomerates are determined. Hess (29) distinguishes between 'soft' and 'hard' agglomerates based on the level of rubber penetration into the agglomerate, but there is probably a whole spectrum of agglomerate varying in size, strength and nature.

In the course of the dispersion stage, the agglomerates are successively broken apart and reduced in size. In this stage the agglomerates are freely suspended in the liquid, which is repeatedly passed over some narrow gap region. In this high shear field, the hydrodynamic forces acting on the agglomerate surface generate internal stresses, and when these exceed the cohesive strength of the agglomerate (eq.3), rupture occurs. The hydrodynamic separating force within a freely suspended axisymmetric particle in shear flow is (30):

$$F_h = \chi \pi \mu \dot{\gamma} c^2 \sin^2 \theta \sin \phi \cos \phi \quad (4)$$

where χ is a numerical constant dependent on particle shape (27), c is characteristic radius μ is the Newtonian viscosity, $\dot{\gamma}$ the local shear rate, and θ and ϕ are instantaneous orientation angles. The condition for rupture is $F_h/F_c > 1$, where F_c is the cohesive strength of the agglomerate evaluated from eq. 3. The ratio F_h/F_c is given by

$$\frac{F_h}{F_c} = Z \sin^2 \theta \sin \phi \cos \phi \quad (5)$$

where

$$Z = \frac{8}{9} \chi(\dot{\mu}) \left(\frac{\epsilon}{1-\epsilon/C_0} \right)^d \quad (6)$$

This dispersion model, proposed by Manas-Zloczower et al (27), predicts, therefore, that rupture depends on shear stress in the liquid, agglomerate porosity and the size and cohesive forces between the particles forming the agglomerate. The size of the agglomerate is conspicuously absent, implying that it is equally likely to break large or small agglomerates, a prediction which seem to have received some experimental support (31). The model also correctly predicts that it is easier to disperse 'high structure' blacks (i.e., larger aggregate) than low structure blacks. Thus, for example the estimate cohesive force F_c of a 100,000 nm agglomerate is $10.6 \times 10^{-3} \text{ N}$ for 150 nm aggregate size, and it is only $3.2 \times 10^{-3} \text{ N}$ for a 500 nm aggregate size ($C_0 = 4.5 \times 10^{-11} \text{ N/nm}$). The former will rupture in a shear field of 0.22 MPa (32psi) and the latter requires only 0.66 MPa (9.6 psi). These shear stress values are well within the practical range considering that the shear rates in the high shear zone are in the range of 200-500 s^{-1} .

Upstream the high shear narrow gap zone, there is a tapered entrance region where strong elongational flow components exist. The exact role of this region is not clear. It may have a critical function in separating closely placed agglomerate fragments, in generating significant hydrodynamic pressure to eliminate slip at the wall in the high shear zone, in pulling apart 'soft' agglomerate, and in providing extensive mixing. Another point of view expressed by Funt (32) is that dispersion is altogether controlled by separation and, therefore, the elongational flow in the entrance zone will play a central role in the process. Yet another dispersion model is the 'onion peeling' model proposed by Shiga and Furuta (33). They suggest a dispersion mechanism based on gradual peeling of the external layers of the agglomerates. Additional detailed experimental and theoretical work is needed to critically test the validity of the various models, to account for the many non-Newtonian phenomena that may exist, and to account for particle-particle interactions including possible reagglomeration. Some of these effects are discussed by Manas-Zloczower et al (27,34).

5.2 Pass Distribution Functions

A basic characteristic of dispersive mixing is that the material

experiences repeated passes over high shear zones in narrow gaps. In order to reduce agglomerates to acceptable sizes (e.g. a typical criterion is 99% below 9μ), virtually all agglomerates must experience a sufficient number of passes.

In between passes the material is transported to other regions of the mixer where, by and large, extensive mixing and a randomization of composition takes place. Hence different material elements experience different number of passes, and passes over the high shear zones are bests characterized by a function that accounts for this effect termed as the Pass Distribution Functions (PDF). Thus, for a batch mixer g_k is defined as the fraction of material volume that experienced k passes over the high shear zones. The mean number of passes is

$$\bar{k} = \sum_{k=0}^{\infty} k g_k \quad (7)$$

The volume fraction of material that experienced k passes or less, is

$$G_k = \sum_{j=0}^k g_j \quad (8)$$

G_k , g_k and $\bar{k}$ are functions of time and by definition $G_{\infty} = 1$. Similarly, for a steady continuous mixer, we define f_k as the volume fraction of exiting flow rate Q , that experienced k passes over the high shear zone. The mean number of passes $\bar{k}$ is

$$\bar{k} = \sum_{k=0}^{\infty} k f_k \quad (9)$$

The volume fraction of exiting flow rate that experienced k passes is

$$F_k = \sum_{j=0}^k f_j \quad (10)$$

and by definition $F_{\infty} = 1$. The function F_k and f_k as well as $\bar{k}$ are functions of

the mean residence time in the mixer. Next we define an internal PDF of a continuous mixer i_k as the fraction of volume of the material in the mixer that experienced k passes. This function is related to F_k via

$$i_k = \frac{Q}{q} (1 - F_k) \quad (11)$$

where q is the total flow rate over the high shear zone. Finally I_k is defined as the fraction of material volume in the mixer that experienced k passes or less

$$I_k = \sum_{j=0}^k i_j \quad (12)$$

5.3 Dispersion Model of the Batch Internal Mixer

The dispersion model of section 5.1 can be combined with the PDF concept to derive a dispersion model for example of a batch internal mixer (27). For this purpose the mixer is considered as a well mixed tank of volume, V (representing the region between the rotors), from which a steady stream q passes over the high shear zone and recycles to the tank. The fraction of agglomerates that rupture per pass, X , is given by

$$X = \int_0^1 W(\xi) f(\xi) d\xi \quad (13)$$

where $W(\xi)$ is the fraction of agglomerates that break at dimensionless location ξ , and $f(\xi)d\xi$ is the fraction of flow rate between ξ and $\xi + d\xi$. Assuming that the axisymmetric agglomerates are randomly oriented at the entrance to the high shear zone X can be computed via Eq. 5 and equations describing the rotation of the particles in the shear flow (35). The computed value of X , in simple shear flow, is a function of only the dimensionless groups Z and L/H where L is the length of the high shear zone, and H is the gap size. The PDF is given by

$$g_k = \frac{1}{k!} \left(\frac{t}{\bar{t}} \right)^k e^{-t/\bar{t}} \quad (14)$$

where t is the mixing time, and $\bar{t} = V/q$ is the mean residence time in the well mixed region. The mean number of passes, from eq. 14, is simply $\bar{k} = t/\bar{t}$. The fraction of agglomerates at any time t , that ruptured j times is given by

$$Y_j = \sum_{k=j}^{\infty} g_k u_{jk} = \frac{(Xt^*)^j}{j!} e^{-Xt^*} \quad (15)$$

where $t^* = t/\bar{t}$ and u_{jk} is the fraction of agglomerate that experienced j ruptures after k passes over the high shear zone. Agglomerate size can be approximately related to the number of ruptures via

$$\frac{D_i}{D_{i+1}} = 2^{1/3} \quad (16)$$

Eq. 15 and 16 permit to calculate agglomerate size distribution as a function of mixing time, and a comparison gave good agreement with experimental data (27). Finally, Eq. 15 suggest Xt^* as a dimensionless scale up criterion (36).

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