TRACE Computer Code Theory and Governing Equations

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Objective

Provide a high level discussion on the TRACE code theory and governing equations.

Outline

- Basic TRACE code theory and governing equations
- Closure relationships
- Code numerical solution scheme
- Code time step control

TRACE Code documentation

TRACE V5.0 Patch 5 Theory Manual, Field Equations, Solution Methods and Physical Models

TRACE V5.0 Patch 5 Assessment Manual

- Fundamental Validation Cases (Appendix A)
- Separate Effects Test Assessments (Appendix B)
- Integral Effects Test Assessments (Appendix C)

TRACE V5.0 Patch 5 User's Manual

- Input Specification (Volume 1 – available on the workshop PCs)
- Modeling Guidelines (Volume 2)

TRACE Theory

TRACE has mathematical models to track transport of mass and energy throughout the system of interest. These equations are discretized in space and time.

- Field Equations
- Closure Models
- Numerical Methods

TRACE Field Equations

TRACE uses what is commonly known as a six equation model for two-phase flow (mass equation, equation of motion, and energy equation for each phase):

1. Conservation of mass, liquid phase
2. Conservation of mass, vapor phase
   - A mixture equation is used to ease calculational requirements for transitions between single and two-phase.
   - Remember that the gas can be a combination of both vapor and non-condensable gases
3. Momentum equation, liquid phase
4. Momentum equation, vapor phase
5. Conservation of energy, liquid phase
6. Conservation of energy, vapor phase
   - Energy source terms are wall heating, direct heat (e.g. radiation) and interfacial heat transfer.
   - Heat to the fluid from the wall is a standard convection form and wall temperatures are obtained from a standard conduction equation.

TRACE Field Equations

Additional equations are used to track mass for:

- non-condensable gases (included with the vapor phase) and
- dissolved boron (included with the liquid phase) when they are present in the fluid.

TRACE solution variables include:

1. void fraction
2. steam and non-condensible gas pressures
3. liquid and vapor velocities
4. liquid and vapor temperatures
5. boron concentration
6. heat structure temperatures

TRACE Constitutive Models

Closure relationships are needed to form a complete set of equations to solve.

These relationships are semi-empirical correlations and equations (not first-principle) representative of the physical properties and processes:

- Equations of State - Vapor and liquid phase pressures, temperatures and densities
- Wall Drag - Irrecoverable pressure loss caused by friction of vapor and liquid phases flowing adjacent to a wall (additional losses may be specified for flow through bends, area changes, etc.)
- Interfacial Drag - Body force between vapor and liquid flowing at different velocities
- Wall Heat Transfer - Energy flow between a structure and the vapor and liquid phases
- Interfacial Heat Transfer - Energy exchange between vapor and liquid phases, with mass transfer resulting from boiling/evaporation of liquid and condensation of steam

New applications and geometries require new models

Slides are available in your notebooks that have more detail on the constitutive models

TRACE Numerical Methods

1. TRACE offers two numerical solution methods:
   - Semi-Implicit, and
   - Stability Enhancing Two-Step (SETS)
2. The analyst should use SETS for most reactor safety problems, which offers improved run-time performance for LOCAs and transients.

   Exception:

   Semi-Implicit (with time step selected to keep Courant number near 1.0 in the region of interest) is recommended if pressure or continuity (convection of void fraction, density, and temperature front) waves need to be tracked and errors caused by numerical diffusion effects may be significant. Relevant phenomena include:
   - Density wave propagation (bubbles traveling though water)
   - Progression of boron concentration or thermal fronts
   - Pressure wave propagation
3. TRACE uses outer iterations to converge the semi-implicit step and minimize mass errors.
4. SETS and Semi-implicit are first-order methods and both are (numerically) diffusive, but SETS is more so.

TRACE Numerical Methods

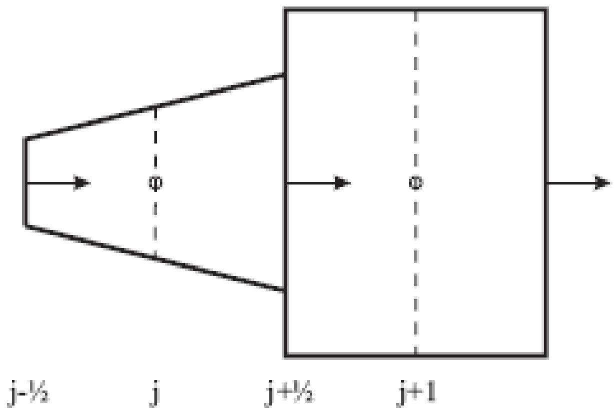
5. The material Courant limit is of primary interest for numerical stability. Considering all fluid cells in the system, the material Courant limit is the shortest time step size for which liquid passes all the way through a cell given the mass flow at the boundaries.
   – SETS time integration allows TRACE to exceed material Courant limit, while the semi-implicit does not.
6. TRACE numerical discretization in time and space are first-order accurate and must be small enough to resolve the time scales and profiles of interest for the applications.
7. Beyond hydrodynamics, appropriate time scales of interest may also be limited by heat transfer within and to structures, and variations in responses of control systems or boundary conditions.

TRACE Solution Uses a Staggered-Mesh Modeling Approach

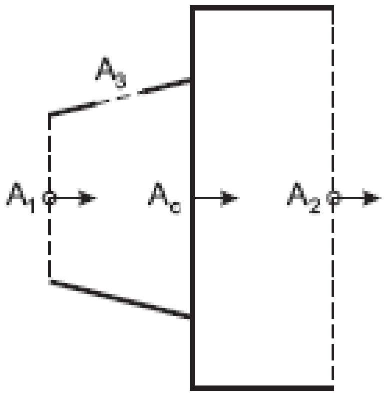
A discrete approximation of the fluid volumes and flow paths of the physical system is specified through input. This represents development of a facility input model.

Thermodynamic fluid state variables (pressure, temperature, etc.) for mass and energy conservation are evaluated as hydrodynamic volume properties.

Momentum equation variables (velocities) are evaluated at the faces between the hydrodynamic volumes.



Two Mass and Energy Conservation Volumes



Corresponding Momentum Conservation Faces

TRACE Time Step Control

The TRACE time step size is determined by the following:

- Material Courant limit (Semi-implicit)
- Rate of change of state variables (void fraction, pressure, fluid and structure temperatures)
- Pressure matrix outer iteration convergence or residual convergence
- Energy conservation error in structure to fluid heat transfer
- Maximum and minimum time step size set by user

TRACE results should be examined to determine whether the relevant physics has been resolved in a particular simulation. Time step size should be adjusted manually where physics is not adequately resolved.

Questions?

Any questions on TRACE code theory and governing equations before moving on?

TRACE Hydrodynamic and Thermal Components

TRACE Thermal-Hydraulic components are the basic building blocks of an input model

There are 22 components available. The most commonly used components include:

- PIPE
- BREAK
- FILL
- VALVE
- PUMP
- TEE
- CONTAN
- HTSTR
- POWER
- CHAN
- JETP
- SEPD
- VESSEL

Dissecting a TRACE Component

- Common Modeling Capabilities
  - Geometry & Orientation
  - Specifying different working fluids
  - Side junctions
  - Power to the fluid
  - Power to the wall
  - Wall heat transfer
  - Wall Friction and Irrecoverable losses
  - Modeling Flags (Choked Flow, CCFL, CHF, etc)

TRACE Component Control

- Pressure and fluid-state boundary condition.
- Velocity or mass-flow and fluid-state boundary condition.
- Reactor-core programmed reactivity or power.
- Reactor-core axial-power shape.
- Energy deposition directly in the coolant.
- Energy generation in the hydro-component wall.
- Pump-impeller rotational speed.
- Turbine power demand.
- Valve flow-area fraction or relative stem position.

Questions?

Any questions on TRACE components?

(Additional details on T/H components are provided on slides in your course notebook)