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Assessment of RELAP5-3D for Future Reactor Designs

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Outline

- System Codes Considered
- Comparison Metrics
  - Conservation Models
  - Closure Relations
    - Critical Heat Flux Calculations
    - Flow Regime Description
    - Interfacial Heat Transfer Calculations
    - Wall-to-fluid heat transfer models
  - Verification & Validation
  - Assumptions
- Conclusions

System Codes Considered

- RELAP5-MOD3.3
- RELAP5-SCDAP
- RELAP5-3D
- TRACE v5.0
- TRAC v3.0
- WCOBRA/TRAC-TF2

Comparison Metrics: RELAP and TRACE Conservation Models

- Six Conservation Equations
  - Liquid and Vapor Field
    - Mass

Volumetric mass exchange rate

$$\frac{\partial}{\partial t}(\alpha_k\rho_k) + \frac{1}{A}\frac{\partial}{\partial x}(\alpha_k\rho_k v_k A) = \Gamma_k$$

Force due to virtual mass

Frictional drag:

iction coefficient x reference area per unit volume x bulk fluid velocity)

Interface frictional drag

Momentum change from fluid acceleration

Body force (gravity and pump head)

$$\alpha_k\rho_k A\frac{\partial v_k}{\partial t} + \frac{1}{2}\alpha_k\rho_k A\frac{\partial v_k^2}{\partial x} = -\alpha_k A\frac{\partial P}{\partial x} + \alpha_k\rho_k B_x A - (\alpha_k\rho_k A)FW_k \bullet v_k + \Gamma_k A(v_{kI} - v_k) - (\alpha_k\rho_k A)FI_k \bullet (v_k - v_r) - C\alpha_k\alpha_r\rho_m A\left[\frac{\partial(v_k - v_r)}{\partial t} + v_r\frac{\partial v_k}{\partial x} - v_k\frac{\partial v_r}{\partial x}\right]$$

Momentum from fluid velocity

Pressure gradient force

Wall friction

Momentum transfer from interface mass transfer

Interface frictional drag:

One of two models (based on flow regime) is used

y

Energy transfer from phase change at wall

- En

$$\frac{\partial}{\partial t}(\alpha_k\rho_k U_k) + \frac{1}{A}\frac{\partial}{\partial x}(\alpha_k\rho_k U_k v_k A) = -P\frac{\partial \alpha_k}{\partial t} - \frac{P}{A}\frac{\partial}{\partial x}(\alpha_k v_k A) + Q_{wk} + Q_{ik} + \Gamma_{ig}h_k^* + \Gamma_w h_k + DISS_k$$

Energy dissipation function ($DISS_k = \alpha_k\rho_k FW_k v_k^2$)

Energy crossing boundary with mass

Phasic interface heat transfer rates

Rate of internal energy change

Phasic wall heat transfer rates

Comparison Metrics: RELAP and TRACE Conservation Models

- Noncondensable Gas Field
  - Mass conservation equation
    $$\frac{\partial}{\partial t}\left(\alpha_g \rho_g X_n\right) + \frac{1}{A}\frac{\partial}{\partial x}\left(\alpha_g \rho_g X_n v_g A\right) = 0$$
  - Simplifying assumptions:
    - Gas has same velocity as vapor field
    - Gas at same temperature as vapor field
  - Assumptions eliminate need for energy and momentum conservation equations
- Dissolved Solute Field
  - Typically Boron
  - Mass conservation equation
    $$\frac{\partial \rho_b}{\partial t} + \frac{1}{A}\frac{\partial\left(\rho_b v_f A\right)}{\partial x} = 0$$
  - Same assumptions as noncondensable gas field

Comparison Metrics: WCOBRA/TRAC-TF2 Conservation Models – 1D Components

- Six-Equation Model
  - Liquid and Vapor Fields – Similar to RELAP and TRACE
  - Noncondensable Gas Field
    - Mass conservation equation
    - Assumed same velocity and temperature as vapor field

Comparison Metrics: WCOBRA/TRAC-TF2 Conservation Models – 3D Components

Mass crossing boundary

Body force

Drag by combined gas on liquid

Viscous effect on momentum

Pressure gradient force

Mass rate of change

Energy crossing boundary with mass

Momentum due to fluid velocity

Momentum exchange from mass exchange

Drag by wall on liquid

Wall heat transfer rate

$Q_{w,l} + (\alpha_l + \alpha_e)\frac{}{\partial t}$

Rate internal energy change

Heat flow to liquid due to change in phase

Heat flow to noncondensables

Heat flow to liquid

Pressure change

– Momentum: $-\alpha_{gas}\nabla P + \alpha_{gas}\rho_{gas}\underline{g} + \nabla\cdot\left[\alpha_{gas}\left(\underline{\underline{\sigma}}_{gas}\right)\right] - \underline{\tau}'''_{w,gas} - \underline{\tau}'''_{i,gl} - \underline{\tau}'''_{i,ge} + \Gamma'''\underline{U}_\Gamma$

– Energy: $\frac{\partial}{\partial t}\left(\alpha_{gas}\rho_{gas}H_{gas}\right) + \nabla\cdot\left(\alpha_{gas}\rho_{gas}H_{gas}\underline{U}_{gas}\right) = -\nabla\cdot\left[\alpha_{gas}\left(\underline{q}_{gas}\right)\right] + \Gamma'''H^i_{gas} + q'''_{i,gas} + q'''_{l,NC} + Q'''_{w,gas} + \alpha_{gas}\frac{\partial P}{\partial t}$

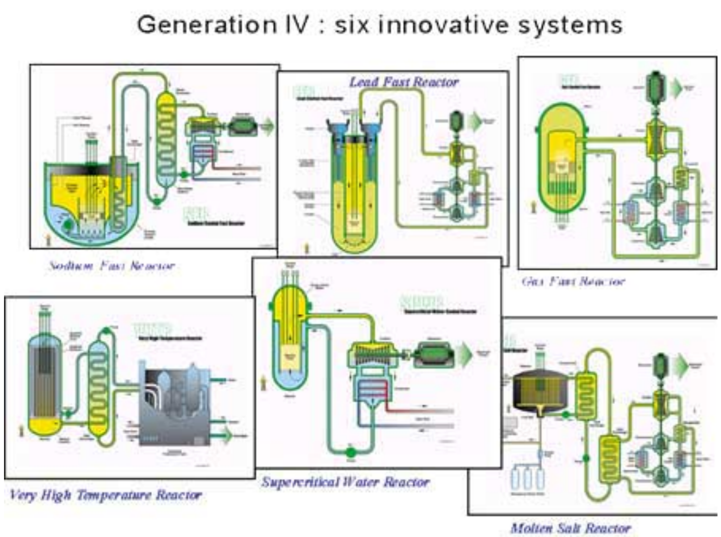
Comparison Metrics: WCOBRA/TRAC-TF2 Conservation Models – 3D Components

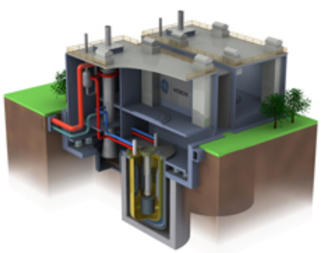
- Entrained Liquid (Droplet) Field
  - Mass: $\frac{\partial}{\partial t}(\alpha_e \rho_l) + \nabla \cdot (\alpha_e \rho_l \underline{U}_e) = -\Gamma'''_e + S'''_{ent} = -\eta \Gamma''' + S'''_{ent}$
  - Momentum: $\frac{\partial}{\partial t}(\alpha_e \rho_l \underline{U}_e) + \nabla \cdot (\alpha_e \rho_l \underline{U}_e \underline{U}_e) = -\alpha_e \nabla P + \alpha_e \rho_l \underline{g} - \underline{\tau}'''_{w,e} + \underline{\tau}'''_{i,ge} - \eta \Gamma''' \underline{U}_\Gamma + S'''_{ent} \underline{U}_{Se}$
  - Energy: Included in liquid field energy equation

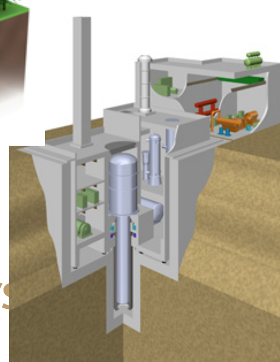
$$\frac{\partial}{\partial t}[(\alpha_l + \alpha_e)\rho_l H_l] + \nabla \cdot (\alpha_l \rho_l H_l \underline{U}_l) + \nabla \cdot (\alpha_e \rho_l H_l \underline{U}_e) = -\nabla \cdot \left[\alpha_l \left(\underline{q}_l + \underline{q}_l^T\right)\right] - \Gamma''' H_l^i + q'''_{i,l} + q'''_{l,NC} +$$
$$Q'''_{w,l} + (\alpha_l + \alpha_e)\frac{\partial P}{\partial t}$$

Assessment of the Conservation Equations For New Designs

- RELAP5-3D is one of the system codes used to analyze next generation plants
  - Sodium-Cooled Fast Reactor (SFR)
  - Lead-Cooled Fast Reactor (LFR)
  - Gas-Cooled Fast Reactor (GFR)
  - Very-High Temperature Reactor (VHTR)
  - Supercritical-Water Cooled Reactor (SCWR)
  - Molten-Salt Reactor (MSR)
  - Small Modular Reactors (SMRs)
    - LWR SMRs
      - W-SMR, NuScale, mPower, etc
    - Other SMRs
      - 4S (Liquid metal coolant), Prism (Na cooled), etc
  - Others







The reactor pictures are obtained from http://www.nrc.gov/reactors/advanced/4s.html

Assessment of the Conservation Equations

- Conservation equations in RELAP5-3D are mainly developed by considering two-phase flow of water coolant. Therefore, supercritical and LWR SMRs can be analyzed with RELAP5-3D's conservation equations.
- WCOBRA-TRAC-TF2 (which is a classified code of Westinghouse) has more realistic representation of entrainment/de-entrainment of two-phase flow in the conservation equations than Relap5-3D equations. Therefore, Loss of Coolant Accident (LOCA) results of Advanced LWRs are expected to be better than Relap5-3D.
- Conservation equations for various coolant types should be verified and validated. For instance, chemical reactions of coolant type should be considered in the conservation equations.

Comparison Metrics: Closure Relations

- Make conservation equations solvable
- Closure relations provide information on
  - Heat transfer between phases
  - Heat transfer from the walls to the fluid(s)
  - Mass exchange between phases
  - Momentum exchange between phases
  - Drag forces
  - Turbulence in continuous fields
  - Determination of flow regime
  - Determination of the Critical Heat Flux (CHF)

Comparison Metrics: Closure Relations/ Critical Heat Flux

- Determines Flow Regime Category
  - “Wetted” flow regimes with liquid in contact with wall
  - “Dryout” flow regimes with limited or no liquid-to-wall contact
- Provides lower wall superheat boundary for transition boiling

Comparison Metrics: Closure Relations/ Computation of Critical Heat Flux

- RELAP5
  - AECL-UO CHF Lookup Table
    - Used by Groenveld and co-workers
    - Includes factors for varying tube sizes or for rod bundles
    - Considers forward/reverse flow
    - Considers axial power shape
    - Incorporates effect of boundary layer changes at bundle inlet and after grid spacers through factors
    - 3D interpolation: Pressure -> Mass Flux -> Quality
  - PG-CHF
    - Only available in RELAP5-3D
    - Replaces CHF table lookup method
    - Data from Czech republic data bank
    - Calculates the Critical Heat Flux Ratio (CHFR) - ratio of critical heat flux to local heat flux

Comparison Metrics: Closure Relations/ Computation of Critical Heat Flux

- TRACE
  - AECL-IPPE look-up table
    - Updated version of AECL-UO used in RELAP5-3D
    - Correction factors for various tube sizes, orientations, and bundle geometries
    - Similar interpolation scheme to what was done in RELAP5-3D
- TRAC
  - Vessel Component
    - AECL-UO CHF
      - Groenveld
  - 1D Components
    - Biasi correlation
      - Rod bundles
      - Generally over-predicts CHF

Biasi:

$$q_{CHF} = \max(q_{CHF1}, q_{CHF2})$$

Hydraulic diameter

Critical heat flux

$$q_{CHF1} = \frac{1.883\times10^{7}}{D_h^n |G|^{1/6}}\left[\frac{f_p}{|G|^{1/6}} - x_e\right]$$

$$q_{CHF2} = \frac{3.78\times10^{7}}{D_h^n |G|^{0.6}} h_p [1 - x_e]$$

Equilibrium quality

Mass flux (g/cm^2-s)

$$n = \begin{cases} 0.4 & D_h \ge 1cm \\ 0.6 & D_h < 1cm \end{cases}$$

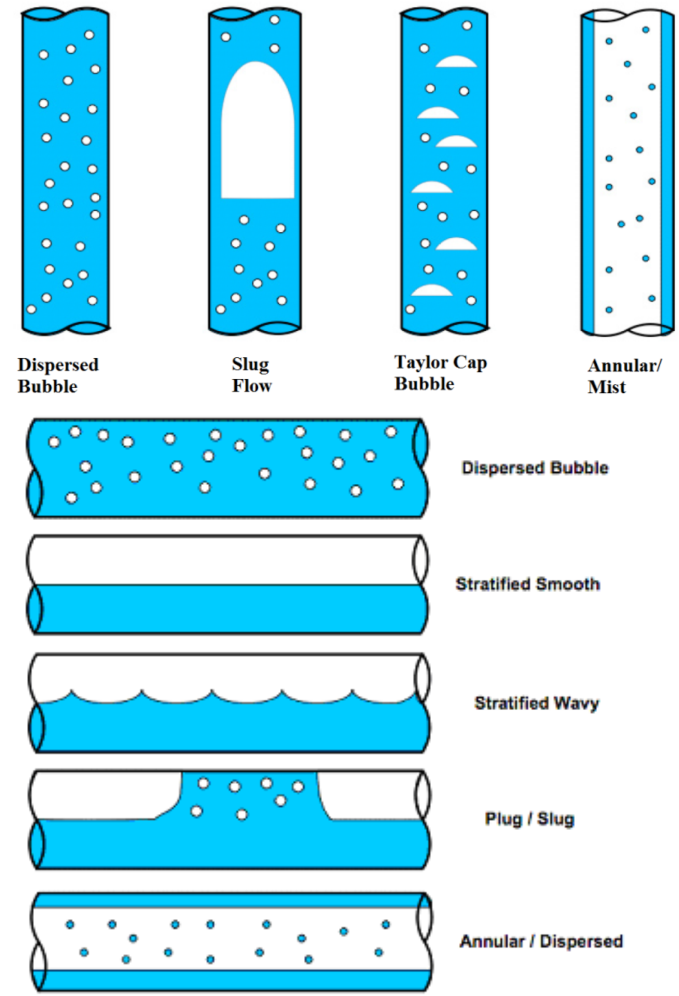
Pressure (bar)

$$f_p = 0.7249 + 0.099P\exp(-0.032P)$$

$$h_p = -1.159 + \frac{8.99P}{10 + P^2} + 0.149P\exp(-0.019P)$$

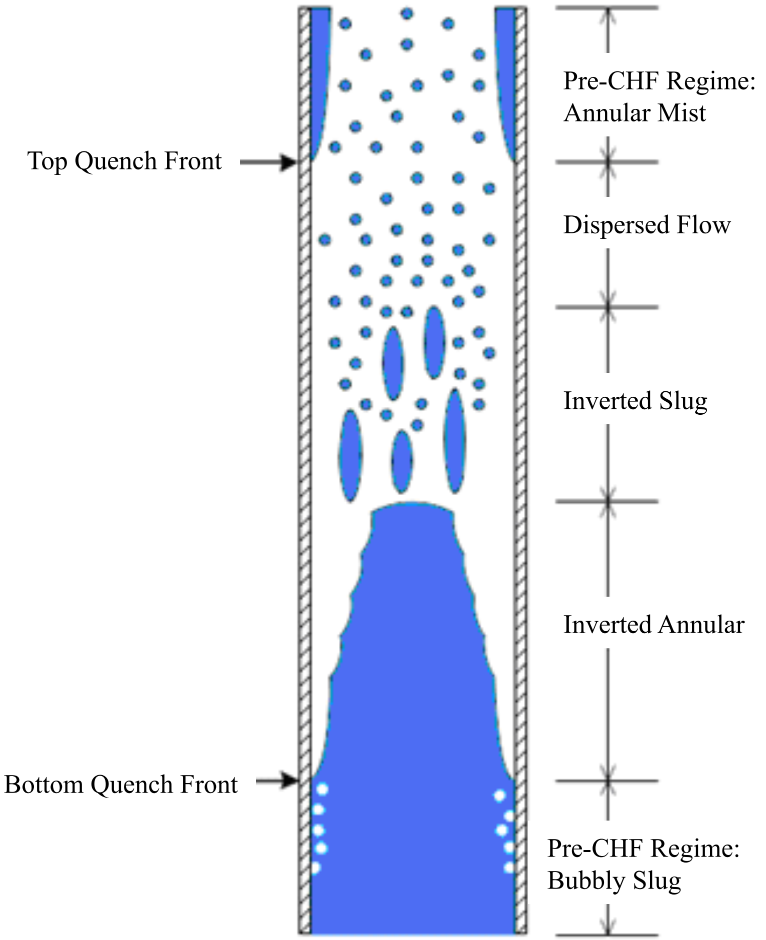
Comparison Metrics: Flow Regimes/Pre-CHF

- Models compute void fraction
  - Specific bubble location/ configuration not modeled
- Vertical
  - Dispersed Bubble
  - Slug Flow
  - Taylor Cap Bubble
  - Annular/Mist
- Horizontal
  - Dispersed Bubble
  - Stratified Smooth
  - Stratified Wavy
  - Plug/Slug
  - Annular/Dispersed



Comparison Metrics: Flow Regimes/Post-CHF

- Models compute void fraction
  - Specific droplet location/ configuration not modeled
- Little or no liquid contact with wall
- CHF point determines transition to “dryout”
  - Post-CHF correlations cover both DNBR and annular dryout



Interfacial Heat Transfer

- Both heat and mass transfer between phases
- Heat transfer computed based on temperature gradients between each phase and the interface

Computation of Interfacial Heat Transfer

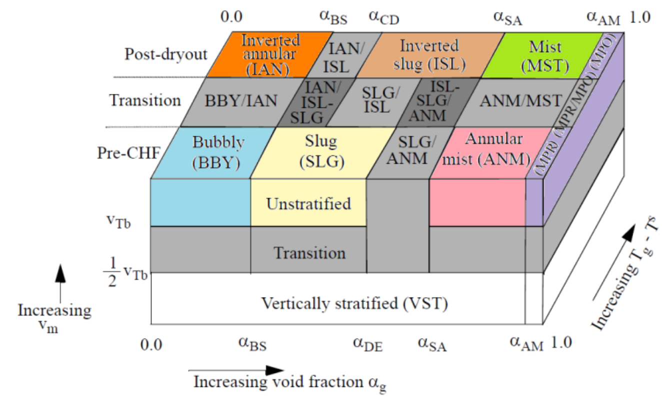
- Superheat and subcooled allowed for both phases
  - heat transfer can be toward or away from interface for each phase
- Energy to interface contributes to vaporization
- Energy from interface contributes to condensation
- Net rate of mass transfer from summation of contributions from each side of the interface
- Heat transfer between phases depends on flow regime
  - Flow regime maps developed to classify flow regimes
  - Heat transfer coefficient correlations specific to each regime
- Differences between codes
  - Correlations used to determine heat transfer coefficients
  - Approximations of interfacial area

Interfacial Heat Transfer Correlations – Bubbly Flow

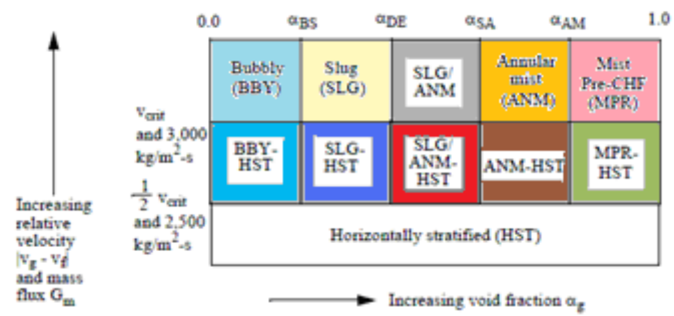
RELAP5-3D	$H_{if} = \left\{ \begin{array}{l} \max \left[\begin{array}{ll} -\frac{k_f}{d_b}\frac{12}{\pi}\Delta T_{sf}\frac{\rho_f C_{pf}}{\rho_g h_{fg}}\beta & Plesset - Zwick \\ \frac{k_f}{d_b}\left(2.0 + 0.74\,\mathrm{Re}_b^{0.5}\right) & Lee - Ryley \end{array} \right] \\ + 0.4\left\lvert v_f \right\rvert \rho_f C_{pf} F_1 \end{array} \right\} \left(a_{gf} F_2 F_3\right)$ $= 0.0 \quad if\ \alpha_g = 0\ and\ \Delta T_{sf} \geq 0$
TRACE	$h_{li,DB} = \frac{k_l}{d_{DB}} Nu_{DB}$ $Nu_{DB} = 2.0 + 0.6 \cdot \mathrm{Re}_{DB}^{1/2} \cdot \mathrm{Pr}_l^{1/3}$
WCOBRA/TRAC-TF2	$Nu = 2.0 + \left(0.4\sqrt{\mathrm{Re}} + 0.06\,\mathrm{Re}^{2/3}\right)\mathrm{Pr}_{liq}^{0.4}$

RELAP Flow Regime Maps

- Flow regime maps determine correct correlation
- RELAP has maps for both horizontal and vertical flow regimes



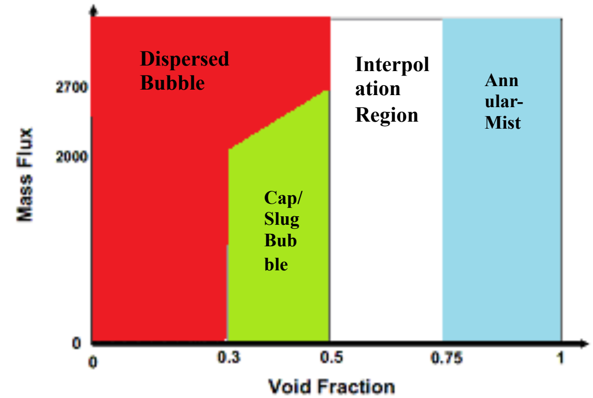
RELAP5-3D Vertical Flow Regime



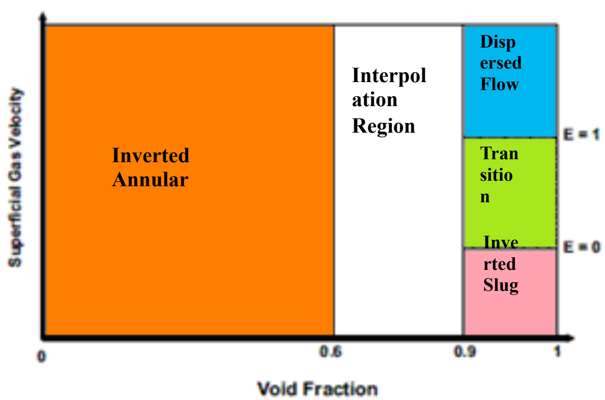
RELAP5-3D Horizontal Flow Regime

TRACE Flow Regime Maps

- Breakpoints between flow regimes differ between codes
- TRACE uses the same flow regime map for both horizontal and vertical regimes, but has specific stratified models used when stratification criteria are met
  - Stratification Criteria
    - Pipes with junctions that have inclination less than 80 degrees
    - Pipes do not have vertical junctions on both sides
    - Taitel-Dukler criterion used to determine stratified flow
- Maps for TRAC code are very similar



Pre-CHF Flow Regime Map



Post-CHF Flow Regime Map

Wall-to-fluid heat transfer

- Selection of correlation depends on characteristic parameters such as:
  - Flow Rate
  - Wall surface temperature
  - Liquid temperature
  - Void fraction in working fluid
  - Heated geometry (Rod bundles, flat plates, tubes)
- Single Phase Heat Transfer Details for Specific Codes
  - RELAP
    - Dittus-Boelter correlation selected by default; others available by user selection
      - RELAP5-MOD3 includes Churchill-Chu, Kays, Shah, McAdams, and ESDU
      - RELAP5-3D adds Gnielinski, Jackson, Petukhov, Sieder-Tate, and others
      - Limited to correlations for circular pipes
      - Large-radius annuli can be used to model parallel plates
      - No spherical shape correlations
    - Laminar, Turbulent, and natural convection correlations for single-phase flows
      - Code selects maximum of the three for use

Wall-to-fluid heat transfer

- TRACE
  - Correlations for Laminar, Turbulent, and natural convection in single-phase flows
    - Code selects maximum of the three for use
  - Gnielinski correlation used for turbulent forced convection
- TRAC
  - Single-phase uses Dittus-Boelter correlation

Wall-to-fluid heat transfer

- Two-Phase Heat Transfer
  - Nucleate Boiling
    - TRACE
      - Combination of pool and forced convection models
      - Gorenflo and Cooper used as pool boiling model
    - RELAP, TRAC, ATHLET
      - Chen correlation for nucleate boiling

Nucleate boiling heat flux

Forced circulation heat flux

Pool boiling heat flux (from Gorenflo)

$$q''_{NB} = \left[q''^3_{FC} + q''^3_{PB}\right]^{\frac{1}{3}}$$

$$h_{pool\_boil\_Gorenflo} = h_0 F_P \left(\frac{q''}{q''_0}\right)^n \left(\frac{R_P}{R_{P0}}\right)^{0.133}$$

Wall-to-fluid heat transfer

- Transition Boiling
  - TRACE defines upper and lower limits of transition boiling regime
    - CHF temperature is set as the beginning of the transition boiling regime
    - The minimum film boiling temperature is used to determine end of the transition boiling regime
    - TRACE interpolates between these two points on the basis of wall superheat
      - Interpolation weighting factor computed as was done in COBRA/TRAC
      - Expected to underpredict the transition boiling heat transfer coefficient
  - TRAC
    - Weighted sum of nucleate-boiling and film-boiling heat transfer terms based on wall area that is wet
  - RELAP
    - CHF point is set as the lower boundary of the transition boiling region
    - The interfacial transition heat transfer coefficient is computed by interpolation between the pre-CHF and the film boiling regimes
    - The wall-to-fluid heat transfer coefficient uses the Chen transition boiling model, which sums components of the wall heat transfer to the liquid and the wall heat transfer to the vapor/gas
    - Computes the transition boiling heat transfer coefficient and the film boiling heat transfer coefficient and takes the maximum value.

Assessment on the Closure Relationships

- CHF lookup tables and correlations are mainly developed for water. Therefore, LWR SMRs and supercritical reactors can use the CHF models.
  - Need for new CHF correlations should be evaluated for non-water cooled reactor designs
- Existing flow regimes are defined for water and they significantly depend on orientation, vapor fraction, velocity etc. Since several of the next generation power plant concepts employ different coolant types, new flow regimes and flow regime dependent correlations are needed. Especially for molten salt reactors RELAP5-3D must include wide range of flow regimes and corresponding correlations/models for heat transfer coefficient and pressure drops.
  - RELAP5-3D has two correlations – Bundle or non-bundle
  - RELAP5-3D uses Petukhov correlation for gas-cooled systems
- There might be various gases in addition He for advanced reactors. Because they have various coolant properties and mixture/drift features, several new correlations are needed in RELAP5-3D. In addition to interfacial features of the combination of these coolants, coolant-wall interface features must be realistically defined in the code. This issue is a serious problem for hypothetical accidents of these power plants.

Assessment on the Closure Relationships - Continued

- New reactor designs may challenge the current closure relations
  - Air and/or vapor distribution in gas-cooled designs in the case of accident transients
  - Accident scenarios with two dissimilar gases
  - Realistic representation of two-phase flow in SMR designs since the size is decreasing with keeping model uncertainties constant

Validation

- Phenomenological Cases
  - Simple problems with exact solutions
  - Address a single code model or capability
- Separate Effects Tests (SETs)
  - Test models against thermal-hydraulic tests of a particular component or geometry
  - Relatively simple experiments addressing one or a few specific phenomena
- Integral Effects Tests
  - Code comparisons to scaled plant models
  - Test overall functionality of the code
- Similar tests used for many of the codes
- V&V Reports that are publicly available do not address:
  - Gas-coolant
  - Pebble-bed spherical heating surfaces
  - Small Modular Reactor Components

Code Major Assumptions

- All codes assume that component approach to modeling reactor systems is appropriate
  - Self-contained components of reactor coolant loop system
  - Components nodalized into physical volumes
    - Fluid conditions averaged within volumes
- TRAC, TRACE, RELAP
  - Noncondensible gas and dissolved solute
    - Move with vapor and liquid as appropriate
    - Minimal interactions with working fluid
    - Isothermal with working fluid
  - Dalton's law of partial pressures applies
- RELAP, TRACE
  - Field equations derived with negligible viscous shear stresses
  - Explicit turbulence modeling not coupled to conservation equations
- WCOBRA\TRAC-TF2
  - Quasi-steady heat transfer coupling between wall and fluid
    - Ignores time dependencies
    - Requires detailed knowledge of fluid parameters

Conclusion

- Available literature lacks detailed V&V of codes for use in future reactor designs
  - Gas-Cooled reactor designs present unique heat transfer and flow modes – correlations for heat transfer coefficients and pressure drops must be verified and validated
  - Small Modular Reactor (SMR) designs use innovative steam generator, pressurizer, pump and heat exchanger designs that must be modeled effectively
  - Natural Circulation is integral to passive safety in most of the SMR designs – codes must be validated for accuracy when computing heat transfer coefficients and loss coefficients for the SMR natural circulation flows.
  - New coolant types including realistic heat transfer and pressure drop correlations/models must be employed, verified and validated in the codes.
  - Realistic simulation of mixture of gas coolant with air and other gases and maybe dry-vapor must be considered in the codes.

Conclusion

- Fuel Performance modeling capabilities are limited
  - SCDAP models fuel melt and oxide spallation
  - Other codes lack this capability
- Effect of containment is modeled by externally coupled codes – system codes do not natively address system containment
- Selection of a system code must be done with care and consider:
  - Closure models used
  - Numerical schemes
  - Validation of the code for the models being exercised
  - Capability of the models to capture effects in “real world” systems