MATHEMATICAL MODELING OF POLYMER MOVEMENT AND MELTING IN THE FEED ZONE OF AN EXTRUDER

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Abstract
The paper presents an analytical solution of a three-dimensional transient equation describing polymer movement and melting in the feed zone, under isothermal and adiabatic conditions. The equation governing the phenomenon is solved analytically using perturbation method and eigenfunctions expansion technique. The results obtained are presented graphically and discussed. It is observed from the results obtained that the polymer temperature increases as the velocity of the solid bed and thermal conductivity increases.

Introduction
Polymers form a very important class of materials without which life may seem very difficult. They are all around us in everyday use; in rubber, in plastic, in resins, and in adhesives and adhesives tapes. The word polymer is derived from two Greek words, poly meaning many and mers meaning parts or units of high molecular mass each molecule of which consist of a very large number of single structural units joined together in a regular manner. In other words, polymers are giant molecules of high molecular weight, called macromolecules, which are build up by linking together of a large number of small molecules, called monomers. The reaction by which the monomers combine to form polymer is known as polymerization (Gowariker *et al.*, 2005).

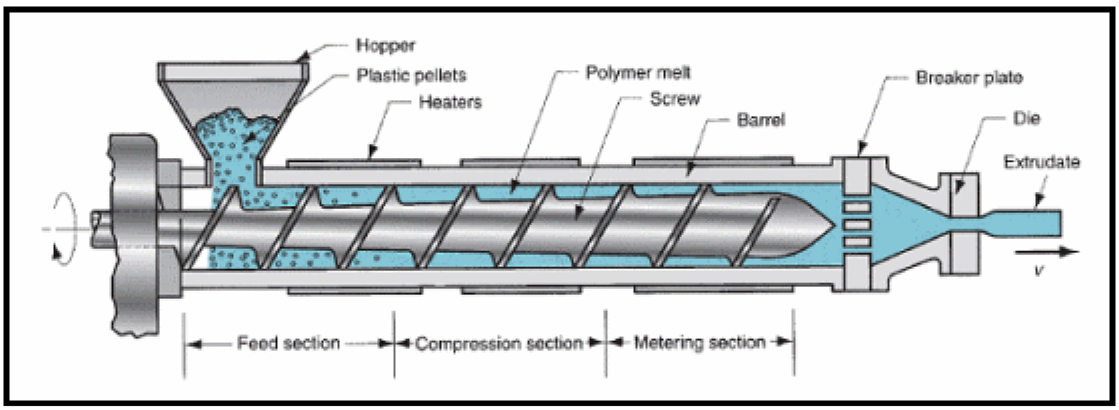

Figure 1: Plasticating Extruder

Most polymeric materials are extruded at least twice in their lifetime, first through a pelletizing die after the reaction and then for final shaping. In simplest terms, screw extruders (figure 1) are polymer pumps with the capacity to melt the material which they are fed.

Screw extruders comprise one or two Archimedean screws rotating in a heated barrel. The single screw extruder (SSE) is the workhorse of the plastics industry. Polymer resins in the form of pellets powders or flakes flow from a hopper to the gap between a rotating screw and a heated barrel. The depth of the conveying channel in the screw is contoured from large to small in the flow direction, to account for the density change from the particulate solid feed to the molten polymer extrudate, and for pressure development. The SSEs normally have diameters between 25 and 250 mm and length/diameter ratios between 20 and 36. Usual rotation speeds range from 20 to 150 revs min^{-1}. A 60-mm diameter machine may deliver up to 200kg h^{-1}, while a 150mm diameter machine can exceed $1000kgh^{1}$ (Vlachopoulos & Wayner, 2001).

In the first or solid conveying zone of the extruder called the feed section, the solid polymer particles are compacted together in the screw channel by the rotating action of the screw to form a solid bed of material. At the start of the next extruder section, the compression (melting) zone, barrel heaters cause a thin film of molten polymer to form in the gap between the solid bed and the barrel wall. The melt film is subjected to intense shearing in the gap, and because of the extremely high viscosities of molten polymers high rates of viscous dissipation result. The generated heat melts the solid bed within a short distance of the start of melting. In the last zone of the extruder, the metering section, the polymer melt flow is stabilized in the shallow screw channels and finally the material passes out through the die at the end of the machine (Vlachopoulos & Wagner, 2001).

The movement of un-deformed solid bed in the feed screw zone has been subjected to intensive experimental investigation since 1960. Tadmore *et al.* (1966) investigated the influence of the barrel temperature and the basic parameters of the granulate movement on the length of the feed zone. They arrived at the conclusion that the length of the feed zone is not confined to the section, in which the barrel temperature reaches the melting point- the effective length of the feed zone is much longer. Aldinkaynak *et al.* (2011) considered a finite height of the solid phase in the melting zone and predetermined constant temperature on the surface of the screw. Shcherbinin *et al.* (2004) proposed quasi-3D approach for describing movement and melting of polymers in a long rectangular channel. Fields of velocity, temperature and pressure in the cross section and along the length of the screw were obtained. Rauwendaal (2004) presented a 2D mathematical formulation taking into account the longitudinal circulation of the polymer melt is presented. Trufanova and Shcherbinin (2014) offered a new theory of polymer melting in screw channels of plasticating extruders. Their proposed approach is based on the numerical solution of complete equations of mass, momentum and energy conservation.

In this paper, an analytical solution for the three-dimensional transient equation describing polymer movement and melting in the feed zone, under isothermal and adiabatic conditions is presented.

Problem Formulation

Following Trufanova and Shcherbinin (2014), constructing a mathematical model of motion and heat transfer in the feed section of the extruder, we assume the following:

(i) The velocity of the solid bed is constant.

(ii) No flow along the cross channel $(y\text{ - axis})$ and the channel depth $(z\text{ - axis})$ directions, $(v = 0, w = 0)$ (see figure 2).

(iii) The screw channel is developed on a plane and the screw rotation is arrested while the barrel continues to rotate with the same speed as the screw but in the opposite sense.

(iv) Diffusion of heat along the channel is neglected.

(v) Transient state is considered.

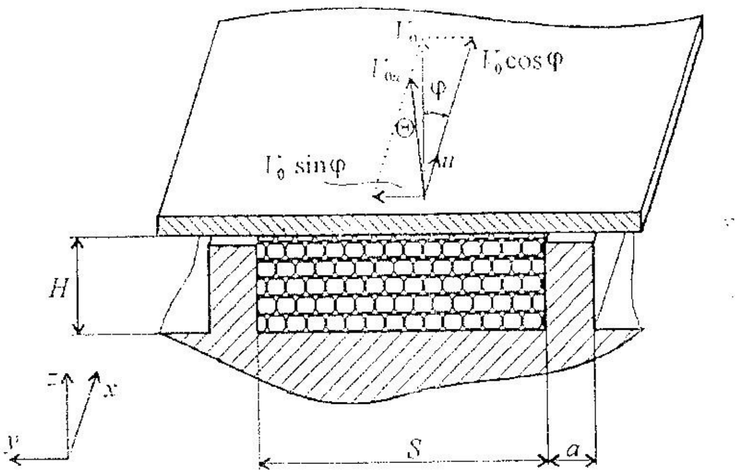

Figure 2: Rectangular Channel of the extruder screw

Based on the above assumptions, the energetic balance in the plug is defined by the transient equation which takes into account the variation of temperature in three directions in the feed zone given as:

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

where ρ is the density of the solid polymer, c_p is the heat capacity of solid polymer, T is the polymer temperature, t is time, x is coordinate along the channel, z is coordinate along the channel depth, U is velocity of the solid bed, k_y is thermal conductivity of the solid polymer along y -axis, k_z is thermal conductivity of the solid polymer along z -axis.

We introduce a new space variable (Olayiwola *et al.* (2014)) as:

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

Then equation (1) transformed into

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

where

$$k = k_y\left(1+\frac{k_z^{\,2}}{k^2_{\,y}}\right)$$

Depending on the initial processing conditions, the boundary conditions of the problem may vary. As a result, equation (3) will be considered in two forms.

Isothermal Condition

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

$$\left.\begin{array}{llll} T(x,\eta,t)=T_0, & x\geq 0, & \eta\geq 0, & t=0 \\ T(x,\eta,t)=T_s, & x=0, & \eta=0, & t>0 \\ \mathrm{T}(\mathrm{x},\eta,\mathrm{t})=\mathrm{T_b}, & \mathrm{x}=\mathrm{L}, & \eta=\mathrm{h}, & t\geq 0 \\ h=S+H\sqrt{\dfrac{k_z}{k_y}} & & & \end{array}\right\}, \tag{4}$$

where T_0 is the temperature of the solid polymer fed into the hopper, T_s is the temperature of the screw surface, T_b is the barrel temperature (in the general case, T_b varies length wise).

Adiabatic Condition

In this case, the barrel temperature is not prescribed, it is necessary to take into account the heat flux to the solid bed as a result of dry friction dissipation. The screw surface is assumed to satisfy adiabatic condition. The initial and boundary conditions are:

$$\left.\begin{array}{l} T(x,\eta,t)=T_0,\ x\geq 0,\ \eta\geq 0,\ t=0 \\ \left.\dfrac{\partial T}{\partial x}\right|_{x=0}=0,\ \left.\dfrac{\partial T}{\partial \eta}\right|_{\eta=0}=0, \quad t>0 \\ \left.\dfrac{\partial T}{\partial x}\right|_{x=L}=0,\ \left.k\dfrac{\partial T}{\partial \eta}\right|_{\eta=h}=q,\ t\geq 0 \end{array}\right\}, \tag{5}$$

where q is the heat flux from the external sources (the extruder barrel), k is the thermal conductivity.

Method of solution

Non-dimensionalization

Here, we non-dimensionalised, (3) - (5) using the following set of dimensionless variables:

$$x'=\frac{x}{\mathrm{L}},\quad \eta'=\frac{\eta}{h},\quad t'=\frac{U_0 t}{L},\quad U'=\frac{U}{U_0},\quad \theta=\frac{T-T_0}{T_S-T_0} \tag{6}$$

and we obtained, after dropping prime

$$\left.\begin{array}{l} \dfrac{\partial\theta}{\partial t}+U\dfrac{\partial\theta}{\partial x}=\lambda\dfrac{\partial^2\theta}{\partial\eta^2} \\ \left.\begin{array}{llll} \theta(x,\eta,t)=0, & x\geq 0, & \eta\geq 0, & t=0 \\ \theta(x,\eta,t)=1, & x=0, & \eta=0, & t>0 \\ \theta(x,\eta,t)=\sigma, & x=1, & \eta=1, & t\geq 0 \end{array}\right\} \end{array}\right\} \tag{7}$$

$$\left.\begin{aligned}
&\frac{\partial\theta}{\partial t}+U\frac{\partial\theta}{\partial x}=\lambda\frac{\partial^2\theta}{\partial\eta^2}\\
&\theta(x,\eta,t)=0, x\ge 0,\quad \eta\ge 0,\quad t=0\\
&\left.\frac{\partial\theta}{\partial x}\right|_{x=0}=0,\quad \left.\frac{\partial\theta}{\partial\eta}\right|_{\eta=0}=0,\quad t>0\\
&\left.\frac{\partial\theta}{\partial x}\right|_{x=1}=0,\quad \left.\frac{\partial\theta}{\partial\eta}\right|_{\eta=1}=\gamma,\quad t\ge 0
\end{aligned}\right\} \tag{8}$$

Analytical Solution

Here, we solve equations (7) and (8), using perturbation method and Eigen-function expansion technique and we obtain

$$\begin{aligned}
\theta(x,y,z,\mathrm{t}) &= 1+\left(\frac{\sigma-1}{2}\right)\left(x+y+\sqrt{\frac{k_z}{k_y}}z\right)+\\
&\sum_{n=1}^{\infty} A_1 e^{-\lambda\left(\frac{n\pi}{2}\right)^2 t}\sin\left(\frac{n\pi}{2}\left(x+y+\sqrt{\frac{k_z}{k_y}}z\right)\right)\\
&+U\left(\sum_{n=1}^{\infty}\frac{4(\sigma-1)\left(1-(-1)^n\right)}{\lambda n^3\pi^3}\left(1-e^{\frac{-\lambda n^2\pi^2}{4}t}\right)\sin\left(\frac{n\pi}{2}\left(x+y+\sqrt{\frac{k_z}{k_y}}z\right)\right)\right)
\end{aligned} \tag{9}$$

$$\begin{aligned}
\theta(x,y,z,\mathrm{t}) &= \frac{\gamma}{4}\left(x+y+\sqrt{\frac{k_z}{k_y}}z\right)+\gamma\left(\lambda t-\frac{2}{3}\right)+\\
&\sum_{n=1}^{\infty}\frac{-4\gamma(-1)^n}{n^2\pi^2}e^{-\lambda\left(\frac{n\pi}{2}\right)^2 t}\cos\left(\frac{n\pi}{2}\left(x+y+\sqrt{\frac{k_z}{k_y}}z\right)\right)+\\
&U\left(\begin{aligned}&-\gamma t+\sum_{n=1}^{\infty}\frac{8\gamma(-1)^n\left((-1)^n-1\right)}{\lambda n^3\pi^3}\left(e^{-\lambda\left(\frac{n\pi}{2}\right)^2\tau}-1\right)+\\
&\sum_{n=1}^{\infty}\frac{\gamma}{2}\left(\begin{aligned}&\frac{4\left(1-(-1)^n\right)}{n^2\pi^2}\left(1-e^{-\lambda\left(\frac{n\pi}{2}\right)^2 t}\right)+\\
&\sum_{n=1}^{\infty}\frac{4(-1)^n\left((-1)^{2n}-1\right)}{n^2\pi^2}\,\mathrm{t}\,e^{-\lambda\left(\frac{n\pi}{2}\right)^2 t}\end{aligned}\right)\cos\left(\frac{n\pi}{2}\left(x+y+\sqrt{\frac{k_z}{k_y}}z\right)\right)\end{aligned}\right),
\end{aligned} \tag{10}$$

where

$$A_1=\frac{-2}{n\pi}$$

The computations were done using computer symbolic algebraic package MAPLE.

Results and Discussion

We solved partial differential equation describing polymer movement and melting in the feed zone, under isothermal and adiabatic conditions analytically using perturbation method and Eigen-functions expansion technique. Numerical solutions of equations (7) and (8) are computed for the values of $\lambda = 0.4,\ 0.6,\ 0.8$, $u = 1,\ 2,\ 4$, $\gamma = 1$, $\sigma = 2$, $k_y = 0.2$ and $k_z = 0.8$.

The following figures explain the polymer temperature distribution in the feed zone for both conditions considered.

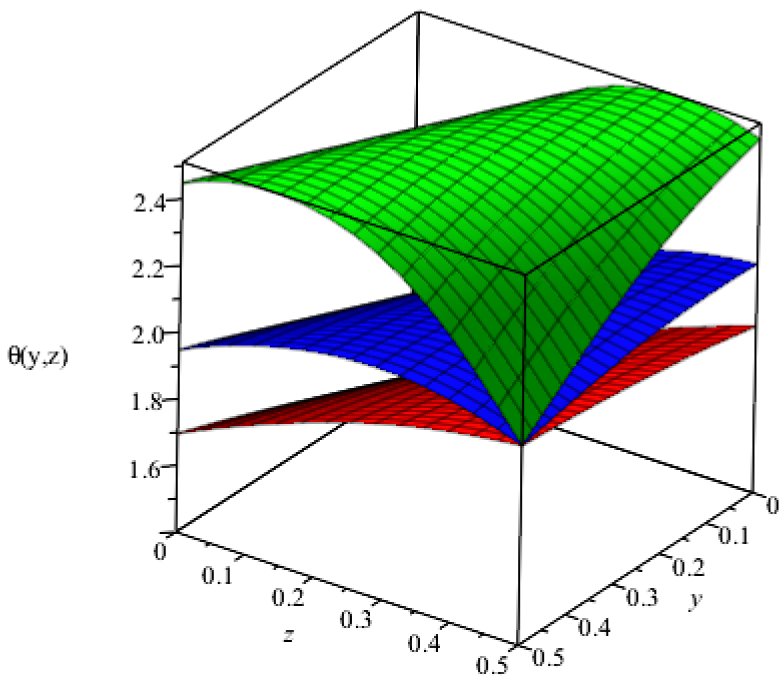

Figure 3: Relation between temperature θ and distances y and z for different values of velocity U under isothermal codition

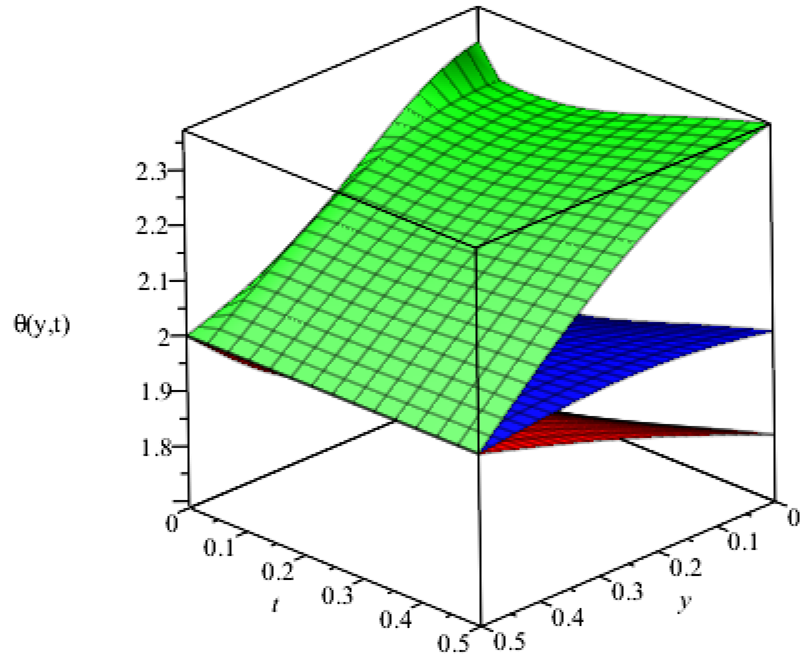

Figure 4 Relation between temperature θ ,distance y and time t for different values of velocity U under isothermal condition

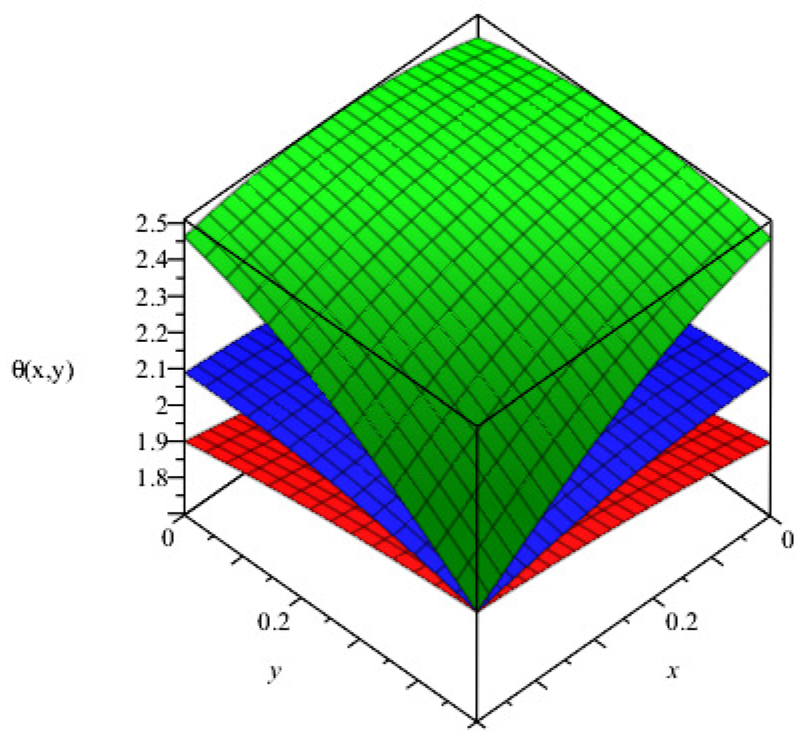

Figure 5: Relation between temperature θ and distances x and y for different values of thermal conductivity λ under isothermal condition

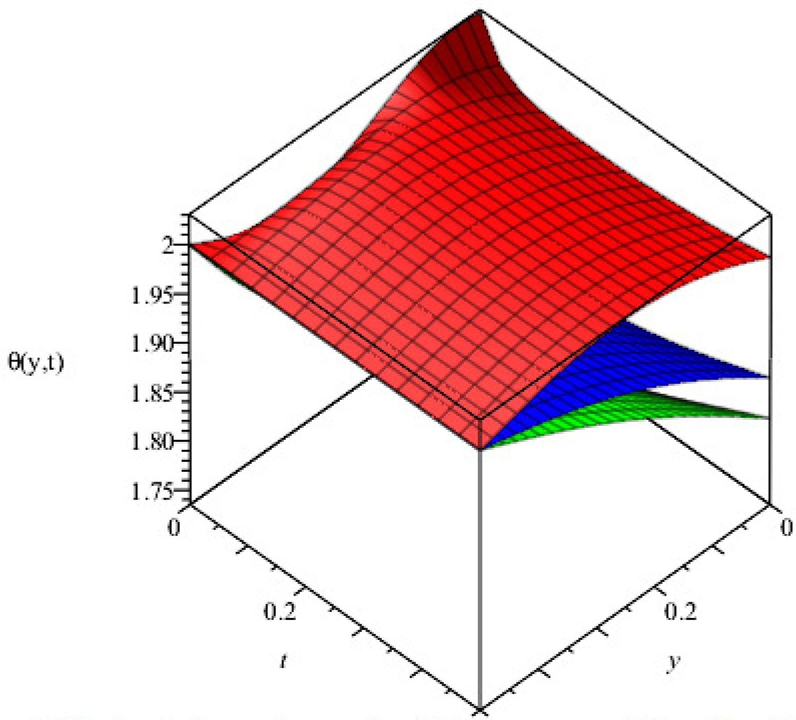

Figure 6: Relation between temperature θ, distances y and time t for different values of thermal conductivity λ under isothermal condition

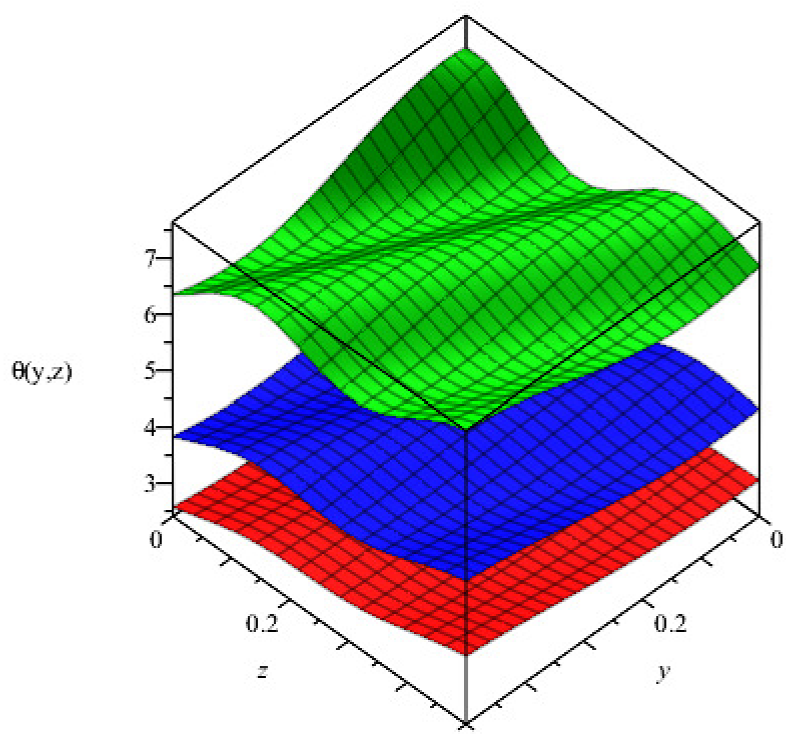

Figure 7: Relation between temperature θ and distances y and z for different values of velocity U under adiabatic condition

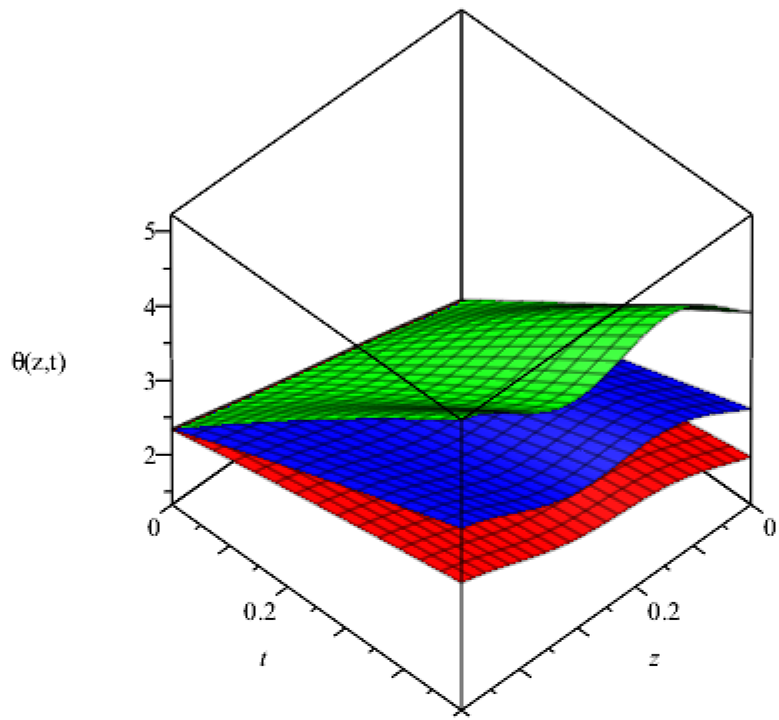

Figure 8: Relation between temperature θ ,distance z and time t for different values of velocity U under adiabatic condition

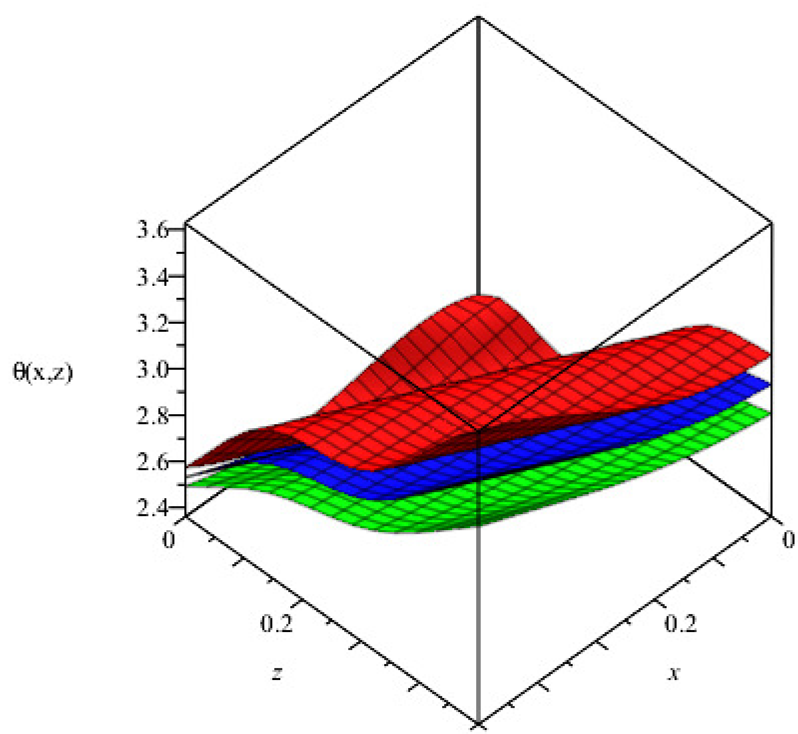

Figure 9: Relation between temperature θ and distances x and z for different values of thermal conductivity λ under adiabatic condition

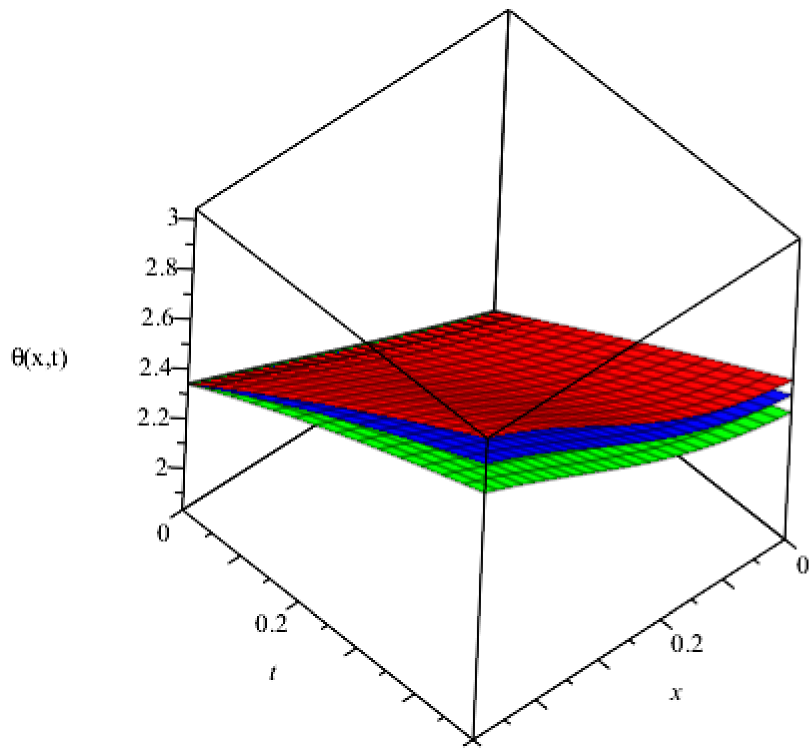

Figure 10: Relation between temperature θ, distance x and time t for different values of thermal conductivity λ under adiabatic condition

Figures 3 to 6 show the effect velocity of the solid bed and thermal conductivity on the polymer temperature distribution along the feed zone under isothermal condition.

Figure 3 shows the effect of velocity of the solid bed (U)on the polymer temperature. It is observed that the polymer temperature decreases along distances x and y but increases as velocity of the solid bed increases.

Figure 4 shows the effect of velocity of the solid bed (U) on the polymer temperature. It is observed that the polymer temperature is steady with time and decreases along distances y but increases as velocity of the solid bed increases.

Figure 5 shows the effect of thermal conductivity (λ) on the polymer temperature. It is observed that the polymer temperature decreases along distances x and y but increases as thermal conductivity increases.

Figure 6 shows the effect of thermal conductivity (λ) on the polymer temperature. It is observed that the polymer temperature is steady with time and increases along distances y but decreases as thermal conductivity increases.

Figures 7 to 10 show the effect velocity of the solid bed and thermal conductivity on the polymer temperature distribution along the feed zone under adiabatic condition.

Figure 7 shows the effect of velocity of the solid bed (U)on the polymer temperature. It is observed that the polymer temperature is steady along distances y and oscillate along distance z but increases as velocity of the solid bed increases.

Figure 8 shows the effect of velocity of the solid bed (U) on the polymer temperature. It is observed that the polymer temperature increases with time and oscillate along distance z but increases as velocity of the solid bed increases.

Figure 9 shows the effect of thermal conductivity (λ) on the polymer temperature. It is observed that the polymer temperature increases along distances x and oscillate along distance z but decreases as thermal conductivity increases.

Figure 10 shows the effect of thermal conductivity (λ) on the polymer temperature. It is observed that the polymer temperature is increases with time and increases along distances x but decreases as thermal conductivity increases.

Conclusion

To study heat transfer in the feed zone of an extruder the three-dimensional transient equation describing polymer movement and melting under isothermal and adiabatic conditions is presented. We used perturbation method and eigenfunctions expansion technique to obtain the analytical solution of the model. The governing parameters for the problem under study are the velocity of the solid bed and thermal conductivity. The polymer temperature profiles are significantly influenced by this parameters.

References

Aldinkaynak, A., Gutpa, M., Spalding, M. A., & Crabtree, S. L. (2011). Melting in a Single Screw Extruder: Experiments and 3D Finite Element Simulations. *International Polymer Processing*, 2,182-196.

Gowariker, V. R., Viswanathan, N. V., & Shreedhar, J. (2005). *Polymer Science*. New Delhi: New Age International.

Olayiwola, R. O., Bello, O. A., & Emuoyibofarhe, O. N. (2014). Mathematical study of contaminant transport with time dependent dispersion coefficient and source concentration in an aquifer. *Journal of Nigerian Association of Mathematical Physics,* 28 (1), 395 – 404.

Rauwendaal, C. (2004). *Polymer extrusion'*, 4th edition, Munich: Hanser.

Shcherbinin, A. G., Trufanova, N. M. & Yankov, V. I. (2004). Spatial mathematical model of a single-screw plasticized extruder. Message I. Mathematical model of heat and mass transfer of polymer in extruder channel Plastics, *Perm State Technical University Plasticheskie, Massy,* 6,38-41.

Trufanova N. M., & Shcherbinin, A. G. (2014). Problem background and mathematical model of polymer movement and melting. *World Applied Science Journal*, 29(3), 441 - 452.

Tadmor, Z. (1966). Fundamentals of plasticating extruder. *Polymer Eng. Sci.*, 6(3), 185-190.

Vlachopulos, J., & Wagner J., JR (ed) (2001). *The SPE guide on extrusion technology and troubleshooting*. Brookfield, CT, Society of Plastics Engineers.