Numerical Simulation of Melting Process in Single Screw Extruder with Vibration Force Field

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Abstract
Melting capacity is always the bottleneck of performance improvement of single-screw extruder, and become the nodus of the extrusion theory. As a novel extrusion technology, the electromagnetic dynamic plasticating (EMDP) extruder for plastics has acquired great economic and social benefit progressively. But the non-linear viscoelastic behavior of polymer and phase change which is a non-linear problem increase the degree of difficulty of the research on the melting mechanism with vibration force field and restrict the exertion of the potential of EMDP extruder in a degree. In this paper, according to the assumption of “flowing solid”, the hydrokinetics is adopted to solve the whole melting problem region, which solves the phase change and the solid-melt interface tracking problems. A 2D melting model is established. This melting model fits for the research on the influence of vibration force field on the melting process. Since polymer has time-dependent non-linear viscoelastic characteristic with vibration force field, and the melting process is a phase change problem, a user-defined program of self-amended non-isothermal Maxwell constitutive equation is developed with the UPFs of ANSYS. This constitutive equation can reflect the relaxation time spectrum of polymer. The responses of melting process to various vibration parameters are simulated. And the rule of the influence of frequency and amplitude on melting process is analyzed.

Introduction
In single screw extruder for plastics, the barrel is immobile, the rotation of the screw pushes polymer conveying toward the extruder head. During this course, the “solid bed” made of solid granules melts owing to the conductive heat and heat of viscous dissipation, and this stage is called melting process. In EMDP extruder, sinusoidal velocity in circumferencial direction is superposed on the steady rotation of screw, and additional vibration velocity can also be introduced in the axial direction, thus the screw can rotate pulsantly. We call the melting process in the EMDP extruder “the dynamic melting process”. The research on the dynamic melting process is different from the traditional melting process by the following three characteristics:
1. the dynamic melting process is periodic, the transient effect should be considered;
2. Since polymer melt will behave time-dependent non-linear viscoelastic characteristic with vibration force field, the hypothesis of pure viscous property of melt won’t be suitable any more;
3. the heat generated by dynamic dissipation is another characteristic of dynamic melting.

Therefore, the dynamic melting process is a non-linear, non-isothermal, close coupled transient problem. To carry out the numerical simulation of dynamic melting process we have to:
1. establish a melting model which not only represent the actual process but also is feasible;
2. solve the phase-change simulation problem;
3. simulate the transient flow of viscoelastic fluid.
Preparation

**Dynamic melting model**

The melting section can be divided into four subsections: upper-melt-film subsection, melt-pool subsection, five-zone melting subsection and solid-bed break-up subsection.

When the screw is not cooled internally, the surface of the screw channel will be covered with thin melt film very soon which is called side melt film and lower melt film, the melting process comes into the five-zone melting subsection, and this subsection occupies the most part of the melting section. The appearance of melt film changes the convey mechanism of solid bed from the solid friction to the shear effect of melt. In this paper, we focus on the five-zone melting subsection. See Figure 1. It shows the schematic diagram of five-zone melting model with unrolled screw. In this Figure the barrel is stationary, the screw rotates, because of the helix angle, the rotation velocity can be decomposed into $V_{\text{screw}z}$ in the down channel direction and $V_{\text{screw}x}$ in the cross channel direction. The solid polymer conveys in the down channel direction at velocity of $V_{sz}$. While in the EMDP extruder periodic velocity components, namely $V_{vibz}$ in the down channel direction and $V_{vibx}$ in the cross channel direction are superposed on $V_{\text{screw}z}$ and $V_{\text{screw}x}$ respectively.

![Figure 1. Schematic diagram of five-zone melting model](image)

Considering the special physical properties of polymer which is different from the other inorganic materials, we put forward an important assumption: “flowing solid phase” to describe the conveying process of solid phase in the melt.

The following will illustrate the rationality of flowing solid phase from the physical structure, properties of polymer and melting behavior during extrusion.

1) the characteristic of physical structure of polymer

Considering the phase state of polymer, the glass state, rubbery state and melt state are all belong to liquid state, because the arrangements between molecule are random. The main difference between these states is the deformability, which is difference of mechanics state.

2) the characteristic of physical property of polymer
Considering the viscoelasticity of material, the difference between solid and liquid is just the difference of relaxation time.

3) the characteristic of melting process of polymer extrusion

During the solid conveying process in the EMDP extruder, the compaction effect of solid pellets is enforced by vibration force field, and the solid pellets are formed into a plug-like continuum. So the polymer solid phase during melting process can be considered as continuous liquid.

From the above explanations, the assumption that using the viscoelasticity property of polymer to describe the melting process after the solid bed is surrounded by melt is rational. According to the assumption of flowing solid phase, hydrokinetics can be applied to solve the whole domain of melting problem which includes the so-called “solid phase zone” and melt zone. So this method not only is rational, but also solves the dynamic tracing problem of solid/melt interface successfully.

Because of the adoption of viscoelastic constitutive equation, more dense meshes are needed to capture the special conveying fashion of melt adjacent to the vibration velocity boundary. And the solid/melt interface where the rheology and physical properties of polymer change sharply is varying along the extrusion direction, which also indicates more dense meshes along the channel depth are needed. Therefore, two-dimensional melting model is used. Considering that the contribution of melt pool to melting ability is neglectable, we use the 2D melting model along the down channel direction. Because our focus is the effect of vibration parameters on the dynamic melting process, it might be as well to further extract the entrance part of 2D melting model to represent the initial stage of melting process. The coordinate frame used in the analysis, which is shown in Figure 2 (a) geometry model, has x axis along the down channel direction and y axis along the channel depth direction.

![Figure 2. 2D melting model](image)

The 2D melting model is meshed into 400 elements with FLUID141, as shown in Figure 2 (c) finite element meshes. And the larger the velocity gradient or temperature gradient is, the denser the meshes are.
**Boundary Conditions**

### Velocity boundary conditions

The average velocity in the down channel direction of solid phase at the entrance can be defined as

\[
    w_x = \frac{\dot{m}}{\rho_s WH}
\]  

(1)

where \( \rho_s \) is the density of the compacted solid polymer, \( W \) is the width of the channel, \( H \) is the depth at the start point of the compression section. The barrel is stationary, while the screw rotates. According to the no-slip assumption, the velocity boundary conditions can be given as:

\[
    v_x|_{y=H} = v_y|_{y=H} = 0
\]  

(2)

where \( v_x|_{y=H} \) and \( v_y|_{y=H} \) are the velocity components at the inner surface of barrel in the downstream direction and transverse direction respectively.

The pulsative velocity boundary condition at the surface of screw can be defined as

\[
    v_x|_{y=0} = 0
\]  

(3)

\[
    v_x|_{y=0} = v_x^0 + v_x^A|_{y=0}
\]  

(4)

\[
    v_x^0 = \text{const}
\]  

(5)

\[
    v_x^A|_{y=0} = a \cdot 2\pi f \sin(2\pi f t)
\]  

(6)

where \( v_x|_{y=0} \) and \( v_y|_{y=0} \) are the velocity components at the surface of screw in the downstream direction and transverse direction, \( v_x^0 \) is the average velocity (namely, steady velocity), \( a \) is amplitude, \( f \) is frequency. The pulsative velocity boundary condition at the surface of screw is applied using the function boundary condition of ANSYS.

### Thermal boundary conditions

1) Apply constant temperature \( T_b \) at the barrel surface.

2) Set the temperature of screw surface the same as that of barrel surface.

3) Assume the temperature of solid phase at the entrance of melting section \( T_{s0} \).

### Pressure boundary conditions

Using the pressure difference between inlet and outlet as pressure boundary condition, apply higher pressure \( p_{out} \) at outlet near extruder head; apply lower pressure \( p_{in} \) at the inlet near the feed section.

See Figure 2 (b) boundary conditions.
Using User-Programmable Subroutines

The molecular motion of polymer is of relaxation. The relaxation spectrum is the most common function to prescribe the relationship of the viscoelasticity of polymer and time or frequency. Microcosmically, it characterize the contribution of different structure units to relaxation time; macroscopically, it connects those viscoelastic function, such as the relaxation modular, dynamic viscosity.

The melting process is considered to be stable in traditional researches of melting mechanism, and non-isothermal pure viscous constitutive equations are mostly used. While during the dynamic melting process, the screw rotates pulsatively, causing the velocity field in melt change periodically, so do the shear rate in melt, which further cause the apparent viscosity and relaxation time change periodically, so the flowing behavior during the dynamic melting process is time-dependent viscoelastic. While simulating the dynamic melting process, constitutive equation that can reflect the time-dependent viscoelastic characteristic must be used.

In recognition of the fact that the viscosity models provided by ANSYS can not satisfy the requests of all users, a user-programmable subroutine (UserVisLaw) is also provided by ANSYS with access to the following variables: position, time, pressure, temperature, velocity component, velocity gradient component. Using the above information, a self-amended MAXWELL viscoelastic constitutive equation was programmed with FORTRAN.

The MAXWELL constitutive equation (Reference 1) is:

$$\tau + \lambda(\dot{\gamma}, T) \frac{\partial \tau}{\partial t} = 2\eta(\dot{\gamma}, T)d$$  \hspace{1cm} (7)

where, $\lambda(\dot{\gamma}, T) = \frac{\eta(\dot{\gamma}, T)}{G}$ is relaxation time, $G$ is bulk modulus, $d = \frac{(L + L^T)}{2}$ is strain rate tensor with $L = (\nabla v)^T, \dot{\gamma} = \sqrt{2d \cdot d^T}$ is shear rate, which is the second invariant of strain rate tensor $d$.

$\eta(\dot{\gamma}, T)$ is the apparent viscosity which is a function of shear rate and temperature. In this paper the apparent viscosity is also used to describe the resistibility of polymer to deformation at temperature lower than melting point. Since the polymer crystal melts within a temperature range, the temperature at which the polymer crystal melts completely is usually called $T_m$, and the temperature range from the start point of melting to the final point of melting is called melting range $T_{mr}$. Thus the apparent viscosity can be described as:

$$\eta(T, \dot{\gamma}) = \begin{cases} 
\eta_0|_{T_m - T_{mr}} & T_g < T < T_m - T_{mr} \\
\exp[b \cdot (T_m - T)] \left( \eta_{T_m} + \frac{\eta_{T_m 0} - \eta_{T_m \infty}}{1 + c \dot{\gamma}^m} \right) & T_m - T \leq T < T_m \\
\exp[b \cdot (T - T_m)] \left( \eta_{T_m} + \frac{\eta_{T_m 0} - \eta_{T_m \infty}}{1 + c \dot{\gamma}^m} \right) & T \geq T_m 
\end{cases}$$  \hspace{1cm} (8)

where $T_g$ is glass temperature, $\eta_0|_{T_m - T_{mr}}$ is viscosity with zero shear rate at temperature $T_m - T_{mr}$, $\eta_{T_m 0}$ and $\eta_{T_m \infty}$ are the viscosity with zero shear rate and second Newtonian viscosity at temperature $T_m$ respectively, $c$ and $m$ are characteristic constants of polymer.

Since the stress can not be described as the explicit function of velocity and gradient of velocity when simulating the viscoelastic flow, the stress is a variable to be solved, which cause the non-linear characteristics of viscoelastic flows and call more challenge and more computer resources than those
numerical simulation of Newtonian flows and generalized Newtonian flows. According to whether the stress is an original variable, the finite element methods for viscoelastic flows can be divided into mixed method and split method.

In this work, the split method (Reference2,3) is adopted; the velocity and pressure are the two variables to be solved. Thus the Galerkin weak form of the above problem can be stated as: to obtain the $n+1$th iterative value $(\mathbf{u}^{(n+1)}, p^{(n+1)}) \in V \times P$, the following equations must be satisfied,

\[
\int_{\Omega} (2\eta_{ref} a^{(n+1)} : \nabla \phi_u - p^{(n+1)} \nabla \cdot \phi_u) d\Omega = \int_{\Omega} F \cdot \phi_u d\Omega + \int_{\partial \Omega} f \phi_u d\Gamma - \int_{\Omega} \tau^* : \nabla \phi_u d\Omega, \forall \phi_u \in V
\]  

\[
\int_{\Omega} (\nabla \cdot \mathbf{v}^{(n+1)}) \rho_p d\Omega = 0, \forall \phi_p \in P
\]  

where $\phi_u$ and $\phi_p$ are the shape functions of velocity and pressure respectively, $V$ and $P$ are function spaces of $\mathbf{v}, p$ defined in $\Omega$ domain, $\eta_{ref}$ is the reference viscosity, namely $\eta(\gamma, T)$, $\tau^* = \tau - 2\eta_{ref} a''$, the extra stress $\tau$ can be solved using the constitutive equation (7) with the former iterative value $(\mathbf{v}^*, p^*)$.

According to the above constitutive equation, we programmed the User-Defined Viscosity program UserVisLaw, and the property type choice of viscosity is USER, the four coefficients NOMI, COF1, COF2, and COF3 are corresponding to $\eta_{T_0}, \eta_{T_{\infty}}, \gamma$ and $m$ respectively. This constitutive program not only takes the viscoelastic characteristic of polymer into account, but also reflects the relaxation spectrum.

**Specifying Fluid Properties for FLOTRAN**

**Thermal conductivity and Density**

The thermal conductivity and density, are represented as piecewise continuous linear functions of temperature as flowing.

\[
k(T) = \begin{cases} 
  k_s, & T < T_m - T_{mr} \\
  k_s + \frac{k_m - k_s}{T_{mr}} (T_m - T), & T_m - T_{mr} \leq T < T_m \\
  k_m, & T \geq T_m 
\end{cases}
\]  

\[
\rho(T) = \begin{cases} 
  \rho_s, & T < T_m - T_{mr} \\
  \rho_s + \frac{\rho_m - \rho_s}{T_{mr}} (T_m - T), & T_m - T_{mr} \leq T < T_m \\
  \rho_m, & T \geq T_m 
\end{cases}
\]  

where, $k_s$ and $k_m$ represents the thermal conductivity of solid phase and melt respectively, $\rho_s$ and $\rho_m$ represents the density of solid phase and melt respectively.
Specific heat

The specific heat, on the other hand, is given in such a way as to include the latent heat of fusion for crystal polymer as the peak that occurs in the melting range.

\[
C_p(T) = \begin{cases} 
  C_{ps}, & T < T_m - T_{mr} \\
  C_{ps} + \frac{\lambda}{T_m - T_{mr}}(T_m - T), & T_m - T_{mr} \leq T < T_m \\
  C_{pm}, & T \geq T_m 
\end{cases}
\]  

(13)

where, \(C_{ps}\) and \(C_{pm}\) represents the specific heat of solid phase and melt respectively, \(\lambda\) is latent heat of fusion. See Figure 3.

![Figure 3. Temperature curve of specific heat](image)

The above fluid properties are specified with fluid property table.

Analysis Results & Discussion

With the completion of the model, transient analyses of dynamic melting are performed, and obtain the velocity and temperature results. See Figure 4. It shows the velocity distribution at the exit of flow channel. See Figures 5 and 6. They show the temperature distribution and density distribution respectively. These results show the clear velocity, temperature and density difference between “solid state” and “liquid state” polymer, which are coincident with those results obtained with traditional method and indicate the validity of new method provided in this paper.
Figure 4. Vector plot of velocity at the exit

Figure 5. Temperature contours
See Figure 7. It shows the instantaneous velocity vector plot along lower melt film at the starting time of a sinusoidal vibration. After this time point the velocity of screw surface increases. See Figure 8. It shows the instantaneous velocity vector plot at the middle time of a sinusoidal vibration. After this time point the velocity of screw surface decreases. See Figure 9. It shows the velocity distribution curves at those above time points and the velocity distribution result obtained from the correspondent steady analysis. As seen from Figure 9, because of the viscoelastic characteristic of polymer, the velocity curve during the velocity increasing stage will not superpose on the velocity curve during the velocity decreasing stage, even though the screw velocities are the same at these time points. And both of these curves don’t superpose on the velocity curve of steady state.
Figure 8. Velocity vector plot along lower melt film at the middle time of a sinusoidal vibration

Figure 9. Velocity distributes along lower melt film at balance position

See Figure 10. It shows the curves of velocity distribution along lower melt film at different time. Velocity distribution differences between velocity increasing stage and correspondent velocity decreasing stage form loops of velocity distribution.
Figure 10. Curves of velocity distribution along lower melt film at different time

As seen from Figure 11, the velocity-varying curves lag behind the velocity-varying curve of the point at the screw surface. And the velocity-varying curves will always lag behind those velocity-varying curves that are closer to the screw surface.

As shear rate is not a direct result available in the postprocessing of ANSYS, a program of shear rate is programmed using APDL. See Figure 12. It shows the difference of average shear rate distribution in the lower melt film along channel depth between steady melting and dynamic melting with different vibration parameters. It is just because the non-linear viscoelastic response of the velocity distribution of polymer
melt with vibration force field makes the average shear rate distribution in the melt change. From Figure 12, it can be seen that the introduce of vibration force field reduces the average shear rate near the screw surface which rotates pulsatively, while increase the average shear rate near the solid/melt interface. Comparing with the temperature result, it is found that the average shear rate increment reaches the maximum near 115°C, which is to say that the introduction of vibration force field into melting process cause change of average shear rate distribution, and make the average shear rate at the interface of solid/melt increase, which is in favor of the removal of the newly-generated melt that is of higher viscosity with lower temperature and accelerate melting process. From the above simulation results, it can be seen that the larger the amplitude or frequency is, the more obvious the effect of reducing average shear rate near driving surface and enhancing average shear rate near solid/melt interface is.

![Figure 12. Difference of average shear rate distribution](image)

**Conclusion**

In this effort, the assumption of flowing solid phase was used to describe the conveying behavior of polymer solid that has relaxation characteristic during melting process. A 2D melting model that can reflect the influence of the parameters of vibration force field on melting process was established. A user-defined viscosity model of self-amended MAXWELL viscoelastic constitutive equation was programmed via UPFs. The dynamic melting processes were simulated.

According to the simulation results of the melting behavior of polymer with vibration force field, it is found that the introduction of VFF into melting process can optimize the time-average shear rate distribution, namely, reduce the average shear rate near the driving interface, enhance the average shear rate near the solid/melt interface and accelerate the dynamic refresh of solid/melt interface, generate a great deal of viscous dissipation heat near the solid/melt interface and promote melting process.
References