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Title: Multiphase Flow Analysis in Hydra-TH

Author(s):
Christon, Mark A.
Bakosi, Jozsef
Francois, Marianne M.
Lowrie, Robert B.
Nourgaliev, Robert

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Multiphase Flow Analysis in Hydra-TH

J. Bakosi, M. A. Christon, M. M Francois, R.B. Lowrie
Los Alamos National Laboratory

R. Nourgaliev
Idaho National Laboratory

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ABSTRACT

CASL Consortium for Advanced Simulation of LWRs

This talk presents an overview of the multiphase flow efforts with Hydra-TH. The presentation begins with a definition of the requirements and design principles for multiphase flow relevant to CASL-centric problems. A brief survey of existing codes and their solution algorithms is presented before turning the model formulation selected for Hydra-TH. The issues of hyperbolicity and well-posedness are outlined, and a three candidate solution algorithms are discussed. The development status of Hydra-TH for multiphase flow is then presented with a brief summary and discussion of future directions for this work.

U.S. DEPARTMENT OF ENERGY Nuclear Energy

OVERVIEW

- Requirements & Design Principles
- Survey of Codes & Solution Algorithms
- Hydra-TH Model Formulation
- Candidate Hydra-TH Solution Algorithms
- Hydra-TH Status
- Summary & Future Directions

HYDRA-TH: requirements & design principles

- Multi-(*N*)-fluid (user-specified) formulation
- (Discrete) mass, momentum, and energy conservation
- Ability to cover all-speeds (from nearly-incompressible to fully-compressible)
- Ability to deal with numerically stiff fluid (water) equation of state
- Robust treatment of phase appearance and disappearance
- Ability to deal with boiling/condensation (tight coupling with energy equation)
- For [1-fluid, ρ=*const*, operator-splitting] option, should reduce to the original HYDRA algorithm (proven to be robust/accurate/efficient)
- Solvability: hyperbolicity/well-posedness
- Efficient for large-scale unstructured-mesh HPC applications (scalable)
- Can be tightly coupled with Next-Generation System Analysis codes

Survey of Codes & Solution Algorithms

- Codes Surveyed: NPHASE, NEPTUNE, CATHARE, StarCD & CCM+, Fluent, CFX, MFIX, CFDLib, TRAC, TRACE, RELAP5, RETRAN, …
  - Documented in "Effective-Field Modeling for Multi-Fluid Flows" working notes
- Basic formulations are similar in terms of ensemble averaged conservation equations, degrees-of-freedom, and closures
  - Volume fractions, multiple velocities, multiple energy eq.'s, etc.
  - Virtually all are using a single-pressure approximation
- Approaches to hyperbolize equations
  - Bulk pressure difference, interface dynamic pressure, added mass
  - 7 equation-model of Saurel, Berry, et al. preserves hyperbolicity -- invisicid
- Solution algorithms
  - Virtually all are pressure-based
  - Many are based on SIMPLE (aka Uzawa iteration)
    - Expect slow convergence rates (ex: many 100's of iterations for small problems)
    - NPHASE combines SIMPLE-like outer iteration with coupled mass-momentum solve
  - All current work-horse T-H codes (RELAP5, TRAC, TRACE, CATHARE, RETRAN) use operator-split algorithms

HYDRA-TH: model formulation

(5*N*)-conservation equations, *N*-field formulation

- **Mechanical & thermal non-equilibrium**
- **Pressure equilibrium**
- **Multiple-bulk-pressure**
- **Hyperbolic (easily provable when *N*=2 fields)**
- **Can implement both acoustically-filtered and fully-compressible forms**
- **EOS: generic; for water – IAPWS-IF97 Standard**
- **Multiphase closures: from NPHASE methods, Lahey, Podowski, et al.**
- [ILES, LES/DES, k-ε and k-ω models in the future]
- [Interfacial area transport (IAT) in the future (from NPHASE/NEPTUNE)]

Application Focus

1. **Subcooled boiling**
2. Departure from nucleate boiling (DNB)
3. Loss-of-coolant accidents (LOCA)
4. Reflooding

In the future

HYDRA-TH: governing equations

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot \left(\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k\right) = \boxed{\Gamma_k}$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k + \boxed{\mathbf{M}'_k} + \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}^{m}_{ki}} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right] \tilde{\mathbf{v}}_k\right) = \boxed{\mathbf{M}'_k} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k + \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}^{Re}_k}\right]\right) + \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v^{e}_{ki}}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W'_k}$$

+ Turbulence equations

To close:

- + ***N*** **equations of state,** $\bar{p}_k\left(\bar{\rho}_k, \tilde{u}_k\right)$
- + **Constitutive physics (for terms in boxes** $\boxed{}$**)**
- + **Compatibility condition,** $\sum_k \alpha_k = 1$
- + **Bulk pressure difference models,** $\Delta \bar{p}_{(ij)}\left(\mathbf{U}\right),\ i \neq j,\ (i,j) = 0, \ldots, N-1$

HYDRA-TH: hyperbolicity/well-posedness

CASL
Consortium for Advanced Simulation of LWRs

Wave/Eigen-structure

$$\bar{p}$$

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot \left(\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k\right) = \boxed{\Gamma_k}$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k + \cancel{\boxed{\mathbf{M}_k}} +$$

$$+ \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}_{ki}^{m}} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right] \tilde{\mathbf{v}}_k\right) = \cancel{\boxed{\mathbf{M}_k}} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k +$$

$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}}\right) - \ldots\right]\right)$$

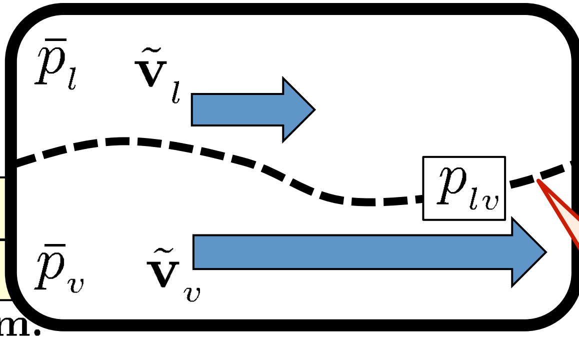
$$+ \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_k} \ldots\right.$$

This is a
non-physical model
(used in TRAC/TRACE)

Non-hyperbolic IF

...RTMENT OF
...ERGY
Nuclear Energy

HYDRA-TH: hyperbolicity/well-posedness



Interfacial dynamic pressure:

$$\boxed{\xi}\hat{\rho}\Delta U^2$$

(Bernoulli effect, [Stuhmiller, 1977])

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \dots$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k]) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k$$

$$\boxed{\delta}\,\alpha_l \alpha_v \frac{\bar{\rho}_l \bar{\rho}_v}{\alpha_l \bar{\rho}_l + \alpha_v \bar{\rho}_v}$$

$$+\nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \dots_{ki} \dots \boxed{\Gamma_k}$$

[Bestion, 1990]

To...

$$\frac{\partial}{\partial_t} \dots \nabla \alpha_k + \dots$$

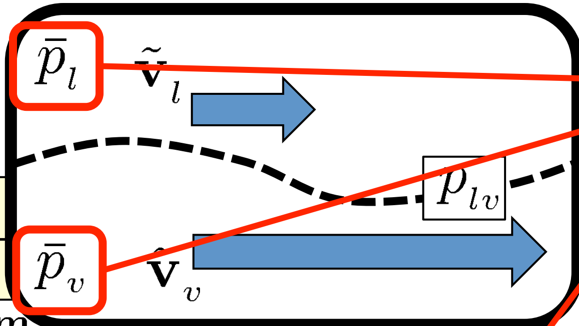
$$+ \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} \dots\right.$$

Conditionally hyperbolic:

$$\delta \geq 1$$

CATHARE
NEPTUNE/OVAP

HYDRA-TH: hyperbolicity/well-posedness



Bulk pressure difference
(e.g., surface tension)

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \cdots$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \boxed{\bar{p}_k}\right]\right) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k + \boxed{\mathbf{M}'_k} + \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}^m_{ki}}\ \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \boxed{\bar{p}_k}\right] \tilde{\mathbf{v}}_k\right) = \boxed{\mathbf{M}'_k} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k + \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}^{Re}_k}\right]\right) + \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v^e_{ki}}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W'_k}$$

HYDRA-TH: hyperbolicity/well-posedness

Added mass:

$$\boxed{\mu\bar{\rho}_c \frac{\mathrm{d}_\mathrm{d}\Delta\vec{U}}{\mathrm{d}t}}$$

Mass:

$$\boxed{\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla\cdot\left(\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k\right)} = \boxed{\Gamma_k}$$

Momentum:

$$\boxed{\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla\cdot\left(\alpha_k\left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right)\nabla\alpha_k + \boxed{\mathbf{M}_k^{'}}} +$$

$$+\nabla\cdot\left(\alpha_k\left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right]\right) + \alpha_k \ldots$$

Total energy:

$$\boxed{\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla\cdot\left(\alpha_k\left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right]\tilde{\mathbf{v}}_k\right) = \boxed{\mathbf{M}_k^{'}}\cdot\tilde{\mathbf{v}}_k \ldots}$$

$$+\nabla\cdot\left(\alpha_k\left[\tilde{\mathbf{v}}_k\left(\boxed{\bar{\tau}_k} + \ldots\right.\right.\right.$$

$$+\alpha_k\bar{\rho}_k\left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k}\cdot\tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k}\left(\boxed{u_{ki}} + \frac{\left(\boxed{v_{ki}^{e}}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W_k^{'}}$$

RELAP5
NPHASE
NEPTUNE

HYDRA-TH: hyperbolicity/well-posedness

Parabolic terms

Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot (\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k) = \boxed{\Gamma_k}$$

Momentum:

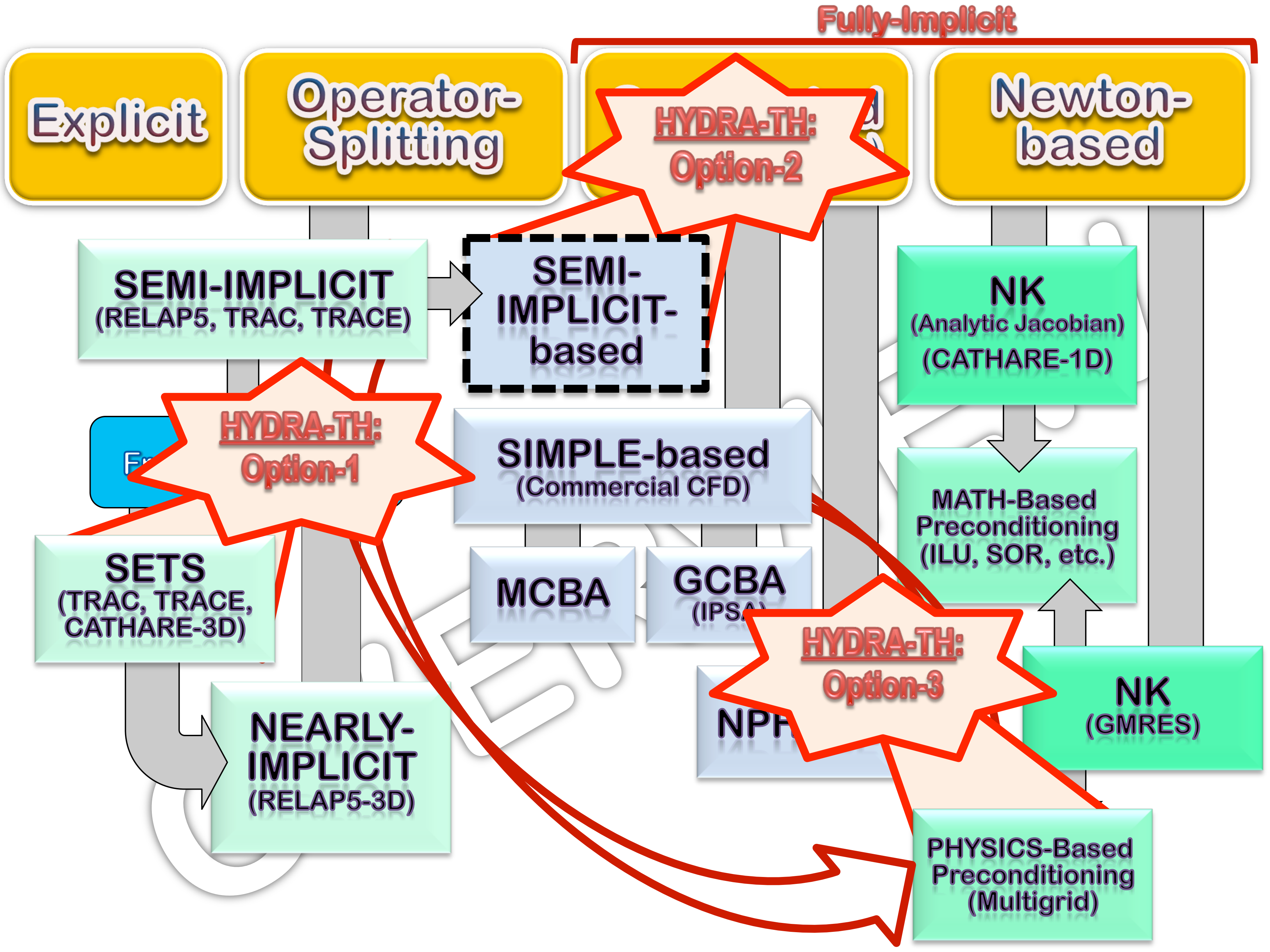
$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k]) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k + \boxed{\mathbf{M}'_k} + \boxed{\nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right]\right)} + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}^m_{ki}} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t} \left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{e}_k + \bar{p}_k] \tilde{\mathbf{v}}_k) = \boxed{\mathbf{M}'_k} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k + \boxed{\nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}^{Re}_k}\right]\right)} + \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v^e_{ki}}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W'_k}$$

HYDRA-TH:

Solution algorithm
(preliminary design)



Fully-Implicit
Explicit
Operator-Splitting
Newton-based
HYDRA-TH: Option-2
SEMI-IMPLICIT (RELAP5, TRAC, TRACE)
SEMI-IMPLICIT-based
NK (Analytic Jacobian) (CATHARE-1D)
HYDRA-TH: Option-1
SIMPLE-based (Commercial CFD)
MATH-Based Preconditioning (ILU, SOR, etc.)
SETS (TRAC, TRACE, CATHARE-3D)
MCBA
GCBA (IPSA)
HYDRA-TH: Option-3
NK (GMRES)
NEARLY-IMPLICIT (RELAP5-3D)
PHYSICS-Based Preconditioning (Multigrid)

HYDRA-TH: solution algorithm, optio

No compatibility enforced

$$res_{\alpha} = 1 - \sum_k \hat{\alpha}^{\star\star}_{k(c)} \neq 0$$

SETS-based operator-splitting (Fractiona

1. Volume fraction update ("mass stabilizer")

$$a^{(k)}_{c,c}\left(\mathbf{U}^{\star}\right)\hat{\alpha}^{\star\star}_{k(c)} + \sum_n^N a^{(k)}_{c,n}\left(\mathbf{U}^{\star}\right)\hat{\alpha}^{\star\star}_{k(n)} = b^{(k)}_c \left(\mathbf{U}\right.$$

Phasic mass

$$\tilde{\mathbf{v}}^{\diamond}_{k(c)} = \frac{b^{(k)}_c + \sum_{m\neq k}^{K} c^{(k,m)}_c \tilde{\mathbf{v}}^{\star}_{m(c)} - \sum_n^N a^{(k)}_{c,n}\tilde{\mathbf{v}}^{\star}_{k(n)}}{a^{(k)}_{c,c} + \sum_{m\neq k}^{K} c^{(k,m)}_c}$$

ILU or AMG

2. Velocity update ("momentum stabilizer", SINCE-based)

$$\hat{\tilde{\mathbf{v}}}^{\star\star}_{k(c)} + \sum_n^N a^{(k)}_{c,n}\hat{\tilde{\mathbf{v}}}^{\star\star}_{k(n)} == \underbrace{b^{(k)}_c + \sum_{m\neq k}^{K}\left[c^{(k,m)}_c \frac{b^{(m)}_c + \sum_{j\neq m,k}^{K} c^{(m,j)}_c \tilde{\mathbf{v}}^{\diamond}_{j(c)} - \sum_n^N a^{(m)}_{c,n}\tilde{\mathbf{v}}^{\diamond}_{m(n)}}{a^{(m)}_{c,c} + \sum_{j\neq m}^{K} c^{(m,j)}_c}\right]}_{\tilde{b}^{(k)}_c}$$

No mass/energy conservation enforced

...interfacial momentum coupling...)

3. Enthalpy update ("energy stabilizer")

$$a^{(k)}\left(\mathbf{U}^{\star}\right)\hat{\tilde{h}}^{\star\star} + \sum^N a^{(k)}\left(\mathbf{U}^{\star}\right)\hat{\tilde{h}}^{\star\star}_{k(n)} = b^{(k)}_c\left(\mathbf{U}^{\star}\right)$$

Compressibility

Phasic energy conservation equations (ILU or AMG)

AMG

5. Turbulence Equations

ion (mass/energy conservation + compatibility)

6. Other scalar transport equations

derivative of [Liles, Reed, 1978] "semi-implicit" (ICE-based) algorithm

HYDRA-TH: solution algorithm, option-2

Fully-Implicit, Segregated (Picard-iteration)

Fractional steps algorithm

1. Volume fraction update ("mass stabilizer")
2. Velocity update ("momentum stabilizer", SINCE-based)
3. Enthalpy update ("energy stabilizer")
4. Pressure-Helmholtz Equation
5. Turbulence Equations
6. Other scalar transport equations

Converged?

HYDRA-TH: solution algorithm, option-3

Fully-Implicit, NK (Physics-based preconditioning)

Fractional step algorithm
(preconditioning)

$$\mathbb{J}_{i,j} \equiv \frac{\partial res_i}{\partial \mathcal{X}_j}$$

Linear solve:

$$\boxed{\mathbb{J}^{\text{it}}}\,\delta\vec{\mathcal{X}}^{\text{it}} = -\vec{res}\left(\vec{\mathcal{X}}^{\text{it}}\right)$$

Start Newton iteration

$$\vec{\mathcal{X}}^{\text{it}+1} = \vec{\mathcal{X}}^{\text{it}} + \boxed{\delta\vec{\mathcal{X}}^{\text{it}}}$$

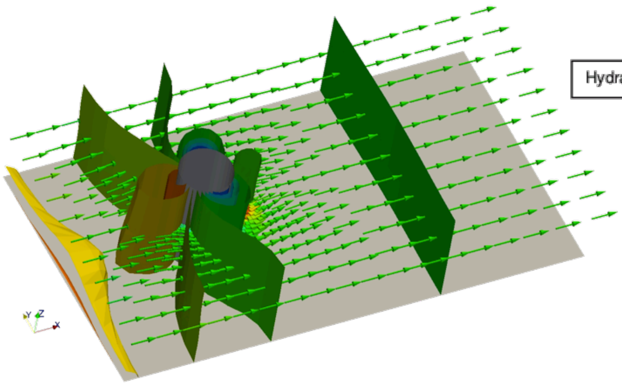
IF $\left|\left|\vec{res}\left(\vec{\mathcal{X}}^{\text{it}}\right)\right|\right|_2 < \text{tol}_\text{N} \left|\left|\vec{res}\left(\vec{\mathcal{X}}^{0}\right)\right|\right|_2$ ELSE

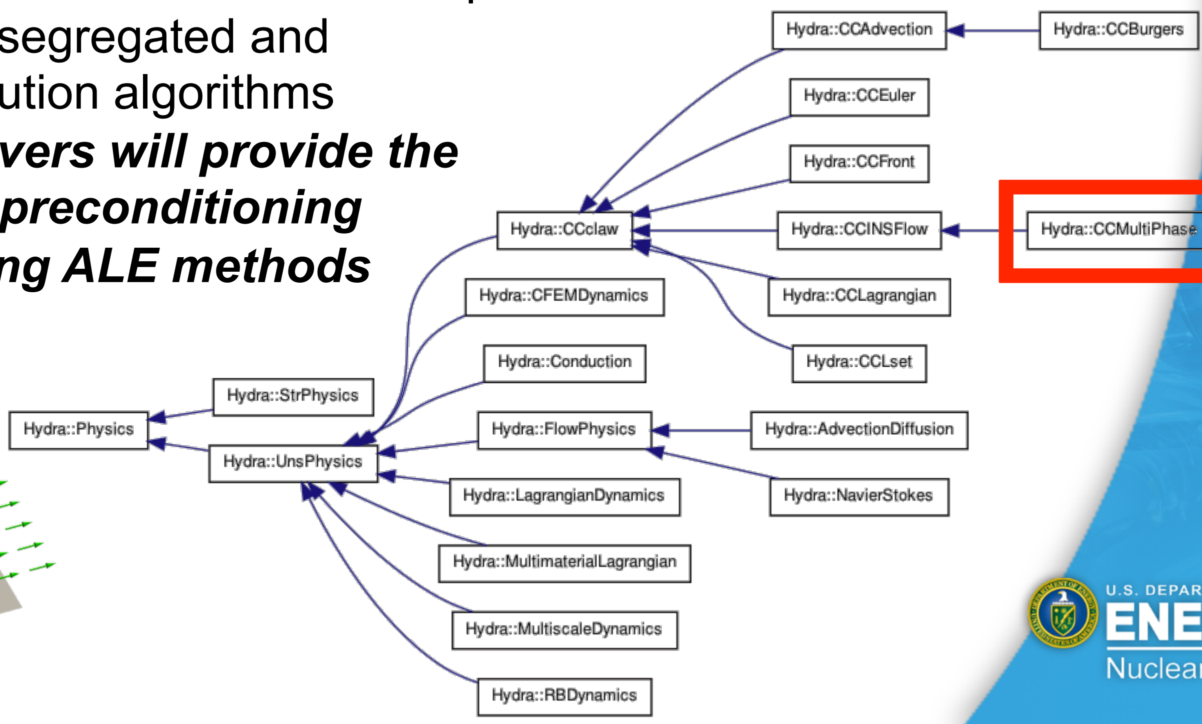
End Newton iteration

HYDRA-TH: Status

- **Prototype multiphase physics is in place**
  - Running simple problems and solving *N*-momentum equations w. single pressure
  - Volume fractions treated as passive scalars for now
  - All keywords, BC's, IC's inherited from the virtual incompressible physics

- **General development plan**
  - Re-use all existing BC's, IC's, materials, transport solvers, and turbulence statistics on a phasic basis
  - Implement both segregated and fully-coupled solution algorithms
  - ***Segregated solvers will provide the physics-based preconditioning***
  - ***Preserve existing ALE methods for FSI***





Summary & Future Directions

- **The basic formulation is relatively well defined at this point**
  - Some questions remain on multiphase closures, e.g., the form of lift forces, mass exchange terms, etc.
    - ➢ May require some additional research to adequately define source terms
  - A number of questions/algorithmic decisions will be answered over the next 3-4 months

- **Prototype multiphase virtual physics is in place**
  - Able to solve multiple momentum equations with identical BC's and obtain correct solutions
  - Volume fraction transport (i.e., continuity) is in place
  - Extension for multiple energy equations appears straightforward
  - Additional effort required to integrate steam tables, additional constitutive and EOS models

- **On-track for L3:THM.CFD.P5.06 milestone**
  - Initial two-phase laminar test case to be based on DEBORA experiments is targeted – time permitting

~ Backup Slides ~

NPHASE Solution Algorithm
a few general notes

- 2 approaches : segregated or coupled mass/momentum
- Coupled mass/momentum approach preferred approach
  - Better stability and robustness
- User routines for closure terms (drag force, lift interfacial force, wall interfacial force, turbulence dispersion interfacial force)
- Closure terms treated differently in segregated and coupled solver
  - Segregated algorithm: linearized drag force, other terms, other terms added as RHS terms held constant during iterations.
  - Coupled algorithm: linearized terms added to LHS and full model term added to RHS

NPHASE Solution Algorithm (Coupled Solver) Coupled Mass/Momentum – Segregated Enthalpy

- Solve for velocity, pressure, volume fractions
  - Variables: (total variables is 5*Nfield)
    - Velocity (3), pressure (1) and volume fraction (1) per field
    - Density held constant → volume fraction equation
  - Equations:
    - Mass (continuity) (1 per field)
    - u, v, w momentum (3 per field)
    - Constraint – sum of volume fractions = 1 (1 total)
    - Jump equations – p_k-p=0 (P equilibrium) (Nfield-1)
- Solve enthalpy, turbulence k-e, species concentration
- Update density as function of T
- Iterate until convergence

NEPTUNE (NURETH10 paper) Pressured-based method with mass/momentum/energy coupling

- predict velocities through partially linearized momentum equations (other variables are frozen and taken at previous time step)
- Mass/momentum/energy coupling
  - Momentum equation using predicted velocity (frozen convective/diffusive parts and pressure and volume fractions treated implicitly)
  - Coupled with mass and total enthalpy equation
  - Iterative solver for pressure, volume fraction, total enthalpy, velocity, density (function of p and h). Enthalpy, thermodynamic properties, volume fractions prediction, pressure equation correction, update velocities, iterate until convergence (convergence is sum volume fractions=1)
- Update other variables (turbulence, interfacial areas)

NEPTUNE CFD V1.0
Interfacial momentum transfer terms

$$\vec{M}_{ki} = \vec{M}_k^D + \vec{M}_k^{MA} + \vec{M}_k^L + \vec{M}_k^{DT}$$

- Drag force

$$\vec{M}_g^D = -\vec{M}_l^D = -\frac{1}{8} a_i \rho_l C_D \left| \vec{u}_g - \vec{u}_l \right| \left(\vec{u}_g - \vec{u}_l \right)$$

- Added mass (virtual mass)

$$\vec{M}_g^{MA} = -\vec{M}_l^{MA} = -C_{MA} \alpha \frac{1+2\alpha}{1-\alpha} \rho_l \left[\left(\frac{\partial \vec{u}_g}{\partial t} + \vec{u}_g \cdot \nabla \vec{u}_g \right) - \left(\frac{\partial \vec{u}_l}{\partial t} + \vec{u}_l \cdot \nabla \vec{u}_l \right) \right]$$

- Lift force

$$\vec{M}_g^L = -\vec{M}_l^L = -C_L \alpha \rho_l \left(\vec{u}_g - \vec{u}_l \right) \times \left(\nabla \times \vec{u}_l \right)$$

- Turbulent dispersion

$$\vec{M}_g^{DT} = -\vec{M}_l^{DT} = -C_{DT} \rho_l K_l \nabla \alpha$$

$C_{MA} = 0.5$

$C_L = 1$

$C_{DT} = 1$ (DEDALE)

$C_{DT} = 2.5$ (DEBORA)

Guelfi A. et al., NEPTUNE: A New Software Platform for Advanced Nuclear Thermal Hydraulics, Nuclear Science and Engineering, 156, 281-324, 2007

NEPTUNE CFD V1.0
Interfacial heat and mass transfer terms

- Interfacial mass transfer

$$\Gamma_g = -\Gamma_l = \frac{-q_{li} - q_{gi} + q_e}{H_g - H_l}$$

- Liquid to interface heat transfer
  - Condensation
  - Evaporation

$$q_{li} = h_{li}(T_{sat} - T_l) \qquad h_{li} = \frac{\lambda_l}{d_s}\mathrm{Nu} \qquad \mathrm{Ja} = \frac{\rho_l C_{pl}(T_l - T_{sat})}{\rho g L}$$

$$\mathrm{Ja} \leq 0 \qquad \mathrm{Nu} = 2 + 0.6\,\mathrm{Re}^{0.5}\,\mathrm{Pr}^{0.33}$$

$$\mathrm{Pe} = \frac{d_s U_r}{a_l}$$

- Interface to vapor heat transfer

$$\mathrm{Ja} \geq 0 \qquad \mathrm{Nu} = Max(\mathrm{Nu}_1, \mathrm{Nu}_2, \mathrm{Nu}_3)$$

$$\mathrm{Nu}_1 = \sqrt{\frac{4Pe}{\pi}} \qquad \mathrm{Nu}_2 = \frac{12}{\pi}\mathrm{Ja} \qquad \mathrm{Nu}_3 = 2$$

$$\mathrm{Re} = \frac{d_s U_r}{\nu_l}$$

$$\mathrm{Pr} = \frac{\nu_l}{a_l}$$

$$q_{gi} = \frac{\alpha \rho_g C_{pg}}{\delta t}(T_{sat} - T_g)$$

NEPTUNE CFD V1.0
wall heat transfer terms

- Wall heat transfer $$q_w = q_c + q_q + q_e$$
  - "single phase" like heat transfer through contact area A_c between the liquid and the duct wall

with heat transfer coefficient $$q_c = A_c h_{\log}\left(T_w - T_l\right)$$

$$h_{\log} = \rho_l C_{pl} \frac{u^*}{T^+}$$

u^* wall friction velocity

T^+ non-dimensional temperature in the wall boundary layer

  - Quenching effect

$$q_q = A_q t_q f \frac{2\lambda_l\left(T_w - T_l\right)}{\sqrt{\pi a_1 t_q}}$$

  - Phase change heat flux (bubbles nucleated on the wall surface)

$$q_e = f \frac{\pi}{6} d_{nuc}^3 \rho_g L N$$

NEPTUNE CFD V1.0
interfacial area equation

$$\frac{\partial a_i}{\partial t} + \nabla \cdot (a_i \vec{u}_i) = \frac{2}{3}\frac{a_i}{\alpha \rho_g}\left(\Gamma_{g,i} - \alpha \frac{d\rho_g}{dt}\right) + \pi d_{nuc}^2 \Phi_n^{NUC} + \Phi_{a_i}^{CO} + \Phi_{a_i}^{BK}$$

mass transfer and density change effect

nucleation

coalescence

breakup

Assume spherical bubbles

$$d_s = \frac{6\alpha}{a_i}$$

Sauter mean diameter

$$n = \frac{\alpha}{\pi d_s^3/6} = \frac{1}{36\pi}\frac{a_i^3}{\alpha^2}$$

Bubble number density

Mass Conservation Algorithm

- 1) estimate velocities – solve momentum equations implicitly using p^n (predictor step)
- 2) Find pressure correction δp_i
- 3) Update pressure, density, velocity

$$\rho^{k+1} \simeq \rho^k + \left(\frac{\partial \rho_J}{\partial p}\right)^k \delta p_i + \left(\frac{\partial \rho_J}{\partial T}\right)^k \delta T_i$$

If weakly compressible

- 4) Solve continuity equation for volume fractions
  - Enforce sum of volume fractions to unity, by ((1-a), renormalization or under-relaxation
- 5) iterate until convergence

Volume Conservation Algorithm (IPSA)

- 1) first estimate of volume fractions by solving implicitly continuity equation using u^n
- 2) first estimate of velocity by solving implicitly momentum equation
- 3) Find pressure correction using $\left(\alpha_1^k + \delta\alpha_1\right) + \left(\alpha_2^k + \delta\alpha_2\right) = 1$ to form equation for δp
- 4) Update pressure, volume fraction, velocity
- 5) iterate until convergence
- 6) if energy equation, solve for T, update density

$$\rho^{k+1} \simeq \rho^k + \left(\frac{\partial \rho_J}{\partial p}\right)^k \delta p_i + \left(\frac{\partial \rho_J}{\partial T}\right)^k \delta T_i$$ If weakly compressible