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COMPUTER SIMULATION OF PLASTICS COMPOUNDING OPERATIONS IN TWIN-SCREW EXTRUDERS

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Abstract

This presentation is concerned with the development of process simulators for the analysis of compounding operations in modular corotating intermeshing twin-screw extruders. Approximate flow and heat transfer models are presented and implemented in a personal computer based software package for the fast simulation of the processing behavior in realistic settings.

Introduction

With progress in polymer processing research and the advent of powerful yet inexpensive personal computers, there is renewed interest in twin-screw process simulators [1,2]. In this presentation we discuss, from a general point of view, the models and techniques used in the development of extrusion process simulators and provide examples of its application and implementation.

Practical computer simulators require a tradeoff of accuracy and detail in the predictions, and computational efficiency. Efficiency involves not only the computer time required to perform the actual simulation but the time required to setup the simulation (generate the mesh, collect material properties, etc.) and analyze the results (from raw data to useful numbers), and the computer hardware (PC, workstation, super computer) and personnel (process engineer, R&D specialist, numerical analyst) required to perform these tasks.

Although the exact tradeoff may differ between specific products, there are some characteristics common to all successful *practical* process simulators:

(1) The simulator should handle all processing steps involved in compounding operations: solids conveying, melting, melt conveying and pressurization, as well as mixing, devolatilization, and reactive processing.

(2) In addition to the flow and thermal characteristics (pressure, temperature, power consumption, heat transfer to the barrel, etc.) the simulator should provide estimates of the mixing characteristics of the extruder and process.

(3) The simulator should handle realistic settings such as multiple feed and vent ports, multicomponent systems (solids fillers and reinforcers, blends, etc.)

(4) The estimates should be accurate enough for practical application. This is a very subjective issue. For the sake of argument, let us say that the simulation results should agree with available experimental data within ± 20%.

(5) A typical simulation run, including setting up the machine configuration, operating conditions and material properties, performing the simulation, and viewing its results should be completed in a short time (e.g., minutes).

(6) Setting up, performing, and analyzing the results of a simulation should not require special computational or mathematical skills. Any plastics engineer must be able to realize the full potential of the simulator.

(7) The simulator should be inexpensive and run on inexpensive hardware (e.g., personal computer).

Methods based on the complete (3D) numerical solution of the equations of motion (mass, momentum, and energy balances) using finite element analysis (FEA) or similar techniques provide an accurate and detailed picture of the flow field, but are too complex, slow, and resource-hungry for general-purpose process simulators. To some extent, the same can be said of 2D methods such as flow analysis network (FAN). They are most suitable for the simulation of short, full, melt conveying extruder sections and have been used to validate simpler models. At the present time, practical process simulators cannot be entirely based on FEA or FAN methods.

Alternatively, one-dimensional lumped-parameters methods, in which the equations of motion are integrated (based on simplified flow models) throughout the cross section, are very fast, versatile, and easy to use. Their only drawback is their relative lack of accuracy and resolution (i.e., the level of detail) and this can be overcome, at least in part, by the use of extensions and modifications. In this presentation we will discuss only simulators based on one-dimensional models.

Modeling

A process simulator must include mathematical models that estimate the axial profiles of pressure, temperature, composition, and related quantities (power, torque, etc.) The term *composition* is understood in its broadest sense, to include not only the concentration of resins, fillers, additives and volatile solvents, but also the fraction of solid (unmolten) resins, etc. Appropriate models must be developed for each processing step: solids transport, melting, and melt transport including mixing, pressurization, devolatilization and reactive processing.

The basic lumped parameter models are very simple. For example, the momentum balance in a melt conveying screw elements can reduced to the sum of two terms:

$$\frac{q}{\rho} = AN - \frac{B}{\eta}\frac{dp}{dz} \tag{1}$$

relating the flow rate (q) to the screw speed (N) and the pressure gradient (dp/dz) along the axial coordinate z. Eq. (1) was developed for single-screw extrusion modeling [3-6]. The simplicity of the basic formulation leads to extremely fast simulation engines, but the geometric complexity of twin-screw extruders results in substantially less accurate estimates than in single-screw extrusion.

One approach to improve the resolution and accuracy of one-dimensional methods is to subdivide the cross-section into different functional zones. Regions can be defined in purely geometrical terms (e.g., screw channels, tip clearances, and intermesh region in conveying screw elements) or in material terms (e.g., melt and solids in partially molten resins). Different values of selected flow parameters may be computed for each zone (e.g., average temperature in the screw channels and tip clearances, or for the melt and suspended solids). Usually, far better models can be developed for carefully defined functional zones than for the overall cross-section, leading to a significant increase in the accuracy. Figure 1 shows a complex axial element.

Another way to improve the accuracy of lumped parameter models is to introduce empirical constants. Using adjustable constants, users can "fine tune" the models for specific extruder components, classes of materials, and/or processes. The systematic use of limited process data can significantly improve the accuracy of the simulation engine. For example, power input/discharge temperature data for a few different operating conditions can be used to tune up heat transfer models quite efficiently.

Finally, alternative models can be built in the simulator and used to provide, if not a single accurate prediction, at least reasonable upper and lower bounds for process parameters. In some situations, this may be the only way to overcome the inherent limitations of one-dimensional models or our lack of knowledge in some areas, such as melting and mixing mechanisms, required for the formulation of sufficiently accurate models.

It is beyond the scope of this presentation to discuss in detail the use of these techniques in the modeling of the different processing steps. We will present instead a few typical examples.

Pressure Gradient in Conveying Screw Elements.

The melt flow in a full screw conveying element can be modeled as:

$$\frac{q}{\rho} = \pm k_D f A N - k_P \left(\frac{g_0 B_0}{\eta(T,\dot{\gamma},w)} \mp \frac{g_1 B_1}{\eta(T',\dot{\gamma}',w')} \right) \frac{dp}{dz} \tag{2}$$

where ρ is the density (a function of the local temperature and composition), and η is the viscosity (a function of the local temperature, composition, and shear rate). Notice that the pressure term includes the contribution of the main flow in the screw channels (index 0) and the leak flow over the screw tips (index 1). The two regions are characterized by (in general) different temperatures, compositions, and prevailing shear rates. We introduce here a series of terms that will allow us to selectively refine the level of approximation:

- A, B_0, B_1 are functions of geometric parameters only, based on approximate theoretical Newtonian flow models (i.e., channel flow, leakage flow, positive displacement intermesh flow, etc.), including geometric "shape factors" for the appropriate *class* of screw component.
- f, g_0, g_1 are semi-empirical functions of the rheological parameters (e.g., power law index), geometric parameters (e.g., pitch for conveying screw elements, disk width for kneading blocks), and operating conditions (e.g., q/N), to account for non-Newtonian behavior and other deviations of the theoretical models.
- k_D, k_P are empirical fitting constants (in general, different for each screw element, machine size, and possibly, each *class* of materials or processes).

The geometric functions (A, B) may be considered an invariant part of the simulator, while the semi-empirical ones (f, g) may differ for optimized versions of the program. The actual values of the fitting constants (k) are not part of the simulator itself, being user-selectable in most cases.

For example, for a full screw conveying element, the classical flow analysis in screw channels adapted to intermesh twin-screw geometry lead to:

$$A = \frac{1}{2}\pi D_0 \left[\left(A_F - P_0 \delta_0 \right) \sin\theta \cos\theta + 2 A_I \tan\theta \right] \tag{3}$$

$$B_0 = \sin^2\theta \, \frac{A_F \bar{h}^2}{12} \tag{4}$$

$$B_1 = \cos^2\theta \left(\frac{w}{e} - 1 \right) \frac{P_0 \delta_F^3}{12} \tag{5}$$

where A_F is the free cross section area, A_I is the intermesh cross section area, P_0 is the barrel perimeter, D_0 is barrel bore diameter, $\bar{h}$ is the average channel depth, δ_F is the flight clearance, w is channel width, e is the flight width, and θ is the flight helix angle.

The following functions has been proposed to account for the non-Newtonian behavior in twin-screw channels and flight clearances [5]:

$$f = \cos^{\frac{1-n_0}{n_0}} \theta \tag{6}$$

$$g_0 = \frac{1}{\cos^{1-n_0} \theta \cdot n_0^{1-\sin\theta\cos\theta}} \tag{7}$$

$$g_1 = \frac{1}{n_1^{0.94}} \tag{8}$$

These functions may be obtained from detailed simulations using FEM or FAN software packages.

Temperature Gradient in Conveying Screw Elements.

The energy balance in a melt conveying screw element leads to:

$$\hat{c}q\frac{dT}{dz} + \frac{q}{\rho}\frac{dp}{dz} = k_V\left\{\phi A_0\dot{e}_V + A_1\dot{e}_V'\right\} - k_H B h_P\left(T - T_B\right) \tag{9}$$

$\dot{e}_V$ and $\dot{e}_V'$ are the net power input per unit volume in the screw channels and tip clearances, respectively, h_P is the polymer-side heat transfer coefficient, ϕ is the local fill factor, $\hat{c}$ is the specific heat, and T_B is the barrel wall temperature. A_0, A_1, and B are functions of the geometry and k_V and k_H are empirical fitting constants.

In this case the geometric function A_0 is simply the total free cross-section area (minus the tip clearances), A_1 is the total tip clearance cross-section area; and B is the barrel perimeter. The viscous dissipation per unit volume can be readily estimated. In the screw channels:

$$\dot{e}_V = \eta(T, \dot{\gamma}, w)\frac{\left(\pi N D_0\right)^2 + \left(q/\rho A_F\right)^2}{\bar{h}^2} \tag{10}$$

and in the tip clearances:

$$\dot{e}_V' = \eta(T', \dot{\gamma}', w')\frac{\left(\pi N D_0\right)^2}{\delta_F^2} \tag{11}$$

There is some uncertainty in the literature regarding the best estimate for the heat transfer coefficient h_P. For example, Todd [7] proposed the correlation:

$$h_P = 0.94 \cdot \frac{k}{D_0}\left\{\frac{\rho N D_0^2}{\eta(T, \dot{\gamma}, w)}\right\}^{0.28}\left\{\frac{\hat{c}\,\eta(T, \dot{\gamma}, w)}{k}\right\}^{0.33} f_T^{0.14} \tag{12}$$

with

$$f_T = \frac{\eta(T, \dot{\gamma}, w)}{\eta\left(\tfrac{1}{2}\left[T + T_B\right], \dot{\gamma}, w\right)} \tag{13}$$

Actually, Eq. (12)-(13) provide a good conservative estimate of the heat transfer performance of the extruder. A more "optimistic" estimate can be obtained by adapting to the twin-screw geometry the well-known model proposed by Janeschitz-Kriegl and Schijf for single-screw extruders [8]:

$$h_P = 2\frac{k}{\delta_F}x \cdot \left\{\frac{\exp\left(-x^2\right)}{\sqrt{\pi}} + \frac{\operatorname{erf} x}{2x} - x\left(1 - \operatorname{erf} x\right)\right\} \tag{14}$$

with

$$x = \tfrac{1}{2}\delta_F\sqrt{\frac{\pi N D_0}{\phi\alpha}} \tag{15}$$

where k and α are the thermal conductivity and diffusivity ($k/\rho\hat{c}$) of the material at the local processing conditions.

Instead of trying to establish the *best* model, the developer of a process simulator may implement both and let users select the most appropriate for the machine-material-process combination at hand, or use *both* models to generate upper and lower bounds for the relevant parameters.

Melting in Kneading Blocks.

A general form of the energy balance in a partially molten (or softened) material is:

$$q\left(\hat{c}_m\frac{dT}{dz} - \lambda_m\frac{dw_S}{dz}\right) = \frac{d\dot{E}_M}{dz} \tag{16}$$

where w_S is the unmolten polymer (solids) fraction, $\hat{c}_m$ is the specific heat of the partially molten material, and λ_m is effective heat of fusion. The standard procedure is to set $\lambda_m = 0$ for amorphous materials and $\hat{c}_m = 0$ (at the melting point $T = T_m$) for semicrystalline ones. E_M is the net power input or rate of energy dissipation.

Several melting models have been proposed to relate the net power input E_M to the relevant design and operating parameters [9-11]. Most are modifications or combinations of two classical models: the solid bed, drag removal, conductive model developed by Tadmor [12] for single-screw extruders, and a simplified version of the dissipative mix-melting model [3] where the energy required to melt the material is provided mostly by viscous dissipation in the already molten material [13].

Recently, a new approach was proposed [14-15] that emphasizes the energy dissipation by plastic deformation of the solid polymer particles (e.g., in the strong elongational fields, in the kneading blocks' intermesh region), along with other more traditional mechanisms such as polymer-wall and polymer-polymer friction, heat transfer, and viscous dissipation. This *advanced dissipate mix melting model* is theoretically sound and well grounded in the available experimental evidence.

A simple, preliminary implementation of the concept add up contributions for the different mechanisms:

$$\begin{aligned}\frac{d\dot{E}_M}{dz} = {} & k_F^{(m)} pF(f, \theta) N w_S + \left\{k_C^{(m)} A_C \sigma_Y + k_S^{(m)} A_S \tau_Y\right\}\frac{N}{q} w_S \\ & + k_V^{(m)}\left\{A_0 \dot{e}_V\left(1 - w_S\right) + A_1 \dot{e}_V'\right\} + k_H^{(m)} B h_M\left(T_B - T\right)\end{aligned} \tag{17}$$

where p is the pressure, F is a function of geometrical parameters and frictional properties [16], σ_Y and τ_Y are the compressive and shear yield stresses at the processing conditions, and h_M is the heat transfer coefficient between the partially molten material and the barrel. The viscous dissipation ($\dot{e}_V$) and associated geometric functions (A_i) are interpreted as in the previous example. The specific melting constants $k^{(m)}$ are determined based on freezing experiments. The geometric functions associated with the plastic compressive and shear contributions can be estimated as a first approximation as:

$$A_C \approx 2n_F\left(1+\frac{A_I}{A_K}\right)A_I \tag{18}$$

$$A_S \approx \left(2n_F - 1\right)\pi\frac{A_K D_0}{\bar{h}} \tag{19}$$

where n_F is the number of flights and A_K is the channel cross-section area defined as:

$$A_F = (2n_F - 1)A_K + A_I \tag{20}$$

The examples presented in this section show how extensible, semiempirical, one-dimensional lumped-parameters models can be developed for some processing steps involved in twin-screw compounding operations. Similar models have been generated for most processing steps, including mixing and devolatilization. Validation of this approach against experimental results will be presented in a companion paper.

Implementation

Once a series of mathematical models is developed, they must be implemented within a computer program. The models must be translated into numerical algorithms, and the algorithms translated (coded) into a computer program. This module becomes the "simulation engine" at the core of the simulator. Details of this process are beyond the scope of this presentation. In any case, the procedures required for one-dimensional simulators such as the ones considered here are relatively simple.

In addition, a process simulator must include an interface to interact with its users, and a series of services to manage internal communications, validate results, handle errors and exceptions, etc. Users often overlook this part of the development (for good reason: successful implementations are based on transparent internals and "natural" user interfaces). However, in practice these components account for most of the computer code and effort (therefore, the cost) dedicated to the development of a *general-purpose* process simulator.

The following discussion is set in general terms, thus applicable to most currently available simulators; examples are taken from the Twin-Screw Extruder Simulator (TXS™) software package. Figure 2 shows the simplified flow chart corresponding to a typical simulation run, involving a straightforward sequence of steps:

(1) A specific extruder is selected from a list of supported machines, allowing the simulator to establish the available components, and the process capabilities and limitations of the machine.

(2) An extruder configuration is generated (or recalled from a database of previously created and saved configurations). The configuration process involves selecting a shaft, a sequence of barrel sections and screw elements, a head adapter, die plate, etc. The modular nature of modern twin-screw extruders allows the simulator to precompute and store most geometric parameters related to individual machines and components in an *Extruder Database*. The *Configurations Editor* enforces simple rules and constraints in order to maintain a one-to-one correspondence between configurations that can be generated within the simulator and configurations that can be assembled in the real world. Appropriate design and suitable graphical user interface can greatly enhance the value and ease of use of the simulator, which then becomes a powerful visualization tool for twin-screw extrusion. Figure 3 shows TXS screw configuration screen illustrating this theme.

(3) Feed materials (resins, fillers, additives, etc.) are selected from a list of available items, and a complete set of operating conditions is imposed. The operating conditions must be consistent with the previously selected extruder and material specifications. Optionally, processing options and other user-selectable simulation parameters can be set at this stage. Figure 4 shows TXS operating conditions screen.

(4) The simulation is performed by the main component of the program, the simulation engine.

(5) The results are displayed on the screen in tabular or graphics form, stored for later analysis, printed, etc. Figure 5 shows a typical axial temperature plot, with the results obtained using two different heat transfer models. Data analysis modules may be loaded at this time to perform a more detailed examination of the results.

External utility programs or internal modules (*Extruder Editor*, *Materials Editor*) can be used to manage the databases, add new entries or modify existing ones. These utilities may be used also input the machine and/or material-specific adjustable parameters discussed in the previous section.

Simulators should not be evaluated based only on the accuracy and reliability of models *currently* implemented. Issues such as how easy (or difficult) is to adjust the models to new materials and processes, add new features or implement alternative models are probably more important in the long term.

Conclusions

A careful selection of modeling techniques allows the development of fast, versatile, and reasonably accurate process simulators for the analysis of plastics compounding operations in twin-screw extruders.

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Keywords: Twin-Screw Extruder, Mathematical Modeling, Process Simulator, Software

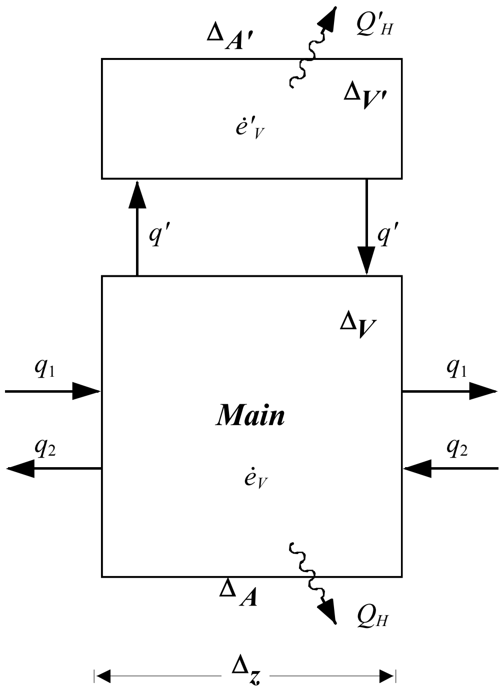


Figure 1. Axial Element.

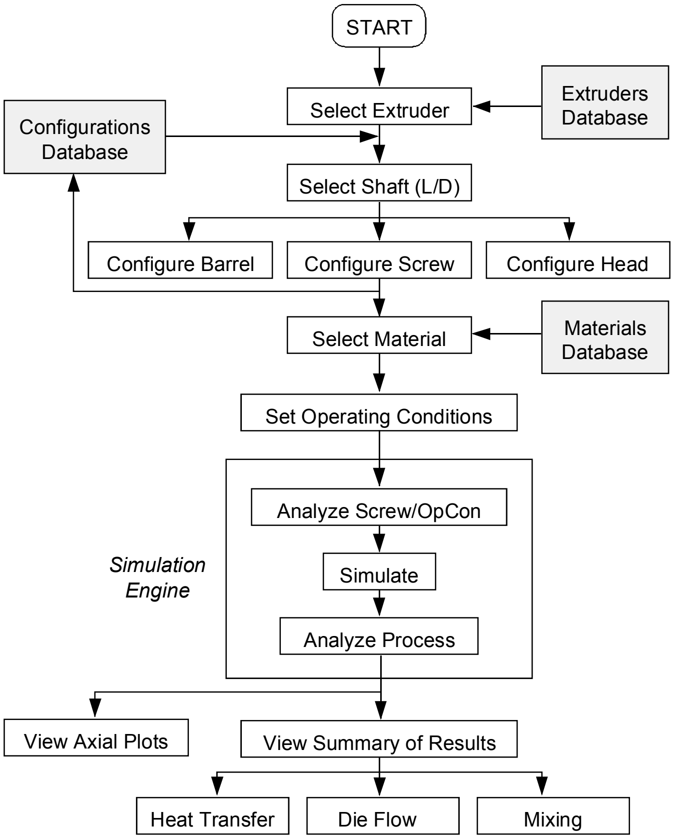
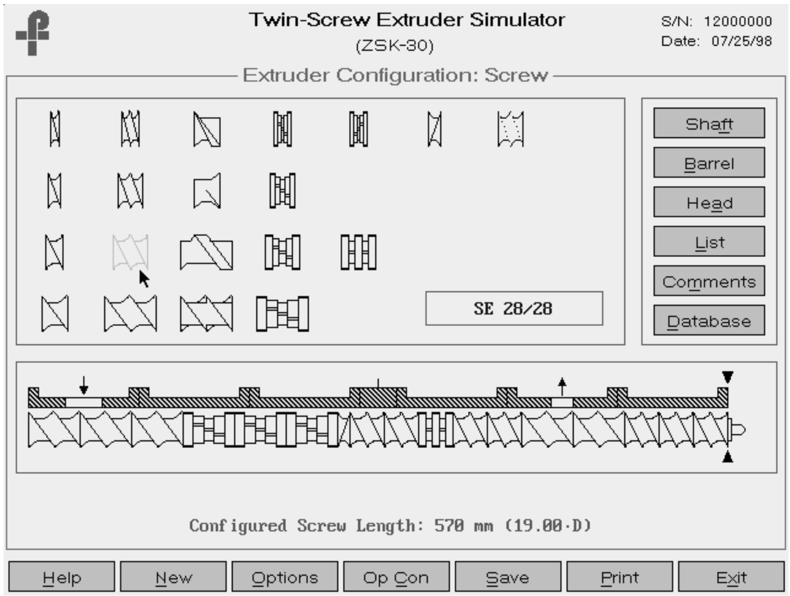


Figure 2. Typical run in Twin-Screw Extruder Simulator (TXS)



Twin-Screw Extruder Simulator
(ZSK-30)

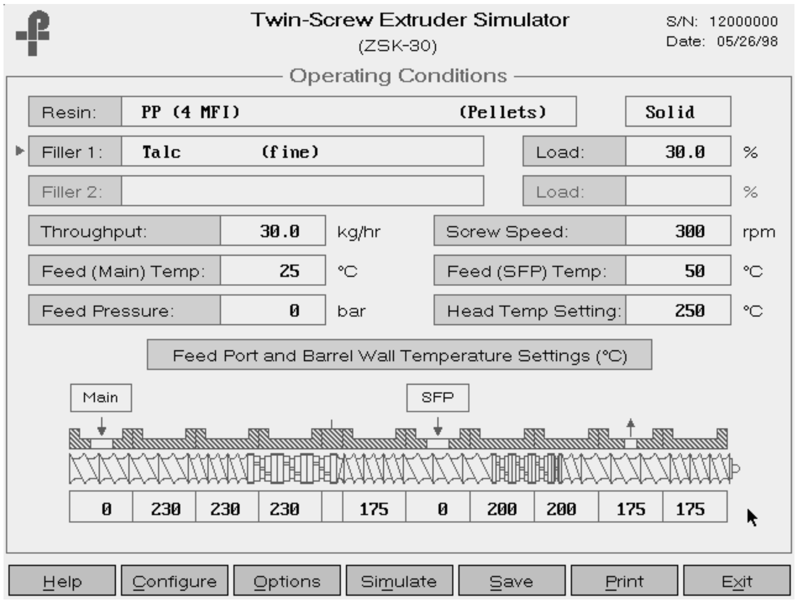
S/N: 12000000
Date: 07/25/98

Extruder Configuration: Screw

SE 28/28

Configured Screw Length: 570 mm (19.00·D)

Figure 3. Typical Extruder Configuration screen (TXS)



Twin-Screw Extruder Simulator
(ZSK-30)

S/N: 12000000
Date: 05/26/98

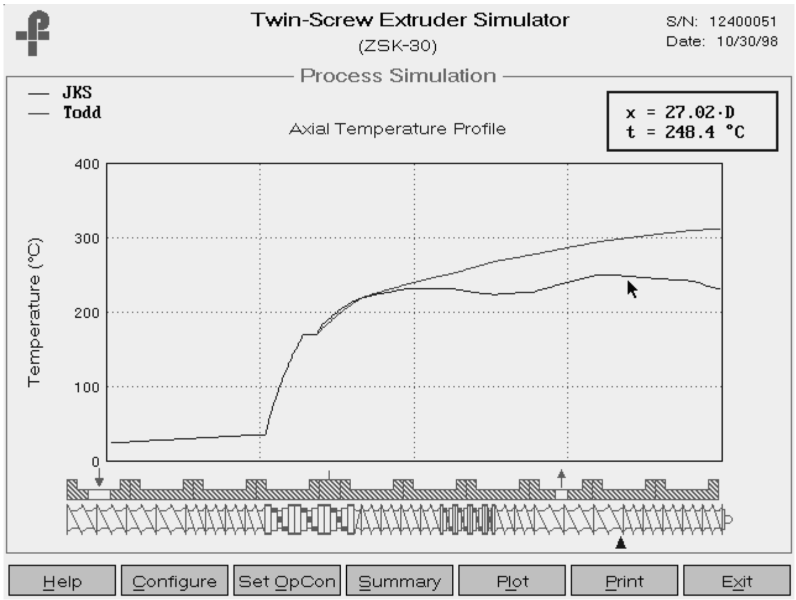
Operating Conditions

Resin: PP (4 MFI) (Pellets) Solid
Filler 1: Talc (fine) Load: 30.0 %
Filler 2: Load: %
Throughput: 30.0 kg/hr
Screw Speed: 300 rpm
Feed (Main) Temp: 25 °C
Feed (SFP) Temp: 50 °C
Feed Pressure: 0 bar
Head Temp Setting: 250 °C

Feed Port and Barrel Wall Temperature Settings (°C)

0	230	230	230		175	0	200	200	175	175

Figure 4. Typical Operating Conditions screen (TXS)



Twin-Screw Extruder Simulator
(ZSK-30)

S/N: 12400051
Date: 10/30/98

Process Simulation

x = 27.02·D
t = 248.4 °C

Figure 5. Typical Simulation Results: Axial Plot screen (TXS)