



TXS™ Simulation Engine

1. Introduction

We present in this document a brief explanation on how flow and heat transfer in a twin-screw extruder processing chamber are modeled, how these models are used by TXS to simulate the process, and how TXS users can control most aspects of the procedure. TXS utilizes simple mathematical models, and simple numerical schemes to solve the model equations, as befits to a fast, general-purpose simulator. Specific process applications often require modifications of models and/or numerical methods, and a *basic understanding* of both is needed to take advantage of the many user adjustable control parameters available within TXS. The only purpose of this document is to provide this basic understanding. It is *not* a general presentation of mathematical models or process simulation techniques for twin-screw extruders. Another brief treatment of the subject, more or less complementary of this one, can be found in the ANTEC 99 presentation by E. L. Canedo, “Computer Simulation of Plastics Compounding Operations in Twin-Screw Extruders”, *SPE Tech. Papers* **45**, 310-316 (1999).

2. A simulation example

Let us consider a very simple twin-screw extrusion process (Figure 1): Q (kg/hr) of a molten polymer is fed at T_F (°C) into a modular corotating twin-screw extruder rotating at N (rpm) and is delivered at the head at p_{HEAD} (MPa). The extruder is configured with a variety of forward and reverse conveying elements and kneading blocks, and the inner surface of the barrel is kept at T_B (°C). Let us assume that material properties (melt density ρ and specific heat \hat{c}) are constant, independent of melt temperature, except the melt viscosity η , which is assumed to be a strong function of temperature and shear rate.

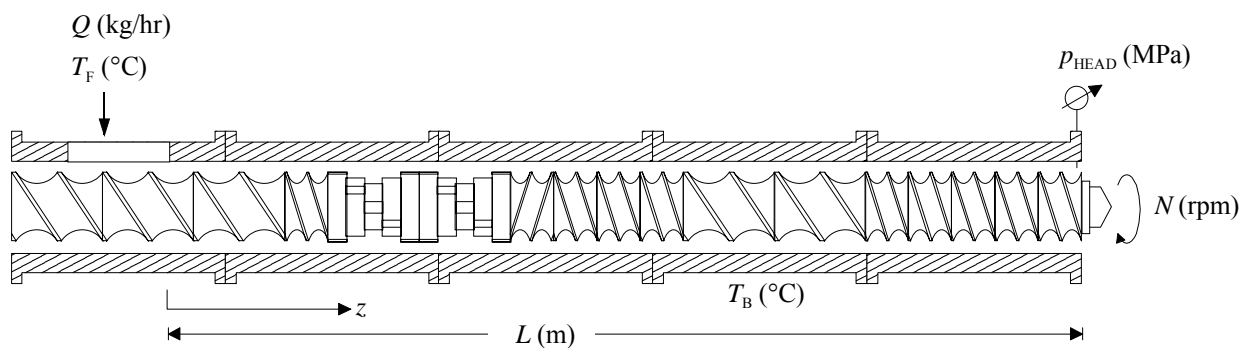


Figure 1

TXS simulates the extruder from the downstream edge of the main feed port to the end of the last configured screw element, excluding the end plug, over an axial length L (m). These are the limits in our conventional definition of “screw flow”. The region within the feed port is considered to be affected too greatly by the open port to be part of the “developed” screw flow, while the region beyond the last screw element is considered to be part of the “head flow”.



This simple example contains all the necessary detail. Solid feed (melting inside the extruder), solid and liquid additives, multiple feed and injection ports, etc. would make the example more realistic, but would also make modeling more complex, and distract from the *essential* features of process modeling and simulation that we wish to consider.

In this case, to simulate the extrusion process means to estimate the axial pressure and temperature profiles, $p(z)$ and $T(z)$, $0 < z < L$, based on the known extruder geometry, material properties and operating conditions. There are many other process variables we could and would estimate, such as power consumption, residence time, etc., but all of them can be computed once melt temperature and pressure profiles inside the extruder processing chamber are estimated. Notice that we consider pressure and temperature to be functions of the axial coordinate alone. There are, of course, significant radial and circumferential gradients (particularly in temperature), but we are considering here only cross-section averages. Thus, when we say “temperature” we should understand “cross-section average temperature”, and so on.

3. Modeling flow and heat transfer in the extruder

Modeling flow and heat transfer in extruders (twin-screw extruders in particular) is a tricky proposition. The geometry of the processing chamber (the extruder channels and gaps), especially in twin-screw extruders, and the rheological behavior of the melt are very complex, to the point that theoretical models are extremely difficult to establish, let alone to solve. Consequently, successful process models consist of a mixture of “oversimplified” theory, semi-empirical correlations, and empirical “adjusting coefficients”, with plenty of exceptions and “special treatments” for this or that particular case. For the present purpose, we are going to keep only the first component, the “oversimplified” theory, that neglects gaps and views the extruder channel as little more than the space between two parallel plates, separated by a distance h (the screw channel depth), one stationary and the other moving at a speed of πND_0 , (where D_0 is the barrel bore diameter) at an angle θ (the real or equivalent helix angle, according to the screw component). Mass, momentum, and energy balances are used to obtain the model equations.

Mass and momentum balances result in the well-known “flow equation”:

$$q = AN + \frac{B}{\eta} \cdot \frac{dp}{dz} \quad 0 < z < L \quad (1)$$

Here, q is the volumetric melt flow, a constant along the extruder in our example (we assumed uniform melt density), N is the screw rotation speed, an operating condition in its own right, and η is the melt viscosity, a function of shear rate and temperature, that varies along the extruder; A and B are functions of the extruder geometry, characteristic of each screw component. For example, the simplest flow model for full conveying elements makes $A = \frac{1}{2} \pi D_0 A_F \sin\theta \cos\theta$, $B = 1/12 h^2 A_F \sin^2\theta$ (A_F is the cross section free area). TXS utilizes more complex flow model, making A and B functions of some material parameters (e.g., power law index n) and operating conditions (e.g., specific rate q/N), but for the sake of this example A and B can be considered as known, albeit complex, functions of the axial coordinate alone.

Physically, Eq.(1) says that the flow rate (left hand side) is the sum of two components: drag flow (first term in the right hand side) and pressure flow (second term in the right hand side). The situation is a little more involved since, even in this simplified case, the pressure flow component depends on the drag flow



through the shear rate dependence of the viscosity. Care should be taken of the signs of each term. For example, in forward conveying screw elements, drag flow is positive (pushes the melt forward), while pressure flow (if the screw channels are full) is usually negative (pushes the melt backwards) making $dp/dz < 0$.

An energy balance leads, in its most simple case, to the expression:

$$q \frac{dT}{dz} = C\phi\eta N^2 - DU(T - T_B) \quad 0 < z < L \quad (2)$$

where ϕ is screw fill level, U is the heat transfer coefficient between the melt and the barrel, T_B is the barrel temperature, and C and D are known functions of geometric parameters and physical properties.

Physically, Eq.(2) says that the rate of increase of the internal energy of the melt (left hand side) is the result of the balance of two opposite factors: the rate of energy “generation” (viscous dissipation) within the melt (first term in the right hand side) and the rate of energy transfer to the barrel (second term in the right hand side). Again, we must say that Eq.(2) is a drastic simplification, but it serves our purpose here.

TXS allows users to modify the model equations using a variety of empirical adjusting coefficients. These “debugging aids”, described in the *TXS User’s Manual* (version 2), are available within the program in the Options screen.

4. Simulation: solving the model equations

The flow and energy balance equations, Eq.(1)-(2) involve the axial gradients of pressure and temperature (dp/dz , dT/dz). Integration of Eq.(1)-(2) with the appropriate boundary conditions leads to the pressure and temperature profiles, $p(z)$ and $T(z)$. We know the pressure at one end (head pressure p_{HEAD} at the discharge end) and the temperature at the other (feed temperature T_F at the feed end), thus appropriate boundary conditions for Eq.(1)-(2) are:

$$p = p_{HEAD} \quad \text{at} \quad z = L \quad (3)$$

$$T = T_F \quad \text{at} \quad z = 0 \quad (4)$$

Straightforward integration of Eq.(1)-(2) with boundary conditions, Eq.(3)-(4), is not possible because (a) the “coefficients” (A , B , etc) depend on the local geometry that changes along a screw composed of different kinds of screw elements (and consequently, the coefficients are complex functions of the axial coordinate z), and (b) the two balance equations are *coupled*, that is, the “pressure” equation, Eq.(1), depends on the temperature through the viscosity (a strong function of the temperature) and the “temperature” equation, Eq.(2), depends on the pressure through the screw fill level ($\phi = 1$ if $p > 0$, $\phi < 1$ if $p = 0$).

As a consequence, the balance equations should be solved using a more involved numerical technique. To that effect, we start by dividing the screw in a series of “slices” (or *computational elements*) resulting in a discretization of the axial coordinate z and, consequently, of all coefficients and processing variables depending on z . TXS automatically divides each screw component in a number of elements (users can affect this subdivision process, as we will see later) with more “points” assigned to more “active”

components (such as kneading blocks and reverse screw elements). Let us call N the total number of computational elements (Figure 2).

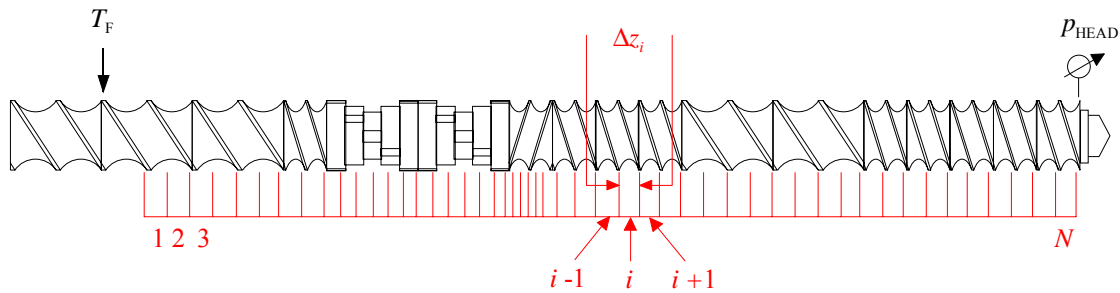


Figure 2

Thus, a discrete set of point values p_i , $i = 0, 1, 2, \dots, N$, replaces the continuous variable $p(z)$, $0 < z < L$, and the same happens with all axial profiles. The differential equations, Eq.(1)-(2), are reduced to two sets of algebraic equations:

$$q = A_i N + \frac{B_i}{\eta_i} \cdot \frac{\Delta p_i}{\Delta z_i} \quad \text{for } i = 1, 2, 3, \dots, N \quad (5)$$

$$q \frac{\Delta T_i}{\Delta z_i} = C_i \phi_i \eta_i N^2 - D_i U_i (T_i - T_B) \quad \text{for } i = 1, 2, 3, \dots, N \quad (6)$$

Boundary conditions, Eq.(3)-(4), are now:

$$p_N = p_{HEAD} \quad (7)$$

$$T_0 = T_F \quad (8)$$

Eq.(5)-(6) are coupled and must be solved using an iterative scheme. TXS uses the following procedure (cf. Figure 3):

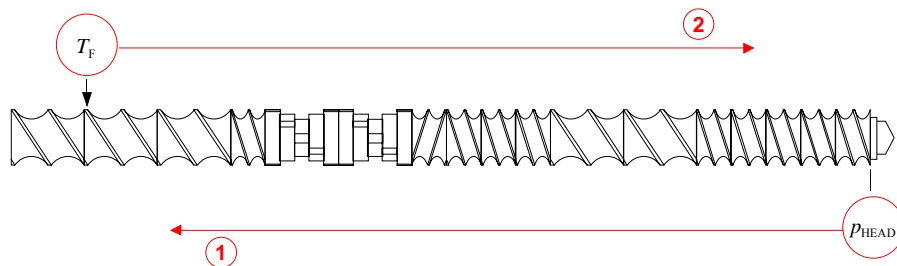


Figure 3

1. A temperature profile T_i , ($i = 0, 1, 2, \dots, N$) is assumed.
2. The “pressure equations”, Eq.(5), are solved successively, from $i = N-1$ to $i = 1$, using the initial condition (at $i = N$), Eq. (7), with viscosities computed at the assumed temperatures, and then the fill factor profile is computed (pass ① in Figure 3).



3. The “temperature equations”, Eq.(6), are solved successively, from $i = 1$ to $i = N-1$, using the initial condition (at $i = 0$), Eq. (8), with the fill factors computed in the previous step 1 (pass ② in Figure 3).
4. The “new” temperature profile computed in step 3 is compared with the “old” temperature profile assumed in step 1. If the two profiles are close enough, according to some tolerance criterion, the iteration procedure ends. The pressure and temperature profiles just computed are taken as “the” pressure and temperature profiles. Auxiliary processing variables (power, residence time, etc.) are computed.
5. If the two temperature profiles are not close enough, a new assumption is made about the temperature profile, based on the “old” and “new” profiles. Steps 1 to 5 are repeated again.

Each repetition of steps 1-5 is called an iteration. If the numerical procedure *converges* the difference between “old” and “new” temperature profiles becomes smaller with each iteration and, eventually, the criterion of step 4 is met. If not, we say that the numerical procedure *diverges* and, after a predetermined (maximum) number of iterations, an error message (“*melt conveying computation failure*”) is returned.

It should be noted that Eq.(5)-(6) are a set of *nonlinear* algebraic equations. Even in the simple example considered here there is no *guarantee*, mathematically speaking, that the numerical procedure outlined above (or any other) will converge to a valid solution in all cases (that is, for all choices of screw configuration, material properties, and operating conditions), or if it converges, that the solution will be unique (independent, for example, of the initially assumed temperature profile). For this reason, TXS provides several control parameters that permit users to modify and adjust, within limits, the actual numerical scheme. For some problems, obtaining a valid solution is essentially a trial-and-error procedure, without the assurances of a “happy ending”.

5. The numerical procedure in detail

Let us examine, step by step, the iterative procedure. In this and the next sections we will use the following notation: $T^{(INIT)}$ will be the initial guess of the temperature profile; $T^{(OLD)}$ and $T^{(NEW)}$ will be the “old” (assumed) and “new” (computed) temperature profiles, within a given iteration; finally, $T^{(NEW OLD)}$ will be the updated temperature profile at the end of given iteration, the one that will have the role of “old” temperature profile in the next iteration.

Step 1:

In some cases, an adequate selection of the initial temperature profile could make the difference and, if the system converges, the closest the initial guess to the “true” (final) profile the fastest the converge. TXS offers several choices (cf. Section 6.2 below):

- (a) $T_i^{(INIT)} = T_F$ for $i = 1, 2, 3, \dots N$
- (b) $T_{ii}^{(INIT)} = T_{OP}$ for $i = 1, 2, 3, \dots N$ (9)
- (c) $T_{ii}^{(INIT)} = T_F + i \cdot (T_{OP} - T_F) / N$ for $i = 1, 2, 3, \dots N$

where T_{OP} is a typical process temperature (a parameter set when the material is specified), which is close, in most cases, to the expected exit melt temperature.

Step 2:

Pressure calculation goes, from the downstream (discharge) end, where $p_N = p_{HEAD}$, to the upstream (feed) end, in $N-1$ steps, for $i = N-1, N-2, \dots, 1$ (pass ① in Figure 3). Within each element, the *pressure increment* in the element is computed from Eq.(5):

$$\Delta p_i = \frac{q - A_i N}{B_i} \eta(T_i) \Delta z_i \quad (10)$$

where T_i is the assumed temperature at the current step. Then, the *pressure* in the element is computed based on the pressure of preceding (downstream) element, taking into account that actual pressure cannot go below the ambient (gauge) pressure:

$$p_i = \max \{0, p_{i+1} - \Delta p_i\} \quad (11)$$

Finally, once the pressure profile is computed, we estimate the *fill level* profile

$$\phi_i = \begin{cases} 1 & \text{if } p_i > 0 \\ \frac{q}{A_i N} & \text{if } p_i = 0 \end{cases} \quad (12)$$

Here we consider that pressurized ($p > 0$) elements are full ($\phi = 1$) while the unpressurized ones ($p = 0$) are only partially filled ($\phi < 1$), and identify the fractional fill level with the partial realization of the drag capacity in the corresponding element.

Step 3:

Temperature calculation goes, from the upstream (feed) end, where $T_1 = T_F$, to the downstream (discharge) end, in $N-1$ steps, for $i = 1, 2, \dots, N-1$ (pass ② in Figure 3). First, the *temperature increment* in the element is computed from Eq.(6):

$$\Delta T_{i+1} = \left[\frac{C_i \phi_i N^2}{q} \eta_i(T_i) - \frac{D_i h_i}{q} (T_i - T_B) \right] \Delta z_i \quad (13)$$

where T_i is the computed temperature at the current step. Then, the *temperature* in the next (upstream) element is computed based on the temperature of preceding (upstream) element:

$$T_{i+1} = T_i + \Delta T_{i+1} \quad (14)$$

Step 4:

There are two main quantitative criteria for convergence. The most common requires the maximum absolute difference between “old” and “new” profiles to be less than some specified tolerance ε :

$$\max_{1 < i < N} \{ |T_i^{(NEW)} - T_i^{(OLD)}| \} < \varepsilon \quad (15)$$



Note that this requires the difference between “old” and “new” be less than the tolerance at each and every point along the screw. A second criteria requires that the profiles differ by less than a specified tolerance only on the average:

$$\sqrt{\frac{\sum_1^N |T_i^{(NEW)} - T_i^{(OLD)}|^2}{N}} < \varepsilon \quad (16)$$

There are few systems that will converge or diverge according to the choice of criteria. However, most systems converge faster on the average than point-by-point.

Sometimes a system will “converge” only in a region of the screw and “diverge” on others. TXS allows some of these “partial converge” criteria to be used (cf. Section 6.4 below), in the understanding that the resulting “solution” is unreliable, even within the region of “convergence”.

Step 5:

The simplest, “naive” approach to updating the “old” temperature profile between iterations is to replace the “new” for the “old”

$$T_i^{(NEW\ OLD)} = T_i^{(NEW)} \quad \text{for } i=1, 2, 3, \dots N \quad (17)$$

However, this is not the best choice. TXS uses a more general expression:

$$T_i^{(NEW\ OLD)} = T_i^{(OLD)} + \omega \{T_i^{(NEW)} - T_i^{(OLD)}\} \quad \text{for } i=1, 2, 3, \dots N \quad (18)$$

$\omega > 0$ is called an “acceleration” factor. Notice that Eq.(17) is a particular case of Eq.(18) with $\omega = 1$.

In many cases, the iterative procedure oscillates, meaning that *if* the “old” temperature underestimates the actual value, *then* the “new” one will overestimate it (and vice versa). The quantity $\Delta T = |T^{(NEW)} - T^{(OLD)}|$ is called the amplitude of the oscillation and, if the iterative procedure converges, the amplitude ΔT will diminish with successive iterations. However, convergence could be very slow, so slow as to make impractical a theoretically “correct” procedure. In those cases, that unfortunately are very common, we need to accelerate the convergence of the procedure by “smoothing” the profile between iterations, that is, adding to the “old” temperature profile *less* than the difference $T^{(NEW)} - T^{(OLD)}$. This approach corresponds to a value $\omega < 1$. The numerical parameter ω is called, in this case, a *smoothing factor*.

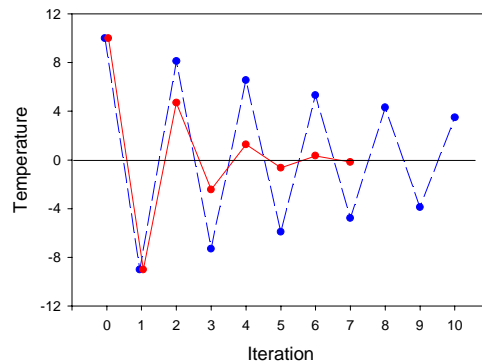


Figure 4



Figure 4 shows a hypothetical example. We have an iterative procedure where $T^{(NEW)} = -0.9 \cdot T^{(OLD)}$. The final “true” value is $T = 0$, and we admit a tolerance of $\varepsilon = 1$. Starting with $T^{(INIT)} = 10$, the blue (broken) line follows the iterations with $\omega = 1.0$, that is $T^{(NEW\ OLD)} = T^{(NEW)}$; the procedure takes 23 iterations to converge within the desired tolerance. The red (solid) line follows the iterations with $\omega = 0.8$, that is $T^{(NEW\ OLD)} = T^{(OLD)} + \omega [T^{(NEW)} - T^{(OLD)}]$; the procedure converges in only 7 iterations within the same tolerance than before. And $\omega = 0.8$ is not the optimum; try $\omega = 0.5$ and see.

In other cases, the iterative procedure converges without oscillation but too slowly, that is, successive iterations all underestimate (or overestimate) the actual value. In these cases it may be convenient to accelerate the convergence of the procedure by adding to the “old” temperature profile *more* than the difference $T^{(NEW)} - T^{(OLD)}$. This approach corresponds to a value $\omega > 1$ of the parameter. The numerical parameter ω is called, in this case, an *overrelaxation factor*.

6. User adjustable numerical parameters

TXS offers the possibility of adjusting, between reasonable limits, most numerical parameters. The user selection must always be made through the inclusion of entries into TXS initialization file (TXS.INI). None of these options is available within the program (Options screen). Remember that TXS.INI entries take the form of lines:

Keyword = Value

with the first three characters of the keyword being recognized by TXS (cf. *User Manual*, Appendix 3). Remember that if you modify the initialization file (you could do that using any text editor, such as NotePad, included with Windows) the modified entries will stay there until you change them again. Since the numerical options and parameters are “invisible” within TXS you should review TXS.INI frequently (again, using any text editor) to see what’s in there. The following are the numerical parameters and options accessible to the user.

1. The subdivision of the screw, increasing the number of computational elements by subdividing each “standard” element in two, three, etc. sub-elements (each of length $\frac{1}{2}$, $\frac{1}{3}$, etc. of the “standard” element length) is obtained by inserting the line:

DIV = n

where n is an integer in the range 1 to 20 (default: 1) into the initialization file. Remember that in the current version of TXS the total number of computational elements (i.e., for the whole screw) is limited to less than 8,000. Increasing the subdivision of the screw could help in some instabilities caused by extreme q/N settings, but could also increase some computational errors; it would always increase the computational time and, sometimes, the required number of iterations.

2. Three different initial temperature profiles can be chosen:

$$(d) \quad T_{INI}(i) = T_F \quad 0 < i < N.$$

$$(e) \quad T_{INI}(i) = T_{OP} \quad 0 < i < N.$$

$$(f) \quad T_{INI}(i) = T_F + i \cdot (T_{OP} - T_F) / N \quad 0 < i < N.$$

This is done by inserting within the initialization file the line:



$$TIN = n$$

where n is -1 for option (a), 0 for option (b), or 1 for option (c) above (default: 0). This option could solve a surprisingly large number of computational instabilities. Just remember that all iterative numerical schemes (and TXS's is no exception) work best when the initial assumption is close to the final solution.

3. The tolerance for the temperature iteration, the maximum acceptable difference between the “old” and “new” temperature profiles to stop the iteration (see item 4 below) is defined by a line in the initialization file:

$$TOL = e$$

where e is a real number in the range 0.01 to 10.00 (default 0.10) representing the tolerance in $^{\circ}\text{C}$. Selecting the right tolerance for a difficult simulation is not easy. Too tight a tolerance may unduly increase the number of iterations without other benefit, while a tolerance too large may hide intrinsic oscillating numerical solutions; this is especially true for complex systems (e.g., reactive systems). For these reasons we recommend to keep the tolerance between 0.1°C and 1.0°C . However, we may increase the tolerance beyond that for otherwise intractable systems, at the potential cost of hiding some “residual” oscillation.

Remember that the iteration tolerance has nothing to do with the accuracy of the predicted temperature profile: a closer tolerance doesn't mean *at all* a more accurate computation. Accuracy of the predictions depends basically on the process models used by TXS (in relation with the specific process application) and on the accuracy of the data provided (geometric parameters, material properties, and operating conditions).

4. Two different criteria for convergence of the temperature iteration can be chosen:

(a) Stop iterations if
$$\max_{1 \leq i \leq N} \{ |T_i^{(NEW)} - T_i^{(OLD)}| \} < e$$

(b) Stop iterations if
$$\sqrt{\frac{\sum_{i=1}^N |T_i^{(NEW)} - T_i^{(OLD)}|^2}{N}} < e$$

where e is the tolerance (see item 3 above). This is done by inserting within the initialization file the line:

$$TOP = n$$

where n is 0 for option (a) or 1 for option (b) above (default: 0). Option (a) is stricter and requires that the two temperature profiles differ point by point by less than the tolerance e ; in particular, it requires that the *maximum* local difference be less than e . Option (b) requires only that the two temperature profiles differ *on the average* by less than the tolerance e , allowing local differences larger than e at some points. Option (a) is always recommended. Option (b) could be used in special circumstances, when option (a) fails or requires an extremely large number of iteration steps (slow convergence), or when we suspect a local convergence problem (i.e., the simulation fails to converge at some particular points). Sometimes option (b) could be combined with a restricted convergence



interval. This restricted interval is set by inserting one (or both) of the following lines into the initialization file:

$$\text{DN1} = N_1$$

$$\text{DN2} = N_2$$

where N_1 and N_2 are positive integers with the condition $N_1 + N_2 < N$. (default, for both: 0). In this case, the convergence criterion (b) above is modified as follows:

$$(b') \text{ Stop iterations if } \sqrt{\frac{\sum_{N_1}^{N-N_2} |T_i^{(NEW)} - T_i^{(OLD)}|^2}{N}} < e$$

This means that we exclude from the convergence requirements an initial (upstream) interval from computational element 1 to computational element N_1 and/or a final (downstream) interval from computational element N_2 to computational interval N . We recommend the use of a restricted convergence interval *only* when the simulation fails to converge by other means and, nevertheless, we wish to obtain results. The results may or may not be meaningful by themselves, but could help diagnose convergence problems.

5. The maximum number of failed iterations before TXS stops the computation and displays an error message is defined by a line in the initialization file:

$$\text{IMX} = I_{MAX}$$

where I_{MAX} is an integer in the range from 1 to 1000 (default: 100). Occasionally, an increase in the number of iterations could help solve the problem in cases with slow (but not too slow) convergence.

6. In order to advance the iterative procedure the “old” (or assumed) temperature profile is updated between iterations using the expression:

$$T_i^{(NEW\ OLD)} = T_i^{(OLD)} + w \{T_i^{(NEW)} - T_i^{(OLD)}\} \text{ for } i=1, 2, 3, \dots N$$

where the control parameter is determined by a line in the initialization file:

$$\text{IRF} = w$$

where w is a real number in the range from 0.01 to 1.90 (default: 0.50). For comments, see Section 5, step 5, above.