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EXISTENCE AND UNIQUENESS OF SOLUTIONS OF MODELS OF THE HYDRODYNAMICS OF POLYMER MOVEMENTS, HEAT AND MASS TRANSFER IN A SINGLE SCREW EXTRUDER.

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Abstract

Screw-type extruders of which there are numerous designs and configurations are widely employed for the extrusion of molten or plasticized polymers to semifinal and final product forms. Although these machines have found wide application, up till now there has been no rigorous theory of polymer melting in screw channels, hence the need for the mathematical treatment of the process. Presented in this paper is the criteria for the existence and uniqueness of the three-dimensional transient mathematical models capable of describing the polymer hydrodynamics and heat and mass transfer in the feed zone (model 1) and in the zone of polymer melting delay (model 2) of a single screw extruder. For both models, accumulation terms is incorporated and no flow along the channel depth $(w=0)$ is assumed. Model 1 is considered under isothermal boundary condition (case 1) and adiabatic boundary condition (case 2). Model 2 is considered under steady state (case 1) and unsteady state (case 2).

Key words: Existence, uniqueness, extruder, melting, transient.

1.0 Introduction

Since 1960, un-deformed solid bed movement in the feed zone of an extruder has been subjected to series of experimental investigation. Klein and Marshall (1965) established that the pressure in the feed zone of the extruder increases along the screw axis up to considerable values. The influence of the temperature of the barrel and the parameters of the granulate movement on the length of the feed zone was investigated by Tadmore and other contributors (Tadmore, 1966). It was concluded that the length of the feed zone goes beyond the section in which the temperature of the barrel reaches the melting point.

Experimental method was used by Schneider (1969) to investigate the behaviour of polymeric materials. He estimated the quantity of the anisotropy of pressure distribution over the solid bed for a number of polymers. Tadmor and Gogos (1984) conducted studies that took into account the obtained estimations by Scneider.

It is worthy of note that most of the studies on this subject matter neglected the melting delay zone. It is quite necessary that the mathematical modeling of this zone should also consider in addition to heat transfer processes, the hydrodynamics of polymer flow in conditions of phase transition (Trufanova and Shcherbinin, 2014). The melting delay zone was first mentioned by Tadmor (1966). The approach and models proposed by Tadmor cannot provide an acceptable description of this zone (Trufanova and Shcherbinin, 2014). A mathematical model of the flow and the transfer of heat in the zone of melting delay was first proposed by (Agur and Vlachopoulos, 1982).

A systematic investigation of melting processes in the screw extruders can be traced back to the study by (Maddock, 1959). This work has been acknowledged as the most outstanding work in this field. He first attempted to describe melting mechanisms operating in the extruder channels using visual observation, the tests were ran for variety of polymers and extruders. Street (1961) using experimental techniques similar to that of Maddock (1959) published the results of experimental investigation of the melting processes. Thus his data served as verification of the melting mechanism proposed by Maddock.

Further studies of the melting zone were mostly based on the Tadmor's model. Lindt (1981) examined the channel of variable height. Rauwendaal (1989) took into account the dependence of polymer viscosity on shear rate and temperature. A finite height of the solid phase in the zone of melting was considered by (Aldinkaynak *et al.,* 2011). They predetermined constant temperature on the surface of the screw. Shcherbinin *et al*. (2004) proposed a quasi-3D approach for describing movement and melting of polymers in a long rectangular channel. They obtained fields of velocity, temperature and pressure in the cross section and along the length of screw. The flow between two infinite plates was considered by (Elbirli *et al*., 1984). Rauwendaal (2004) presented a 2D mathematical formulation with longitudinal circulation of the polymer melt captured in the study.

In the work of Olayiwola *et al*. (2013), a mathematical model for the free radical polymerization in the presence of the material diffusion is presented. They assumed that temperature of the mixture and the initial monomer concentration depends on the space variable. They obtained the analytical solution of the model via parameter- expanding method and eigenfunctions expansion method.

Jemada *et al*. (2017) studied anterior polymerization in two adjacent thin layers. They examined the properties of solution and solved the model equations analytically using parameter-expanding method and eigenfunctions expansion technique. Trufanova and Shcherbinin (2014) presented a mathematical model of polymer melting in screw channels of plasticating extruders.

Most existing literature on three – dimensional polymer flow and heat transfer assumed steady state. But, no system occurs initially under steady state conditions nor can a system remain permanently under unsteady state condition. Therefore in this work, simplified models of polymer movement in the feed zone, and in the zone of melting delay of a single screw extruder incorporating velocities and temperature accumulations will be presented and both steady and unsteady state conditions of polymer flow and heat transfer will be considered.

2. 0 Mathematical Formulation of the Problem

In single screw extruders, the initial polymer is fed to the feed zone of the extruder through the hopper. The polymer is entrapped by the screw flights and transported along the channel by friction at the inner surface of the barrel.

Model 1 (Case 1): The equation of polymer movement in the feed zone of a single screw extruder under isothemal condition

The equation of polymer movement in the feed zone of an extruder by Trufanova and Shcherbinin (2014) is extended based on the above assumptions as:

$$\rho c_p \left(\frac{\partial T}{\partial t} + U \frac{\partial T}{\partial x} \right) = k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} \quad (1)$$

To reduce the three dimensional problem in (1) to a two dimensional problem, a new space variable (Olayiwola *et al*. (2014)) was introduced as:

$$\eta = y + z\sqrt{\frac{k_z}{k_y}} \quad (2)$$

Equation (1) is transformed into :

$$\rho c_p \left(\frac{\partial T}{\partial t} + U \frac{\partial T}{\partial x} \right) = k \frac{\partial^2 T}{\partial \eta^2} \quad , \quad (3)$$

where

$$k = k_y \left(1 + \frac{k_z^2}{k_y^2} \right) \quad (4)$$

In this case, the screw surface is assumed to satisfy isothermal conditions while the barrel temperature is fixed. The initial and boundary conditions are:

$$\left.\begin{aligned} &T(x,\eta,t) = T_0\,, \quad x \ge 0, \quad \eta \ge 0, \quad t = 0 \\ &T(x,\eta,t) = T_s\,, \quad x = 0, \quad \eta = 0, \quad t > 0 \\ &\mathrm{T}(\mathrm{x},\eta,\mathrm{t}) = \mathrm{T_b}\,, \quad \mathrm{x} = \mathrm{L}\,, \quad \eta = \mathrm{h}\,, \quad t \ge 0 \\ &h = S + H\sqrt{\frac{k_z}{k_y}} \end{aligned}\right\} \quad (5)$$

Model 1 (Case 2): The equation of polymer movement in the feed zone of a single screw extruder under adiabatic condition

In this case, the barrel temperature is not prescribed; it is pertinent to account for the solid bed's heat flux resulting from dry friction dissipation. The screw surface is assumed to satisfy adiabatic condition. Thus we consider (4) under the initial and boundary conditions:

$$\left.\begin{aligned} &T(x,\eta,t) = T_0, \quad x \ge 0, \quad \eta \ge 0, \quad t = 0 \\ &T_x(0,\eta,t) = 0, \quad T_\eta(x,0,t) = 0, \quad t > 0 \\ &T_x(L,\eta,t) = 0, \quad \mathrm{k}T_\eta(x,h,t) = q, \quad t \ge 0 \end{aligned}\right\} \quad (6)$$

Model 2 (Case 1): The Equation of polymer movement in the zone of melting delay of a single screw extruder under unsteady state condition

Following Trufanova and Shcherbinin (2014), the system of equations for a liquid phase is simplified as:

$$\rho \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = \frac{\partial}{\partial z}\left(\mu \frac{\partial u}{\partial z} \right) \quad (10)$$

$$\rho \frac{\partial v}{\partial t} + \frac{\partial p}{\partial y} = \frac{\partial}{\partial z}\left(\mu \frac{\partial v}{\partial z} \right) \quad (11)$$

$$\rho \int_0^H u dz = G \quad (12)$$

$$\int_0^H v dz = 0 \quad (13)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = k_z \frac{\partial^2 T}{\partial z^2} + k_y \frac{\partial^2 T}{\partial y^2} + \mu \left(\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right) \quad (14)$$

The relationship between the melt viscosity, the shear rate and temperature is expressed as (Trufanova and Shcherbinin, 2014):

$$\mu = \mu_0 \exp(-\beta (T - T_m)) \left(\frac{I_2}{2} \right)^{\frac{n-1}{2}}, \quad (15)$$

To reduce the three dimensional problem to a one dimensional problem, a new space variable (Olayiwola *et.al*., (2014)) was introduced as:

$$\varepsilon = x + y + z \sqrt{\frac{k_z}{k_y}} \quad (16)$$

Equations (10) to (14) was transformed into

$$\rho \frac{\partial u}{\partial t} + \frac{\partial p}{\partial \varepsilon} = b \frac{\partial}{\partial \varepsilon}\left(\mu \frac{\partial u}{\partial \varepsilon} \right), \quad (17)$$

where

$$b = \frac{k_z}{k_y} \quad (18)$$

$$\rho \frac{\partial v}{\partial t} + \frac{\partial p}{\partial \varepsilon} = b \frac{\partial}{\partial \varepsilon}\left(\mu \frac{\partial v}{\partial \varepsilon} \right) \quad (19)$$

$$G = \frac{\rho}{\sqrt{b}} \int_0^H u d\varepsilon \quad (20)$$

$$\int_0^H v d\varepsilon = 0 \quad (21)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + (u + v) \frac{\partial T}{\partial \varepsilon} \right) = k \frac{\partial^2 T}{\partial \varepsilon^2} + b\mu \left(\left(\frac{\partial u}{\partial \varepsilon} \right)^2 + \left(\frac{\partial v}{\partial \varepsilon} \right)^2 \right), \quad (22)$$

where

$$\mathrm{k} = \mathrm{k_y} \left(1 + b^2 \right) \quad (23)$$

The initial and boundary conditions are formulated as:

$$\left.\begin{array}{lll} u(\varepsilon,0)=0, & u(H,t)=V_0\cos\varphi, & u(H-h,t)=\mathrm{U} \\ v(\varepsilon,0)=0, & v(H,t)=V_0\sin\varphi, & v(H-h,t)=0 \\ T(\varepsilon,0)=T_0, & T(H,t)=T_b, & T(H-h,t)=T_m \end{array}\right\} \quad (24)$$

Model 2 (Case 2): The Equation of polymer movement in the zone of melting delay of a single screw extruder under steady state condition

In this case, equations (15) - (22) reduce to:

$$\frac{\partial p}{\partial \varepsilon}=b\frac{\partial}{\partial \varepsilon}\left(\mu\frac{\partial u}{\partial \varepsilon}\right) \quad (23)$$

$$\frac{\partial p}{\partial \varepsilon}=b\frac{\partial}{\partial \varepsilon}\left(\mu\frac{\partial v}{\partial \varepsilon}\right) \quad (24)$$

$$G=\frac{\rho}{\sqrt{b}}\int_0^H u\,d\varepsilon \quad (25)$$

$$\int_0^H v\,d\varepsilon=0 \quad (26)$$

$$\rho c_p(u+v)\frac{\partial T}{\partial \varepsilon}=k\frac{\partial^2 T}{\partial \varepsilon^2}+b\mu\left(\left(\frac{\partial u}{\partial \varepsilon}\right)^2+\left(\frac{\partial v}{\partial \varepsilon}\right)^2\right) \quad (27)$$

With boundary conditions:

$$\left.\begin{array}{ll} u(H,t)=V_0\cos\varphi, & u(H-h,t)=\mathrm{U} \\ v(H,t)=V_0\sin\varphi, & v(H-h,t)=0 \\ T(H,t)=T_b, & T(H-h,t)=T_m \end{array}\right\} \quad (28)$$

3.0 Results

Here the proof of existence of unique solution of the models are presented

For models 1 (Cases 1 and 2):

The proof of existence of unique solution of the system of parabolic equation (4) satisfying (5) and (6) will be analogous to the proof of Ayeni (1978).

Theorem 1: There exists a unique solution θ of equation (4) which satisfies (5) and (6).

Proof:

We let $\varepsilon = x+\eta$ and rewrite the equation (4) as

$$\frac{\partial \theta}{\partial t'}+U\frac{\partial \theta}{\partial \varepsilon}=\lambda\frac{\partial^2\theta}{\partial \varepsilon^2}+f(\varepsilon,t,\theta), \quad \varepsilon\in R^n, t>0, \quad (7)$$

where

$$f(\varepsilon,t,\theta)=0 \quad (8)$$

Ignoring the second term at the right hand side, the fundamental solution of equation (4) is (Toki and Tokis, 2007):

$$F(\varepsilon,t)=\frac{\varepsilon}{2\pi^{\frac{1}{2}}\lambda^{\frac{1}{2}}t^{\frac{3}{2}}}\exp\left(\frac{U}{2\lambda}\varepsilon-\frac{U^2t}{4\lambda}-\frac{\varepsilon}{4\lambda t}\right) \tag{9}$$

Clearly, $f(\varepsilon,t,\theta)=0$ is Lipschitz continuous. This completes the proof.

For model 2 (Case 1)

To examine the properties of solution of equations (17) - (24), we consider the following asymptotic expansions of velocities u', v' and temperature θ in β_1.

Let

$$\left.\begin{aligned} u' &= \mathrm{u}_0' + \beta_1 u_1' + \dots \\ v' &= \mathrm{v}_0' + \beta_1 v_1' + \dots \\ \theta' &= \theta_0 + \beta_1 \theta_1 + \dots \end{aligned}\right\}, \tag{25}$$

where

$$\mu'=\left(\frac{\mathrm{I}_2}{2}\right)^{\frac{n-1}{2}}e^{-\beta_1(\theta-1)}=\left(\frac{\mathrm{I}_2}{2}\right)^{\frac{n-1}{2}}e^{-\beta_1}e^{-\beta_1\theta}\approx A(1-\beta_1\theta) \tag{26}$$

$$A=\left(\frac{\mathrm{I}_2}{2}\right)^{\frac{n-1}{2}}e^{-\beta_1} \tag{27}$$

Substituting (25) to (27) into (3.199) to (3.201) and collecting like powers of β_1:

$$\frac{\partial u_0'}{\partial t'}+\frac{\partial p'}{\partial \varepsilon'}=\frac{A}{\mathrm{Re}}\frac{\partial^2 u_0'}{\partial \varepsilon'^2} \tag{3.205}$$

$$\frac{\partial v_0'}{\partial t'}+\frac{\partial p'}{\partial \varepsilon'}=\frac{A}{\mathrm{Re}}\frac{\partial^2 v_0'}{\partial \varepsilon'^2} \tag{3.206}$$

$$\frac{\partial \theta_0}{\partial t'}+(u_0'+v_0')\frac{\partial \theta_0}{\partial \varepsilon'}=\frac{1}{Pe}\frac{\partial^2 \theta_0}{\partial \varepsilon'^2}+\frac{EcA}{\mathrm{Re}}\left(\left(\frac{\partial u_0'}{\partial \varepsilon'}\right)^2+\left(\frac{\partial v_0'}{\partial \varepsilon'}\right)^2\right) \tag{3.207}$$

Theorem 3: Let $\frac{\partial p'}{\partial \varepsilon'}=c_2=$ constant, $\frac{\partial \theta}{\partial \varepsilon'}=\frac{\partial \theta_m}{\partial \varepsilon'}=c_3=$ constant and $\bar{\varepsilon}=\varepsilon'+a-1$. Then there exists unique solutions $u_0'(\bar{\varepsilon}.t')$, $v_0'(\bar{\varepsilon}.t')$ and $\theta_0(\bar{\varepsilon}.t')$ of equations (3.187) – (3.191) satisfying (3.192).

Proof: We rewrite equations (3.187), (3.188) and (3.191) respectively as:

$$\frac{\partial u_0'}{\partial t'}=\frac{A}{\mathrm{Re}}\frac{\partial^2 u_0'}{\partial \varepsilon'^2}+f(\bar{\varepsilon},t',u_0',v_0',\theta_0) \tag{3.208}$$

$$\frac{\partial v_0'}{\partial t'}=\frac{A}{\mathrm{Re}}\frac{\partial^2 v_0'}{\partial \varepsilon'^2}+g(\bar{\varepsilon},t',u_0',v_0',\theta_0) \tag{3.209}$$

$$\frac{\partial \theta_0}{\partial t'}=\frac{1}{Pe}\frac{\partial^2 \theta_0}{\partial \varepsilon'^2}+h(\bar{\varepsilon},t',u_0',v_0',\theta_0), \tag{3.210}$$

where

$$f(\bar{\varepsilon},t',u_0',v_0',\theta_0)=-c_2 \quad (3.211)$$

$$g(\bar{\varepsilon},t',u_0',v_0',\theta_0)=-c_2 \quad (3.212)$$

$$h(\bar{\varepsilon},t',u_0',v_0',\theta_0)=\frac{EcA}{\mathrm{Re}}\left(\left(\frac{\partial u_0'}{\partial \varepsilon'}\right)^2+\left(\frac{\partial v_0'}{\partial \varepsilon'}\right)^2\right)-c_3(u_0'+v_0') \quad (3.213)$$

Ignoring the second term at the right hand side, the fundamental solutions of equations (3.208), (3.209) and (3.210) are (see Toki and Tokis (2007)):

$$F(\bar{\varepsilon},t')=\frac{A^{\frac{1}{2}}\bar{\varepsilon}}{2\mathrm{Re}^{\frac{1}{2}}\pi^{\frac{1}{2}}t^{\frac{3}{2}}}\exp\left(-\frac{\mathrm{Re}}{4A}\frac{\bar{\varepsilon}^2}{t'}\right) \quad (3.214)$$

$$G(\bar{\varepsilon},t')=\frac{A^{\frac{1}{2}}\bar{\varepsilon}}{2\mathrm{Re}^{\frac{1}{2}}\pi^{\frac{1}{2}}t^{\frac{3}{2}}}\exp\left(-\frac{\mathrm{Re}}{4A}\frac{\bar{\varepsilon}^2}{t'}\right) \quad (3.215)$$

$$H(\bar{\varepsilon},t')=\frac{Pe^{\frac{1}{2}}\bar{\varepsilon}}{2\pi^{\frac{1}{2}}t^{\frac{3}{2}}}\exp\left(\frac{Pe}{4}\frac{\bar{\varepsilon}^2}{t'}\right) \quad (3.216)$$

Clearly, $f(\bar{\varepsilon},t',u_0',v_0',\theta_0)$, $g(\bar{\varepsilon},t',u_0',v_0',\theta_0)$ and $h(\bar{\varepsilon},t',u_0',v_0',\theta_0)$ are Lipschitz continuous. Hence by lemma (2.1), the result follows. This completes the proof.

For model 2 (Case 2)

Here, the existence and uniqueness of solution of equation (4) satisfying (7) is presented.

Theorem 4: Let $\mu'=\frac{\partial p'}{\partial \varepsilon'}=c_0=$constant and $\bar{\varepsilon}=\varepsilon'+a-1$, then the equations (3.120) – (3.124) satisfying (3.126) has a unique solution.

Proof: Let $\mu'=\frac{\partial p'}{\partial \varepsilon'}=$constant and $\bar{\varepsilon}=\varepsilon'+a-1$ and $\phi(\bar{\varepsilon})=u'(\bar{\varepsilon})+v'(\bar{\varepsilon})$, we obtain,

$$\frac{\partial^2\phi}{\partial\bar{\varepsilon}^2}=2\mathrm{Re} \quad (3.196)$$

$$\phi(0)=1,\quad \phi(a)=\alpha(\cos\varphi+\sin\varphi) \quad (3.197)$$

By direct integration, we obtain the solution of (3.196) and (3.197) as:

$$\phi(\bar{\varepsilon})=\mathrm{Re}\bar{\varepsilon}^2+\frac{1}{a}\left(\alpha(\cos\varphi+\sin\varphi)-\mathrm{Re}a^2-1\right)\bar{\varepsilon}+1 \quad (3.198)$$

Then we obtain

$$u'(\bar{\varepsilon})=\left(\mathrm{Re}\bar{\varepsilon}^2+\frac{1}{a}\left(\alpha(\cos\varphi+\sin\varphi)-\mathrm{Re}a^2-1\right)\bar{\varepsilon}+1\right)-v'(\bar{\varepsilon}) \quad (3.199)$$

$$v'(\bar{\varepsilon})=\left(\mathrm{Re}\bar{\varepsilon}^2+\frac{1}{a}\left(\alpha(\cos\varphi+\sin\varphi)-\mathrm{Re}a^2-1\right)\bar{\varepsilon}+1\right)-u'(\bar{\varepsilon}) \quad (3.200)$$

$$\theta(\bar{\varepsilon}) = \int \begin{pmatrix} e^{\int Pe\phi(\bar{\varepsilon})d\bar{\varepsilon}} \int_0^{\bar{\varepsilon}} e^{-\int Pe\phi(\tau)d\tau} \left(\frac{-EcPe\mu'}{\mathrm{Re}}\right)\left(\left(\frac{\partial u'}{\partial \tau}\right)^2 + \left(\frac{\partial v'}{\partial \tau}\right)^2\right) \mathrm{d}\tau \\ + ce^{\int Pe\phi(\bar{\varepsilon})d\bar{\varepsilon}} \end{pmatrix} \partial\bar{\varepsilon} + c_1, \qquad (3.201)$$

Where $\theta(0) = 1$, $\theta(a) = \gamma$ are the corresponding boundary conditions.

Hence, there exists a unique solution of problem (3.120) to (3.126). This completes the proof.

4.0 Conclusion

The criteria for the existence and uniqueness of solutions of the formulated models of the hydrodynamics of polymer movements and heat, mass transfer in a single screw extruder have been established.

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