Impurity Ti Model in TRANSP (SLVTX)

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Subroutine SLVTX in TRANSP advances the current radial profile of impurity ion temperature (XXTIMP) in time, based on the local heating power density delivered to impurities (including beam heating, RF heating, compressional heating, viscous heating, and "fast ion" heating from fusion products), power flows due to particle convection, and a local model of conductive losses.

The equations that describe the time evolution of impurity energy density and hydrogenic energy density are:

$$\frac{\partial}{\partial t}(1.5n_xT_x) = q_x - c\nabla \cdot (\Gamma_xT_x) + \frac{1.5n_x(T_i - T_x)}{\tau_{xi}} + \frac{1.5n_x(T_e - T_x)}{\tau_{xe}} \quad (1)$$

$$-\frac{1.5n_xT_x}{\tau_E}$$

$$\frac{\partial}{\partial t}(1.5n_iT_i) = q_i - c\nabla \cdot (\Gamma_iT_i) + \frac{1.5n_i(T_x - T_i)}{\tau_{ix}} + \frac{1.5n_i(T_e - T_i)}{\tau_{ie}} \quad (2)$$

$$-\frac{1.5n_iT_i}{\tau_E}$$

where subscripts x and i indicate impurity and main ion, repectively, q is the total heating power density, Γ is the particle flux, derived from the continuity equation for each species, c is the convective multiplier (supplied by the user), τ_{xi} is the temperature relaxation time for impurities on the main ions (see NRL plasma formulary or Spitzer's little book), τ_{ix} is the temperature relaxation time for the main ions on impurity ions, τ_{xe} is the temperature relaxation time of impurities on electrons, τ_{ie} is the temperature relaxation time of main ions on electrons, and τ_E is a "local" ion energy confinement time whose value will be determined self-consistently.

To determine the proper expression for τ_E which makes Eqs. 1 and 2 a self-consistent local model of the ion energy balance, we will sum the equations,

making use of the following identities and definitions

$$0 = \frac{1.5n_x(T_x - T_i)}{\tau_{xi}} + \frac{1.5n_i(T_i - T_x)}{\tau_{ix}}$$

$$q_{ei} \equiv \frac{1.5n_x(T_e - T_x)}{\tau_{xe}} + \frac{1.5n_i(T_e - T_i)}{\tau_{ie}}$$

$$q_h \equiv q_i + q_x + q_{bth}$$

$$q_{conv} \equiv c\nabla \cdot (\Gamma_x T_x + \Gamma_i T_i)$$

$$w_i \equiv \frac{3}{2}(n_i T_i + n_x T_x)$$
(3)

where q_{ei} represents the total power density transfer from electrons to all thermal ions (hydrogenic + impurity), q_h is the total heating power density to the thermal ions, q_{conv} is the total convective power flow, and w_i is the total thermal ion energy density. The sum of Eqns. 1 and 2 becomes

$$\frac{\partial w_i}{\partial t} = q_h + q_{bth} + q_{ei} - q_{conv} - \frac{w_i}{\tau_E}.$$
(4)

Since all of the terms in this equation are available to TRANSP except τ_E , we can solve for it:

$$\tau_E = \frac{w_i}{q_h + q_{bth} + q_{ei} - q_{\text{conv}} - \frac{\partial w_i}{\partial t}}.$$
(5)

For each TRANSP transport time step, The SOLVTX routine in TRANSP advances Eq. 1 in time, using the τ_E determined from Eq. 5.

Some physics details

Note that there are no local sources of impurities (except at the plasma edge), so the continuity equation for impurities reduces to $\frac{\partial n_x}{\partial t} = -\nabla \cdot \Gamma_x$. If we expand the LHS of Eq. 1 and the divergence term on the RHS ($\nabla \cdot (\Gamma_x T_x \equiv T_x \nabla \cdot \Gamma_x + \Gamma_x \cdot \nabla T_x)$), we can combine the terms involving $\frac{\partial n_x}{\partial t}$ to obtain:

$$1.5n_x \frac{\partial T_x}{\partial t} + T_x \frac{\partial n_x}{\partial t} (1.5 - c) = q_x - c\Gamma_x \cdot \nabla T_x + \frac{1.5n_x(T_i - T_x)}{\tau_{xi}} + \frac{1.5n_x(T_e - T_x)}{\tau_{xe}} - \frac{1.5n_xT_x}{\tau_E}$$
(6)

This equation clarifies how the impurity temperature evolution is affected by impurity particle transport and the time derivative of impurity density. If one chooses c = 1.5, then the term involving $\frac{\partial n_x}{\partial t}$ drops out, leaving only the term

 $c\Gamma_{\mathbf{x}} \cdot \nabla T_x$. Note that n_x typically rises rapidly at the start of beam injection (paralleling the rise in \overline{n}_e at constant Z_{eff}), implying a large negative $\Gamma_{\mathbf{x}}$. Since ∇T_x is also negative, the term $-c\Gamma_{\mathbf{x}} \cdot \nabla T_x$ is negative and will tend to decrease the time derivative of T_x . This simply reflects the physical situation that if particles are convected with their average energy (i.e., $q_{\text{conv}} \equiv \frac{3}{2}\Gamma T$), an inward particle flux carries particles from a colder region of the plasma into a hotter region.

Another interesting limit to consider is Eq. 2 (for the hydrogenic ions), when the plasma density and beam thermalization rates have reached steadystate. We restrict our attention to the center of highly beam fuelled plasmas (i.e. supershots), for which the dominant source term for ions is the beam fuelling rather than ionization of wall neutrals. Neglecting charge-exchange losses, we then have $S_{bth} = \nabla \cdot \Gamma_i$, where S_{bth} is the beam thermalization rate per unit volume. We must add to the local heating rate q_i a term due to beam ion thermalization, $S_{bth} \times \frac{3}{2}T_i$. So Eq. 2 becomes:

$$1.5n_{i}\frac{\partial}{\partial t}(T_{i}) = q_{i} + \frac{3}{2}S_{bth}T_{i} - \nabla(c\Gamma_{i}T_{i}) + \frac{1.5n_{i}(T_{x} - T_{i})}{\tau_{ix}} + \frac{1.5n_{i}(T_{e} - T_{i})}{\tau_{ie}} - \frac{1.5n_{i}T_{i}}{\tau_{E}}$$
$$= q_{i} + T_{i}S_{bth}(\frac{3}{2} - c) - c\Gamma_{i} \cdot \nabla T_{i}$$
$$+ \frac{1.5n_{i}(T_{x} - T_{i})}{\tau_{ix}} + \frac{1.5n_{i}(T_{e} - T_{i})}{\tau_{ie}} - \frac{1.5n_{i}T_{i}}{\tau_{E}}$$
(7)

Under the standard assumption $c = \frac{3}{2}$, the term involving S_{bth} drops out, i.e. the beam thermalization power cancels the convective power (no great surprise, if beam ions thermalize at $\frac{3}{2}T_i$ and thermal particles convect with the same average energy). There will remains a term $-c\Gamma_i \cdot \nabla T_i$ which is positive in this case (Γ_i is positive and ∇T_i negative), reflecting the fact that the convected particles have slightly less energy than the average $\frac{3}{2}T_i$ within a plasma shell, because they carry only the $\frac{3}{2}T_i$ at the outer edge of the shell, where the T_i is slightly lower due to the temperature gradient.

Some numerical details

TRANSP's calculation of $\frac{\partial w_i}{\partial t}$ is typically derived from (noisy) measurements of $T_i(R, t)$, $n_e(R, t)$, and $Z_{\text{eff}}(t)$. Thus there is no numerical guarantee that $\frac{\partial w_i}{\partial t}$ will not occasionally exceed the net power input to ions, thereby yielding a negative τ_E from Eq. 5, particularly at the start of neutral beam injection. It is also possible to obtain $\tau_E < 0$ even when $\frac{\partial w_i}{\partial t} = 0$, if the ion-electron power transfer plus convective losses exceeds the power input to ions (this can occur in the core of supershots).

I have chosen to impose the constraint that if the computed value of τ_E is less than zero, then τ_E will be set to a large number, 100 seconds, to represent "near-perfect" ion energy confinement. This is probably the correct choice in the quasi-steady state portion of supershots, where the condition $\tau_E < 0$ typically results from the ion heating being less than the nonconductive losses (q_{ie} + convection). There, although the power balance is questionable, SLVTX will still obtain a physically meaningful result for T_x – it will be the impurity temperature that is limited only by impurity-ion and impurity-electron coupling. If SLVTX had used its negative value of τ_E in the calculation of T_x , then in addition to the beam power input, there would be a physically meaningless (positive) term $-n_x T_x/\tau_E$, that would tend to further increase the calculated T_x .

At the start of neutral beam injection, when $\tau_E < 0$ can result from $\frac{\partial w_i}{\partial t} > q_{bi}$, the hack that sets τ_E to 100 sec will *not* give the proper time history of $T_x - T_i$ – effectively, the condition $\tau_E < 0$ implies that the thermal ions' energy density is increasing *faster* that it possibly could give the computed power sources. But by setting τ_E to 100 seconds, we effectively constrain the T_x to increase only as fast as the deposited power allows (i.e. neglecting radial transport).

TRANSP does not actually use the measured $T_i(r,t)$ directly, rather it "computes" a radius- and time-dependent multiplier on χ_i^{neo} which reproduces the measured temperature as best it can. There are limits to the multiplier (default minimum = 0.1, maximum = 40; controllable through namelist), in particular the multiplier is typically constrained to be positive. So the $T_i(r,t)$ used in TRANSP for all calculations *also* cannot rise faster than the transport=0 limit, hence the treatment of T_x in SLVTX and T_i are consistent; SLVTX should compute a meaningful temperature difference $T_x - T_i$ even during periods when the input ion temperature TIPRO rises faster than physically possible with the available beam power.

The version of SLVTX implemented as of April 1991 does not check that the time step is short compared to the characteristic time scales in Eq. 1 that advances T_x in time. In principle, we should use a Δt that is short compared to the impurity-ion and impurity-electron coupling times, and also short compared to the computed value of τ_E . I was a little worried, in particular, about the value of τ_E ; since it is derived from noisy data, it might be possible to (transiently) get a very short value of τ_E , which would then drop T_x considerably in one time step. In practice, this does not seem to be a problem; looking at TRANSPs for 35782, 55851 and 45950, the absolute value of τ_E seemed to stay above ~ 50 ms across the entire plasma. Nevertheless, to avoid potential difficulties, I also impose the constraint that τ_E be less than a minimum value, currently defined to be 20 ms in a data statement.

Doug McCune has pointed out that TRANSP's treatment of the ion power

balance uses a single ion temperature. Thus, for example, when TRANSP is asked to *compute* an ion temperature profile from some model (say $\chi_i = 2 \chi_e$), the temperature array TI it computes represents NOT the temperature of the "majority" species per se, but rather some mean temperature averaged over all of the ion species. It is not easy to write down the weighting of each species in this mean temperature, since the weighting depends on the ratio of conductive to convective losses. Therefore, it would be difficult to ask SLVTX to infer the appropriate "majority" and "impurity" temperature given as input the mean temperature.

In the more customary case, TRANSP is given as input some measured temperature profile time history TIPRO, which typically represents the carbon temperature. In this case the power balance will assume that all ions have the temperature of the carbon impurity; this will lead to some underestimate of the inferred χ_i . However in this case the temperature array TI passed into SLVTX is at least well defined; it's the carbon temperature. SLVTX has been amended to calculate both the "majority" temperature that would be consistent with a given impurity temperature, as well as the impurity temperature that would be consistent with a given majority temperature.

The proper procedure to analyze the early time history of ion temperature in supershots would be to run TRANSP in the usual analysis mode, allowing SLVTX to calculate the time-dependent profile of majority ion temperature (\equiv TMJ) that is consistent with the measured (carbon) temperature. Then run TRANSP again using TMJ as the "input" temperature of the majority species.

This procedure has two limitations. First, in the first iteration TRANSP uses the carbon temperature as the "ion" temperature, and thus overestimates the ion temperature used to calculated the the beam thermalization power (since beam ions thermalize at 1.5 Ti). Effectively this gives more power to the thermal ions than they actually get, underestimates the temperature difference between majority ions and impurity ions, and thereby overestimates the majority ion temperature. The beam thermalization power will be almost correct on the second iteration, but the "base" temperature is now the slightly-overestimated majority temperature. The net effect is that I expect this procedure to slightly overshoot the original measured carbon temperature. Of course, comparing the calculated impurity temperature from the second iteration to the original measurement gives a good indication of the self-consistency of the model.

The second limitation has to do with the constraint imposed by TRANSP, both in SLVTX and in the ion power balance, that the ion temperature array is not allowed to increase faster than the transport=0 limit, i.e. χ_i is not allowed to go negative. At the very start of supershots, we might expect the transport=0 limit to be approached. We expect the carbon temperature (i.e., TIPRO) to rise faster than the majority temperature due to the preferential beam coupling to impurities, but TRANSP's power balance will limit the rate of increase of the TI array to be the expected rate of rise of the *averaged* ions. Using this artificially -low TI as the temperature of the *impurity* species, SLVTX will then compute a similarly artificially low majority temperature. So on the second iteration, I would expect TRANSP to undershoot the impurity temperature, i.e. its calculation of TX should be less than the original TIPRO. The net effect is that the two-cycle TRANSP model may tend to indicate that there is some heat conduction going on at the start of supershots in situations where the heat conduction could really be negligible. The solution of the dilemma would be to modify SLVTX to use the TIPRO array as the temperature of the "impurity" in its calculation of the time history of the majority ion temperature.

Because SLVTX effectively computes a *local* difference between the impurity and hydrogenic temperature, it is more sensitive to noise on the beam power deposition than would be a corresponding prediction of $T_i(R)$ only (which would represent a double integral of the heating profile). Preliminary TRANSP runs with only 1000 particles gave factor ~2-3 fluctuations in the computed temperature difference $T_x - T_i$ over periods of only 10s of milliseconds. Presumably the output can be smoothed to yield a meaningful mean difference $T_x - T_i$, but if good time resolution is required then the number of Monte Carlo beam particles must be increased, or else the Fokker Planck package should be employed to eliminate the noise altogether. As of April 18, the Fokker Planck code needed a minor upgrade (to pass back the fraction of power delivered to impurities) to make it compatible with SLVTX.

The LATEX source text for this memo is stored in RX1:[SCOTT.TEX]-SLVTX.FOR. Last modified April 18, 1991.