



TXS™ Advanced Features

Users can, in some instances, modify the appearance or alter the execution of TXS to suit their particular needs through user-selectable program options. Program options are used to change the display, control the printing operations, add special features, or modify the computations performed by the simulation engine.

All available program options can be set in TXS initialization file (TXS.INI). The initialization file is an ordinary text file and can be edited by the user with any text editor, such as EDIT (that comes with MS-DOS version 4 or later) or NOTEPAD (that comes with Microsoft Windows 3.x and Windows 95). Most word processing programs can also be used to edit TXS.INI, provided the changes are saved as text without special formatting codes. Entries in the initialization file must follow the format:

```
keyword = value
```

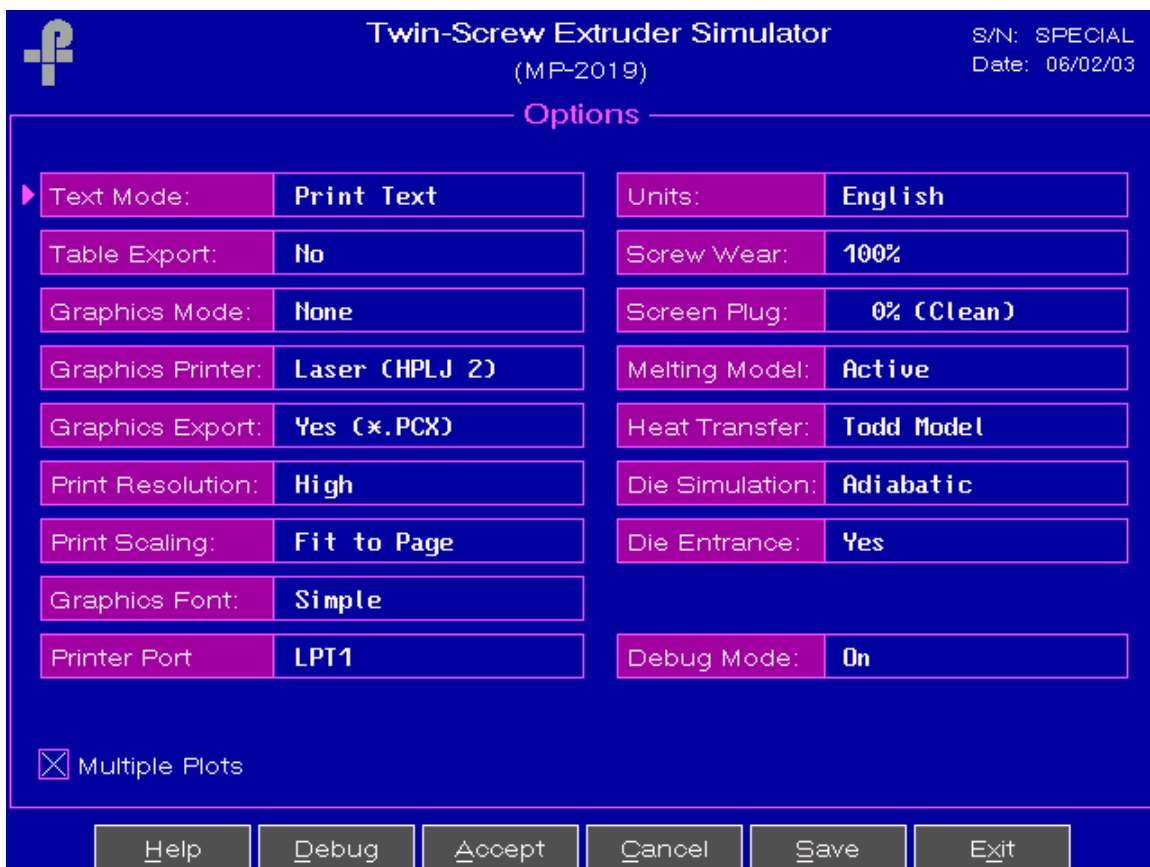


Figure 1 Options screen

A few program options can be modified at run time using the **Options** screen (Figure 1), which can be opened from the **Extruder Configuration** or **Operating Conditions** screens with



the **Options** command. Changes to program options made in this way can be saved to the initialization file. The **Options** screen includes selection boxes and buttons to show the current value of several program options and to allow users to modify them. On the left, there are nine selection boxes to set the printing control parameters: **Text Mode**, **Table Export**, **Graphics Mode**, **Graphics Printer**, **Graphics Export**, **Print Resolution**, **Print Scaling**, **Graphics Font**, and **Printer Port** (these features are disabled in the demo version). On the bottom left corner, the **Multi-Plot** selection button enables or disables the Multi-Plots option, allowing the representation of several simulation runs in the same axial plot. On the right, there are eight selection boxes to set the **Units** used by TXS to display the operating conditions and the results of the simulations, to select processing options: **Screw Wear**, **Screen Plug**, **Melting Model**, **Heat Transfer**, **Die Simulation**, and **Die Entrance**, and to activate the **Debug Mode** (see below).

The screen also includes six command buttons: **Help** (shortcut ALT-H or F1) to open the **Help** screen, **Debug** (shortcut: ALT-A) to set the debug calibration factors, **Accept** (shortcut: ALT-A) to accept the current settings, **Cancel** (shortcut: ALT-C) to disregard all changes, **Save** (shortcut: ALT-S) to accept the current settings and save them to TXS initialization file (TXS.INI), and **Exit** (shortcut: ALT-X or ESC) to exit the program. The **Accept**, **Cancel**, and **Save** commands close the screen and return control to the place where the **Options** screen was open, either the **Extruder Configuration** or the **Operating Conditions** screens.

To select a particular box, click with the mouse on the box once or move the selection pointer (▶) using the UP/DOWN or TAB/SHIFT-TAB keys. Selected boxes with more than two choices (e.g., **Screw Wear**, **Screen Plug**, **Heat Transfer**, **Die Simulation**) are opened by pressing the ENTER key, to display a drop-down menu with its own selection pointer. When a selection box is open, all user input is directed to that particular box until it is closed. You can navigate the drop-down menu using the mouse or the UP/DOWN arrow keys (unavailable items are skipped). To complete a selection and close the box, press the ENTER key or double-click with the mouse on a particular choice. To restore the previous assignment press the ESC key. Double-clicking with the mouse combines selection and opening. Selected boxes with only two choices (e.g., **Units**) use the ENTER key to switch between the choices. Selection buttons control two states to enable (box with ✕) or disable (box empty) a feature; use the ENTER key to switch between the two states.

TXS's speed and "user-friendliness" encourages its use on a trial and error basis, to explore and test new ideas and perform quick and inexpensive "computer experiments". To facilitate this process TXS offers, whenever possible, user-controlled alternative paths of execution. As a partial embodiment of this design philosophy, the standard version of TXS includes six processing options that can be rapidly set or modified at run time, using six selection boxes in the **Options** screen: **Screw Wear**, **Melting Model**, and **Heat Transfer**, which affect the main extruder simulation if enabled, and **Screen Plug**, **Die Simulation**, and **Die Entrance**, which affect the extruder head simulation if enabled.

Screw wear may significantly affect the processing condition in twin-screw extrusion. In its first stages, it involves an increase in the tip clearances, resulting in a diminishing conveying capacity. TXS allow users to simulate this condition to obtain a more realistic appraisal of processing characteristics over the life of the extruder.

In TXS, the screw wear is set as the percent fractional increase in screw tip clearance; for example, a screw wear of 50% means that the simulation will be performed assuming that the screw tip clearances are 1.5 times the tip clearance values stored in the Extruders Database for new extruders. In the initialization file (TXS.INI), you can set the increase in tip clearances to any integer value between 0 (new screw) and 200% (that is, a tip clearance three times the original). The **Screw Wear** selection box lets you choose between four settings 0 (default), 20%, 50%, and 100% screw tip increase.

Heat transfer in twin-screw extruders is not a completely settled issue and several models are presently available that claim to represent the heat transfer characteristics of operating extruders. Since it is difficult at this time to choose between conflicting claims (that may well depend on extruder size), TXS offers several alternatives. The following heat transfer models are currently supported by TXS and can be selected in the **Heat Transfer** box:

- **Isothermal.** The simulations are performed assuming that the material is always at a constant temperature equal to the feed temperature. Thermal effects are not taken into account by the simulation engine. Axial temperature, viscous dissipation and heat transfer profiles are not available for isothermal simulations, which can only be performed for melt-fed extruders. This model is intended for use in comparative studies and is *not* a realistic representation of most processing conditions.
- **Adiabatic.** The simulations are performed assuming that there is no heat transfer to or from the barrel. Axial temperature and viscous dissipation plots are available for adiabatic simulations; heat transfer data is not. This model may be useful for comparative studies, in special circumstances, and for large extruders, where heat transfer is minimal.

With the next options TXS performs a complete calculation of the thermal effects based on the barrel wall temperature profile set in the operating conditions and a suitable model to evaluate the polymer-side heat transfer coefficient. TXS supports three models:

- **Todd Model.** The polymer side heat transfer coefficient is computed based on the semi-empirical model developed by Todd (1988)*. Todd's model is a conservative approach to the problem and provides a lower bound to the heat transfer capacity of the extruder. This selection is set as the default heat transfer model.
- **JKS Model.** The polymer side heat transfer coefficient is computed based on a custom modification of the classic model developed by Janeschitz-Kriegl and Schijf (1956)* for single-screw extruders. JKS model is an optimistic approach to the problem and provides an upper bound to the heat transfer capacity of the extruder.



- **JKS/DJ Model.** This model, based on original unpublished developments, is a modified version of the JKS model that addresses, in a more realistic way, viscous heat dissipation and heat transfer in screw tip clearances; the acronym DJ acknowledges the influence of a recent paper by Domschke and Justus (1993)** in this work. This model, which appears to be an improvement over the traditional JKS approach, has yet to be experimentally verified.

* D. B. Todd, “Heat Transfer in Twin-Screw Extruders”, *SPE Tech. Papers* **34**, 54-58 (1988).

* H. Janeschitz-Kriegl and J. Schijf, “A Study of Radial Heat Transfer in Single-Screw Extruders”, *Plastics and Polymers* **37**, 523-528 (1969).

** T. Domschke and C. Justus, “Heat Transfer in Single and Twin Screw Extruders”, *Intern. Polymer Proc.* **8**, 294-307 (1993).

It is recommended that first-time simulations in small or medium size extruders (under 100 mm nominal diameter) be performed with both the Todd and JKS models. Our experience indicates that the heat transfer characteristics of the extruder will be bounded by the two results.

Screens are used as melt filtering devices to prevent unmolten polymer, undispersed solid agglomerates, and debris from reaching the die and either contaminate the pellets, negatively affecting product quality, or plug in the die openings, causing a complete system failure. In the course of its intended use, screens become clogged and must be replaced with new, clean screens usually by means of manual or automatic screen changers. Dirty screens greatly affect the performance of the extruder, increasing both the head pressure (which in turn affects the screw simulation) and the head temperature rise. In TXS, partial screen clogging is set as the percent fraction of the screen area unavailable for melt flow; for example, a screen plug of 20% means that the head flow simulation will be performed assuming that the screens, if configured, have only 80% of the normal cross-section area. In the initialization file (TXS.INI), you can set the decrease in screen area to any integer value between 0 (clean screen) and 80% (that is, one fifth of the normal screen area available for melt flow). The **Screen Plug** selection box lets you choose between four settings 0 (default), 10%, 20%, and 50% screen clogging.

TXS offers two alternative models to evaluate the thermal effects in head, which can be selected in the **Die Simulation** box:

- **Isothermal.** The head simulation is performed assuming that the material is always at a constant temperature equal to the temperature at the discharge end of the screw. How this temperature is established depends on the selected *extruder* simulation heat transfer model.
- **Adiabatic.** The head simulation is performed assuming that there is no heat transfer to or from the head.

Melting in twin-screw extruders is the least understood process step. No satisfactory *quantitative* model is presently available. TXS offers two alternatives selected through the **Melting Model** box:

- **Passive Bed.** The melting process is simulated using the classical melting model developed by Zehev Tadmor for single-screw extruders in the 1960s, adapted to the twin-screw extruder geometry. The version implemented in TXS is based in the published work of Prof. White and Prof. Potente*. This model does not require specific empirical coefficients and may be utilized in cases where little information on the melting behavior of the polymer is available.
- **Active Bed.** The melting process is simulated using a custom model based on the ideas developed by Zehev Tadmor, Costas Gogos, and collaborators at Polymer Processing Institute (PPI) in past several years**. Several energy dissipation mechanisms are considered: heat transfer from the barrel, plastic deformation of the particulate solid by compressive and shear stresses, polymer/wall and polymer/polymer friction, and viscous dissipation in the partially melt. This model may be considered the one that best represents the physics of the melting process, but the approximate nature of the models used to estimate the contribution of each melting mechanism requires the use of material-dependent empirical coefficients (Melting Coefficients) stored in the Materials Database.

4.13.2. Debugging

TXS let users temporarily modify the values of some physical properties, material parameters and process variables utilized by the simulator. The feature may help “debugging” problem simulations, and should be used with extreme care, only if you suspect that the physical properties of the materials and/or the general purpose process models utilized by TXS might be incorrect in a particular case. This new feature is controlled by the **Debug** flag set within the **Options** screen. Setting the flag to ON enables the use of user selected empirical calibration factors in the current simulation (setting it to OFF disables the use of the calibration factors, no matter their current value). The debug flag can be preset in the initialization file TXS.INI by adding to it the following line:

debug = n

where **n** = 0 (OFF, the default) or **n** = 1 (ON).

The factors themselves are set in the **Calibration Factors** window (Figure 2), that can be opened using the **Debug** (shortcut: ALT-D) command button in the **Options** screen. The window

* S. Bawishkar and J. L. White, “Melting Model for Modular Self Wiping Co-Rotating Twin Screw Extruders”, *Polym. Eng. Sci.* **38**, 727-740 (1998).

** C. C. Gogos, Z. Tadmor and M. H. Kim, “Melting Phenomena and Mechanisms in Polymer Processing Equipment”, *Adv. Polymer Technol.* **17**, 285-305 (1998).

contains eight input boxes that allow users to set up the values for calibration factors, and three command buttons: **Set** (shortcut: ALT-S) to accept the current values, **Reset** (shortcut: ALT-R) to reset all factors to their default values (see below), and **Cancel** (shortcut: ALT-C) to undue recent changes and return to the previous values. All commands close the **Calibration Factors** window and return to the main **Options** screen.

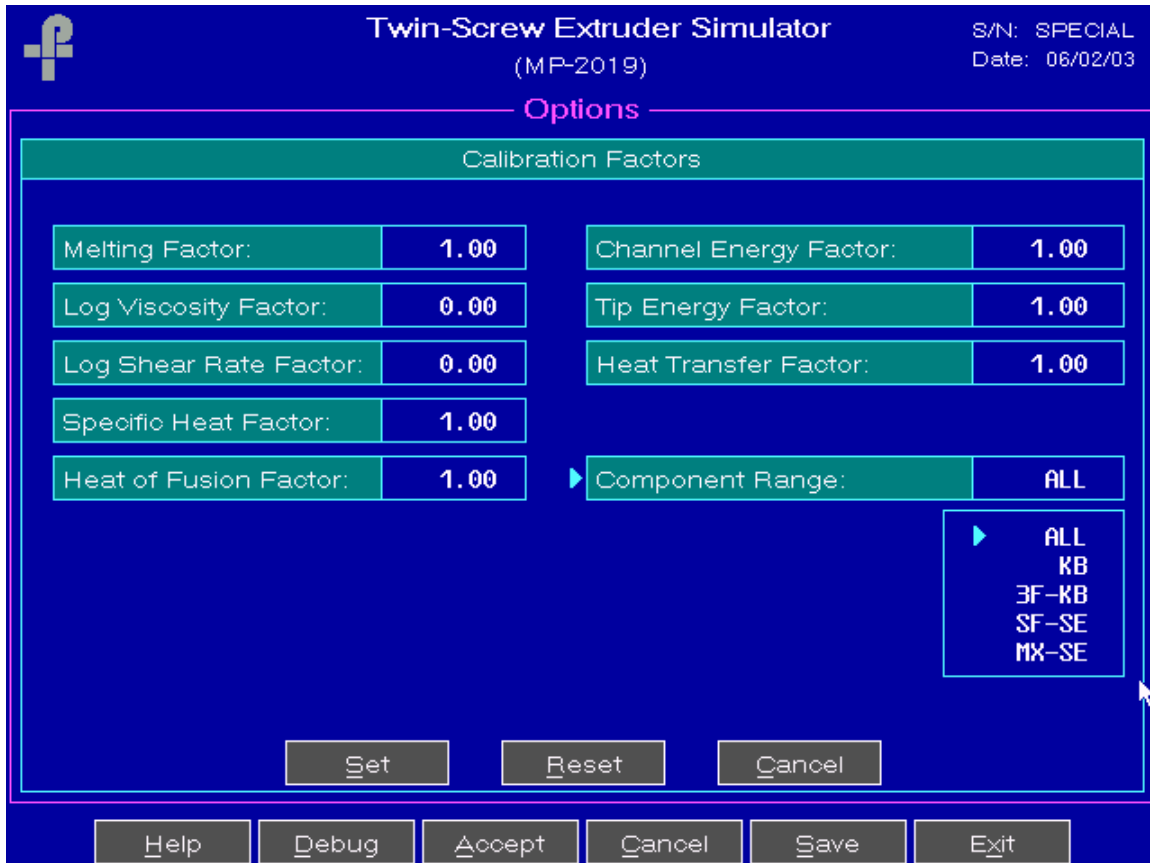


Figure 2 Calibration Factors window

The following calibration factors are currently supported:

1. **Melting Factor** (keyword: **km0**) affects the active-bed melting model coefficients.
2. **Log Viscosity Factor** (keyword: **km1**) affects the material viscosity.
3. **Log Shear Rate Factor** (keyword: **km2**) affects the shear rate (only for viscosity calculations).
4. **Specific Heat Factor** (keyword: **km3**) affects the material specific heat
5. **Heat of Fusion Factor** (keyword: **km4**) affects the latent heat of fusion of semicrystalline resins.
6. **Channel Energy Factor**(keyword: **ks0**) affects the rate of energy dissipation in the screw channel.
7. **Tip Energy Factor** (keyword: **ks1**) affects the rate of energy dissipation in the flight tip gaps.
8. **Heat Transfer Factor** (keyword: **ks2**) affects the polymer-side heat transfer coefficient.

All factors (except 2 and 3, **Log Viscosity Factor** and **Log Shear Rate Factor**) have an acceptable range of 0.02 to 50, with a default value of 1. All are “multiplicative” factors, applied as:



$$p_{\text{eff}} = k \cdot p$$

where p is a property, material parameter of process variable and k is the factor. **Log Viscosity Factor** and **Log Shear Rate Factor** are “additive” factors, working as,

$$\log_{10} \phi_{\text{eff}} = k + \log_{10} \phi$$

where ϕ is the viscosity or shear rate and k is the factor. The acceptable range for these factors is -5 to 5 , and the default value is 0 .

All factors can be preset in the initialization file TXS.INI using the familiar construct:

keyword = value

where **value** is an integer or real number within the acceptable range, using the appropriate **keyword** (see above).

The first five factors (those with keywords **km...**) correspond to material-dependent parameters and are applied (when enabled) to the whole screw. The last three (those with keywords **ks...**) correspond to machine-dependent process variables and could be applied only to certain screw components. The range of applicability of these factors is selected with the **Component Range** box in the **Calibration Factors** window. Currently there are five options (default is **ALL**):

0. **ALL** Applies to all screw components (except spacer rings).
1. **KB** Applies only to all kneading blocks. Does not affect other screw components.
2. **KB-3F** Applies only to trilobe kneading blocks (eccentric or not) when used in double-flighted extruders. Does not affect other screw components.
3. **SE-SF** Applies to single-flighted screw elements. Does not affect other screw components.
4. **SE-MX** Applies to slotted-flight (SME, ZME) and gear (turbine) mixing elements. Does not affect other screw components.

The component range can be preset using the keyword **kss**. Factors (and component range) settings can be stored into the initialization file using the **Save** command in the **Options** screen.

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