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Professor Wallis and Professor Ransom:

I have read parts of the transcripts from the February 15 2005 meeting of the T/H Subcommittee regarding the TRACE code. I have additional comments as follows.

It seems to me that the NRC and ACRS and its T/H subcommittee should give serious consideration to enlisting assistance from persons who have in fact developed V&V and QA software for engineering analyses of nuclear-powered electricity generating plants.

1. Solution for the void fraction

The method used in TRACE does not solve for the void fraction. At best it might be a rough approximation for the void, and not a very good one at that. So far as I know there have been no investigations into the behavior of the TRACE code relative to the void fraction "solution" and the equation of state.

The four equations that provide the correct solution for the void, and the new-time liquid and vapor temperature and the pressure are

$$
\begin{aligned}
&<(1-\alpha_v)\rho_l(P,T_l)> - (1-\alpha_v)\rho_l(P,T_l) = 0 \\
&<\alpha_v\rho_v(P,T_v)> - \alpha_v\rho_v(P,T_v) = 0 \\
&<(1-\alpha_v)\rho_l(P,T_l)e_l(P,T_l)> - (1-\alpha_v)\rho_l(P,T_l)e_l(P,T_l) = 0 \\
&<\alpha_v\rho_v(P,T_v)e_v(P,T_v)> - \alpha_v\rho_v(P,T_v)e_v(P,T_v) = 0
\end{aligned} \tag{1.1}
$$

Four implicit non-linear equations for the four unknowns α_v, P, T_l, T_v. As stated in the manual, these equations are not solved for the final new-time values of these quantities. Instead they are linearized, as they would be for almost all numerical solution methods, and the results from the first iterate for the void fraction is retained and used in subsequent calculations.

A Newton-Raphson method applied to the equation system, and solved for the change in the variables across an iterate can be written

$$
\begin{bmatrix}
\left(\frac{\partial F\rho l}{\partial \alpha v}\right) & \left(\frac{\partial F\rho l}{\partial P}\right) & \left(\frac{\partial F\rho l}{\partial Tv}\right) & \left(\frac{\partial F\rho l}{\partial Tl}\right) \\
\left(\frac{\partial F\rho v}{\partial \alpha v}\right) & \left(\frac{\partial F\rho v}{\partial P}\right) & \left(\frac{\partial F\rho v}{\partial Tv}\right) & \left(\frac{\partial F\rho v}{\partial Tl}\right) \\
\left(\frac{\partial Fel}{\partial \alpha v}\right) & \left(\frac{\partial Fel}{\partial P}\right) & \left(\frac{\partial Fel}{\partial Tv}\right) & \left(\frac{\partial Fel}{\partial Tl}\right) \\
\left(\frac{\partial Fev}{\partial \alpha v}\right) & \left(\frac{\partial Fev}{\partial P}\right) & \left(\frac{\partial Fev}{\partial Tv}\right) & \left(\frac{\partial Fev}{\partial Tl}\right)
\end{bmatrix}
\begin{bmatrix}
(\Delta\alpha_v)^{k+1} \\
(\Delta P)^{k+1} \\
(\Delta T_v)^{k+1} \\
(\Delta T_l)^{k+1}
\end{bmatrix}
=
\begin{bmatrix}
-(F\rho l)^k \\
-(F\rho v)^k \\
-(Fel)^k \\
-(Fev)^k
\end{bmatrix} \tag{1.2}
$$

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where $(\Delta\Upsilon)^{k+1} = \Upsilon^{k+1} - \Upsilon^{k}$ for each of α_v, P, T_l, T_v.

The important aspect is that the derivatives in the Jacobian matrix on the left-hand side and the functions on the right-hand side, are all functions of the unknown quantities and thus a first guess is needed to start the iterative method. What is used for these is in the code, but there are at least two options; the last old-time value or the tentative values obtained in a previous step of the SETS method. The first guess could be either (1) based on the pressure and temperatures with calls to the EOS to get the density and internal energy, or (2) these latter values directly from a previous step. The manual does not report what are used for first guesses.

Because only the results of the first iterate for the void are used in TRACE, that value of the void will be determined by the values for the first guess of all the unknown quantities. The effects of this approach are difficult to determine without actually using TRACE and investigating the impact of the first guess on the void. The two different values mentioned above could be used in two successive runs and the change in the void observed. An every-time-step edit is suggested for observing the effects.

But here is a most radical suggestion. Carry out the Newton-Raphson procedure to completion in TRACE and see what the void fraction really should be. This would also give the correct values for the new-time level of the liquid temperature, vapor temperature, and the pressure. At the present time, TRACE uses the last tentative values for these quantities from a previous step in the SETS method.

It can not be over-stated that the void fraction is not solved in TRACE. Additionally, the equation system (1.1) will not be satisfied by the void calculated as it is TRACE. Finally, the void determined as in TRACE will not satisfy the equation of state in which the tentative values of temperatures and the pressure from a previous SETS step are also used.

The TRACE code does not satisfy the equation of state.

You can investigate the effects of the "solution" of non-linear equations as used in TRACE for the EOS with the following simple equation system:

$$\begin{aligned} 3X^2 + 2Y^2 &= 7 \\ -9X^2 + Y^2 &= 0 \end{aligned} \tag{1.3}$$

The solution of which is $X = \sqrt{1/3}$ and $Y = \sqrt{3}$.

The derivatives needed for the Jacobian are

$$\frac{\partial F_1}{\partial X} = 6X \quad \frac{\partial F_1}{\partial Y} = 4Y$$
$$\frac{\partial F_2}{\partial X} = -18X \quad \frac{\partial F_2}{\partial Y} = 2Y \tag{1.4}$$

And the equations for the change in the independent variables over an iterate are

$$\begin{bmatrix} 6X & 4Y \\ -18X & 2Y \end{bmatrix} \begin{bmatrix} (\Delta X) \\ (\Delta Y) \end{bmatrix} = \begin{bmatrix} -F_1 \\ -F_2 \end{bmatrix} \tag{1.5}$$

and Cramer's rule can be used to get the algebraic expressions for $(\Delta X)^{k+1}$ and $(\Delta Y)^{k+1}$. The determinant of the Jacobian is D = 84XY.

Equations (1.3) through (1.5) and the determinant show that the first iterate value is a function of the numerical values for the first guess for X and Y. The effects of small differences between the correct solution and a first guess can be easily investigated analytically by hand or in a spreadsheet.

2. Verification of the Finite Difference Equations

The discussion about the scale over which the continuous 3-D equations are averaged in order to get the continuous 1-D formulation is not relevant to the solution of the finite-difference equations. The continuous 1-D equations, for example, do not contain any information whatsoever regarding the smallest scale to which they can be applied. They are not limited in any way by the mathematical forms, and the codes typically do not limit the scale to which a user can apply the equations. In fact, users will always use whatever scale they wish.

The problem is that many people confuse and try to mix the continuous and discrete problems when in fact they are two separate and distinct problems. The solution of the discrete equations is a pure mathematics problem. This is in contrast to the development of the continuous 1-D equations into which much engineering is incorporated. So, the numerical solution methods used in the TRACE code should only be viewed from a mathematical focus. Hand waving over fictitious issues serves only to divert attention from real issues.

If the continuous 1-D equations are limited relative to the smallest scale to which they can be applied, then the code needs to ensure that users cannot violate this restriction. And this restriction should be applied to all the model equations used in the codes; heat conduction, power production, algebraic models and correlations, engineering equipment models, equation of state, etc.

Verification of a code is a series of mathematical processes, without appeal to engineering and the derivations of the finite difference equations. Demonstration of the order of accuracy and order of convergence for the numerical methods is conducted by way of only mathematics.

So far as the available literature shows the TRACE code has not been verified to determine that the coded equations are in fact correctly solved. Validation calculations, and applications, that precede verification of the coding and numerical solution methods are more or less meaningless.

3. Condensation in the presence of Non-condensables

It was not clear from Dr. Kelly's presentation that the incorrect partial-pressure weighting of the effects of non-condensables in the basic differential energy equations for the liquid and vapor has been removed from the TRACE code.

4. V&V and QA Plans

It is clear from Dr. Murray's presentation that while the NRC might have QA plans they are not in general use. The industry standards for QA plans does not include a staff member having to somewhat remember seeing an e-mail and having to dig it up to then find the title of a governing document. As was mentioned during the presentation, the documents are not in place for all staff who should have them.

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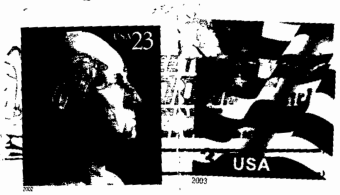

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