CHAPTER III

TEXAS CODE

This chapter consists of five sections. The first section introduces the concept of TEXAS code. Conservation equations for the Eulerian vapor and liquid fields, and only momentum and energy equations for the Lagrangian fuel panicle field are described in the next section. The third section discusses the phase change model used in the TEXAS code. The fourth section is Switch Void Fraction (SVF) in Pressure Iteration. And finally, the modification of TEXAS code for simulation of two-phase natural circulation will be presented.

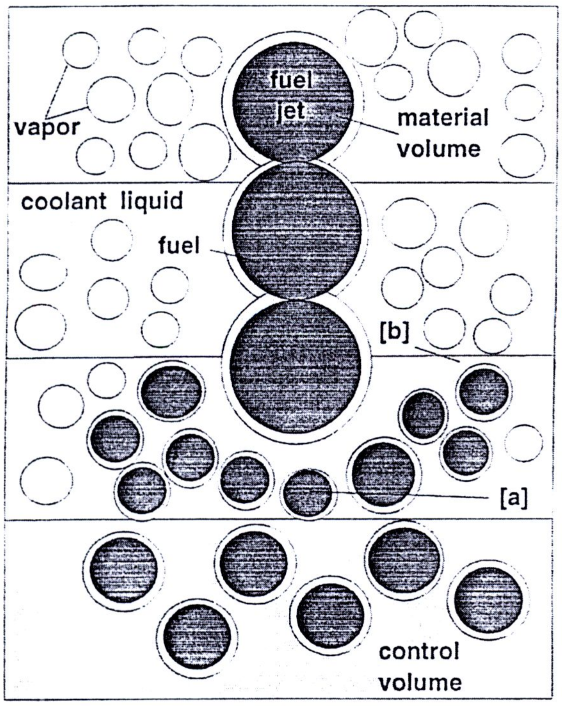
3.1 Brief description of TEXAS code

The TEXAS computer model is one of the major tools used at the Department of Engineering Physics, University of Wisconsin for simulations of fuel-coolant interaction during its mixing, triggering and explosion phases. TEXAS is a model based on a one-dimensional hydrodynamics code originally developed at Los Alamos National Laboratory as part of the SIMMER development, adapted at Sandia National Laboratories and finally modified by the University of Wisconsin for fuel-coolant interactions. The original TEXAS code was a parametric model developed by Young [24] for the design and analysis of fuel-coolant interaction experiments for LMFBR safety related issues. In an attempt to extend the capabilities of TEXAS, Chu and Corradini [25] incorporated a dynamic fragmentation model and a complete set of constitutive correlations for interfacial mass, momentum, and energy transport term; i.e., TEXAS-II. Since then, several improvements to the explosion propagation modeling, in particular, have been introduced by Tang [26]. A chemical reaction model to account the heat generation by oxidation of metallic melt was added by Murphy [27]. These updates, together with the complete model of the fragmentation of the fuel during the mixing phase, warranted a new release of the code, TEXAS-V.

The TEXAS code is a transient, three fluid, one-dimensional models capable of simulating fuel-coolant mixing interactions. The three fields include two Eulerian fields for coolant liquid and vapor, and one Lagrangian field for fuel particles.

The multifield feature of the code allows it to model thermal and mechanical nonequilibrium between coolant liquid and vapor which is very likely the case for fuel-coolant interactions. Fig. 3.1 shows conceptual picture of current TEXAS mixing model. The code has the ability to handle flow regime transitions, which is also important to realistically model the heat transfer process. The "Lagrangian" treatment for the fuel field makes it easier to track the fuel particle movement, and eliminates some numerical difficulties encountered in pure Eulerian codes. The fragmentation model used in the code is based on hydrodynamic instabilities (i.e., Rayleigh-Taylor). The code also provides choices of velocity, pressure, and reflective (or closed) boundary conditions, giving more flexibility to users in different applications. A semi-implicit numerical technique is used in TEXAS which is a modified version of the SIMMER-II method, the actual forerunner of the TEXAS hydrodynamic formulation. With this method, the pressure iteration is done in a loop in which the energy and momentum equations are solved semi-implicitly, whereas the continuity equations are solved implicitly by adjusting the pressure distribution such that the errors of the continuity equations for all cells are reduced to a given tolerance. The Newton-Raphson method is employed in this pressure iteration.

In the following discussion, we briefly review the basic governing conservation equations and the two key constitutive fragmentation models: the fragmentation model for mixing and the explosion and the phase change model. In addition to these two constitutive models, interfacial exchange terms of mass, momentum, and energy are needed to couple the conservation equations among different fields. The complete set of constitutive relations for these interfacial exchange terms have been developed and incorporated into the code. All these exchange terms are modeled in three different flow regimes: bubbly flow, droplet flow, and transition flow. For detailed descriptions of all these terms, readers are referred to Chapter 4 of Chu's PhD thesis [28]



RTI breakup of fuel at front of the coherent jet
[a] fuel jet leading edge of intact master pcls.
[b] fuel jet trailing edge of discrete master pcl

Fig. 3.1 Conceptual picture of current TEXAS mixing model[25]

3.2 Conservation Equations

Conservation equations are the bases of all hydrodynamic computer models. In TEXAS, there are mass, momentum, and energy equations for the Eulerian vapor and liquid fields, and only momentum and energy equations for the Lagrangian fuel panicle field. The macroscopic densities for the vapor and liquid ($\rho_g^{'}$ and $\rho_l^{'}$) are used in these conservation equations. $\rho_g^{'}$ and $\rho_l^{'}$ are defined as:

$$\rho_g^{'} = \alpha_g \rho_g \tag{3.1}$$

$$\rho_l^{'} = \alpha_l \rho_l \tag{3.2}$$

Where α_g and α_l are the volume fractions of the vapor and liquid with respect to the total volume of coolant in an Eulerian cell. With this definition of the macroscopic densities (Equations (3.1) - (3.2)), the conservation equations are listed below:

3.2.1 Mass Equations

Vapor:

$$\frac{\partial \rho_g'}{\partial t} + \nabla \cdot \left(\rho_g' \vec{u}_g \right) = \Gamma_e - \Gamma_c \qquad (3.3)$$

Liquid:

$$\frac{\partial \rho_l'}{\partial t} + \nabla \cdot \left(\rho_l' \vec{u}_l \right) = \Gamma_c - \Gamma_e \qquad (3.4)$$

Where:

$\vec{u}_g$ = velocity of vapor field

$\vec{u}_l$ = velocity of liquid field

Γ_e = evaporation rate

Γ_c = condensation rate

3.2.2 Momentum Equations

Vapor:

$$\begin{aligned} \rho_g' \frac{\partial \vec{u}_g}{\partial t} + \rho_g' \vec{u}_g \frac{\partial \vec{u}_g}{\partial z} = -\rho_g' g - \alpha_g \frac{\partial P}{\partial z} &+ K_{gl} \left(\vec{u}_l - \vec{u}_g \right) \\ &- K_{wg} \vec{u}_g - V_g + A_m \frac{\partial}{\partial t} \left(\vec{u}_l - \vec{u}_g \right) \qquad (3.5) \\ &- \Gamma_e \left(\vec{u}_g - \vec{u}_l \right) + M_{gp} \end{aligned}$$

Liquid:

$$\begin{aligned} \rho_l' \frac{\partial \vec{u}_l}{\partial t} + \rho_l' \vec{u}_l \frac{\partial \vec{u}_l}{\partial z} = -\rho_l' g - \alpha_l \frac{\partial P}{\partial x} &+ K_{gl} \left(\vec{u}_g - \vec{u}_l \right) \\ &- K_{wl} \vec{u}_l - V_l + A_m \frac{\partial}{\partial t} \left(\vec{u}_g - \vec{u}_l \right) \qquad (3.6) \\ &- \Gamma_c \left(\vec{u}_l - \vec{u}_g \right) + M_{lp} \end{aligned}$$

Fuel particle:

$$M_{pk}\frac{du_{pk}}{dt}=-M_{pk}g+D_k\left(u_g-u_{pk}\right)+E_k\left(u_l-u_{pk}\right) \tag{3.7}$$

Where:

g = gravity

P = pressure

K_{gl} = vapor-liquid macroscopic drag coefficient

K_{wg} = wall-liquid friction coefficient

K_{wl} = wall-vapor friction coefficient

V_g = viscous loss term for vapor field

V_l = viscous loss term for liquid field

A_m = transient virtual mass force coefficient

M_{gp} = summation of vapor-Lagrangian particle drags

M_{lp} = summation of liquid-Lagrangian particle drags

D_k = vapor-Lagrangian particle drag term

E_k = liquid-Lagrangian particle drag term

3.2.3 Energy Equations

Vapor:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho_g' I_g\right)+\frac{\partial}{\partial t}\left(\rho_g' I_g\vec{u}_g\right)&=-P\left[\frac{\partial\alpha_g}{\partial t}+\frac{\partial}{\partial t}\left(\alpha_g\vec{u}_g\right)\right]\\&\quad+W_g+Q_{gw}+Q_{gp}+Q_{gi}\\&\quad-C_g+S_g+\left(\Gamma_e-\Gamma_c\right)h_{gs}\end{aligned} \tag{3.8}$$

Liquid:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho_l' I_l\right)+\frac{\partial}{\partial t}\left(\rho_l' I_l\vec{u}_l\right)&=-P\left[\frac{\partial\alpha_l}{\partial t}+\frac{\partial}{\partial t}\left(\alpha_l\vec{u}_l\right)\right]\\&\quad+W_l+Q_{lw}+Q_{lp}+Q_{li}\\&\quad-C_l+S_l+\left(\Gamma_c-\Gamma_e\right)h_{ls}\end{aligned} \tag{3.9}$$

Fuel particle:

$$\begin{aligned} M_{pk}\frac{dI_{pk}}{dt} &= R_{lk}\left(T_l - T_{pk}\right) + R_{gk}\left(T_g - T_{pk}\right) \\ &\quad + R_{ik}\left(T_{sat} - T_{pk}\right) + R_{wk}\left(T_w - T_{pk}\right) + S_{pk} \end{aligned} \tag{3.10}$$

Where:

I_g = internal energy of vapor field

I_l = internal energy of liquid field

I_{pk} = internal energy of Lagrangian particle

W_g = viscous work for vapor

W_l = viscous work for liquid

Q_{gw} = wall-vapor heat transfer term

Q_{lw} = wall-liquid heat transfer term

Q_{gp} = vapor-Lagrangian particle heat transfer term

Q_{lp} = liquid-Lagrangian particle heat transfer term

Q_{gi} = vapor-interface heat transfer term

Q_{li} = liquid-interface heat transfer term

C_g = conduction heat transfer term for vapor

C_l = conduction heat transfer term for liquid

h_{gs} = vapor enthalpy at saturation temperature

h_{ls} = liquid enthalpy at saturation temperature

S_g = heat source term for vapor

S_l = heat source term for liquid

S_{pk} = heat source term for Lagrangian particle

T_g = vapor temperature

T_l = liquid temperature

T_{pk} = Lagrangian particle temperature

T_w = wall temperature

T_{sat} = saturation temperature

R_{gk} = macroscopic heat transfer coefficient between vapor and Lagrangian particles of k^{th} group

R_{lk} = macroscopic heat transfer coefficient between liquid and Lagrangian particles of kth group

R_{ik} = macroscopic heat transfer coefficient between vapor-liquid interface and Lagrangian particles of kth group

R_{wk} = macroscopic heat transfer coefficient between wall and Lagrangian particles of kth group

3.3 Phase Change Model

The phase change model is another important constitutive relation in TEXAS-V, which calculates the vaporization or condensation rate, and in turn, determines the local pressure. The technique employed in the model is similar to the simple vaporization-condensation model used in SIMMER-II. But the phase change model in TEXAS-V is fully implicit in the pressure iteration.

The model assumes that the phase change occurs at the interface of the coolant liquid and vapor, and considers all forms of heat transfer between the fuel and coolant under different flow regime conditions. Generally, there are three ways in which the fuel heat is used:

1. to increase the internal energy of the coolant liquid;
2. to increase the internal energy of the coolant vapor:
3. to vaporize the coolant liquid.

Using an energy balance, the model calculates the net heat flow, which becomes the energy associated with the generated vapor, i.e.:

$$\dot{q}_{net,f} = \dot{q}_f - \dot{q}_l - \dot{q}_g \tag{3.11}$$

Where $\dot{q}_f$ is the heat lost by the fuel; and $\dot{q}_l$ and $\dot{q}_g$ are the heat received by the coolant liquid and coolant vapor respectively, which becomes the internal energy of the coolant. The detailed description of these heat transfer terms is given in Chapter 4 of Chu's PhD thesis [28].

Knowing the net heat flow, $\dot{q}_{net,f}$ one can easily calculate the phase change rate per unit volume, i.e.:

$$\dot{m}_g = \frac{\dot{q}_{net,f}}{h_{fg} V_{cell}} \qquad (3.12)$$

Where the h_{fg} is the latent heat for the coolant; and V_{cell} is the cell volume.

If the net heat flow, $\dot{q}_{net,f}$ is positive, there is vapor generated, and the vaporization rate is:

$$\Gamma_e = \dot{m}_g, \qquad \Gamma_c = 0$$

If the net heat flow, $\dot{q}_{net,f}$ is negative, there is vapor condensed into liquid, and the condensation rate is:

$$\Gamma_c = -\dot{m}_g, \quad \Gamma_e = 0$$

Because this model is based on the assumption that phase changes occur at the interface of the coolant liquid and vapor, it allows the vapor to be produced under subcooled as well as saturated conditions.

3.4 Switch Void Fraction (SVF) in Pressure Iteration

As described in the previous section, TEXAS is a multifluid model, which allows the liquid and vapor to exist at different temperatures. However, the same macroscopic pressure is assumed for both the liquid and vapor within one control volume. The temporal pressure change is found by solving either the liquid or vapor mass equation. The new pressure is then substituted into the other mass equation to find the void fraction. The new pressure is also used to calculate other physical variables. The newly calculated void fraction and other variables are then used in the next pressure iteration until convergence occurs. There is a "switch void fraction (SVF)" given by the user, which determines whether to solve the liquid or vapor mass continuity equation. If the void fraction in a cell is smaller than the SVF, the liquid mass equation is solved otherwise, the vapor equation is solved. In TEXAS-V, the value of 0.5 (or 50%)

was chosen as the switch value (SVF). This value has a significant impact on the convergence efficiency. Because the compressibility of the vapor is much greater than that of the liquid, the local pressure is primarily determined by the vapor density change when a certain amount of vapor is present locally. Therefore, the compressibility difference for the liquid and vapor should be taken into consideration in choosing the appropriate value for SVF. Analysis has been done to select such a value so that at this value, the same change of volume fraction for liquid or vapor will give some pressure change.

The pressure change due to the liquid and vapor density changes are

$$\frac{\Delta P}{\Delta \rho_l} \cong \frac{\partial P}{\partial \rho_l} \qquad (3.13)$$

$$\frac{\Delta P}{\Delta \rho_g} \cong \frac{\partial P}{\partial \rho_g} \qquad (3.14)$$

For given void fraction change, the corresponding density changes for the liquid and vapor are:

$$\Delta \rho_l = -\rho_l \frac{\Delta \alpha_l}{\alpha_l} \qquad (3.15)$$

$$\Delta \rho_g = -\rho_g \frac{\Delta \alpha_g}{\alpha_g} \qquad (3.16)$$

and

$$\alpha_l + \alpha_g = 1 \qquad (3.17)$$

Combining these equations, one obtains the expression of the appropriate value for SVF, α_g

$$\alpha_g = \frac{\rho_g \Big/ \frac{\partial \rho_g}{\partial P}}{-\rho_l \Big/ \frac{\partial \rho_l}{\partial P} + \rho_g \Big/ \frac{\partial \rho_g}{\partial P}} \qquad (3.18)$$

and

$$\rho_l \Big/ \frac{\partial \rho_l}{\partial P} \cong \rho_g \Big/ \frac{\partial \rho_g}{\partial P} \tag{3.19}$$

Therefore one has:

$$\alpha_g \approx \left| \frac{\rho_g \cdot \dfrac{\partial \rho_l}{\partial P}}{\rho_l \cdot \dfrac{\partial \rho_g}{\partial P}} \right| \tag{3.20}$$

At a pressure of 10 MPa, α_g is about 0.004. Using the new switch void fraction, α_g we have greatly improved the calculation efficiency, especially during the propagation phase when the calculation becomes more sensitive due to the large pressure changes.

3.5 Modification of TEXAS code

TEXAS code was modified to simulate the two-phase rectangular natural circulation. Fig. 3.2 and Fig. 3.3 show the TEXAS program and the modification of TEXAS program respectively. The modifications of TEXAS code are as follow:

- The code related to fuel particles was commented in the program.
- The continuous boundary condition (rectangular loop) was added to the computer program as shown in Fig. 3.3.
- The total run time was changed from milliseconds for thermal explosion to seconds for natural circulation.
- The equation of state for liquid was modified to obtain more accurate result.

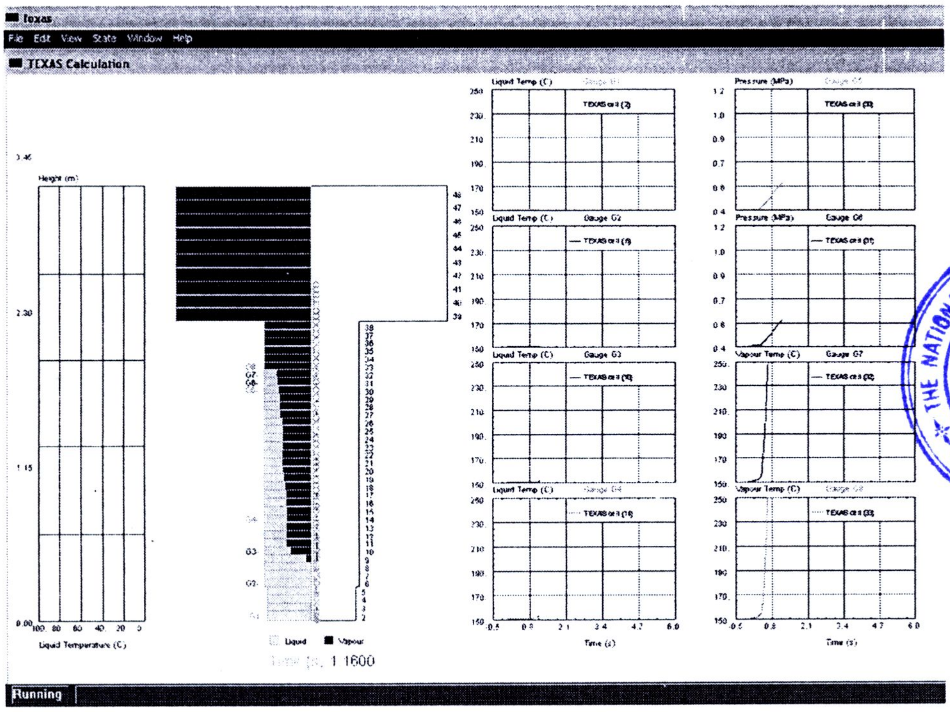
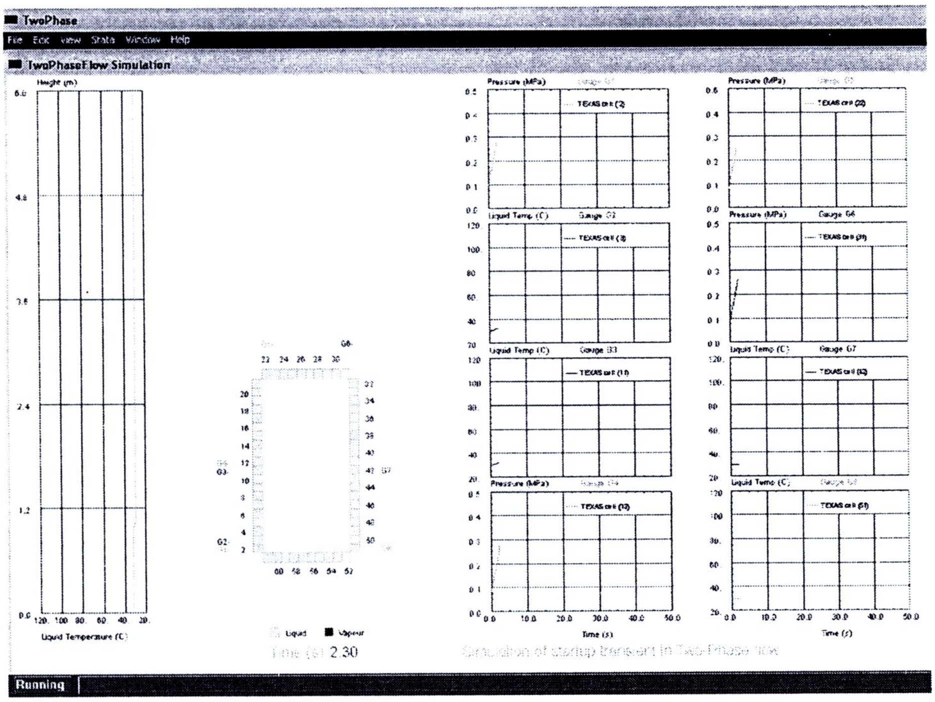


Fig. 3.2 The TEXAS program



Simulation of startup transient in Two-Phase flow

Fig. 3.3 The modification of TEXAS program