

On the Behavior of Natural Circulation Loops with Phase Change

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Outline

1 Background

Motivation

RCCS

Literature

2 Thermohydraulics

3 Discretization of Conservation Equations

4 JFNK

5 Stability

6 Results



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1 Background

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Goals

Simulate a simple closed-loop with naturally circulating water in both single and two-phase regimes using

- Non-ideal equation of state for water
- Simple but accurate models for frictional pressure losses
- Modern, nonlinear solver with complete residual convergence
- Rigorous discretization that allows for exact integration of conservation equations over physical domain

And ultimately determine the linear stability of the system under consideration.



Stability

What is stability?

- Often used term
- Used with many definitions (both implicit and explicit)



Stability

One definition:

Transient (possibly oscillatory) thermal hydraulic phenomenon stemming from nonlinear-geometric-multiphase feedback that could lead to system excursions causing dangerous mechanical or thermal damage and possibly human harm.



Stability

Another definition:

A system of the form

$$\partial_t q = f(t, q) \quad (1)$$

is stable if $q \in [q_{\text{low}}, q_{\text{hi}}]$ for all time.



Stability

Another definition:

A system of the form

$$\partial_t q = f(t, q) \quad (1)$$

is stable if $q \in [q_{\text{low}}, q_{\text{hi}}]$ for all time.

Definition for here:

A system of the form

$$\partial_t q = Aq \quad (2)$$

is stable if all eigenvalues of A are less than or equal to zero.



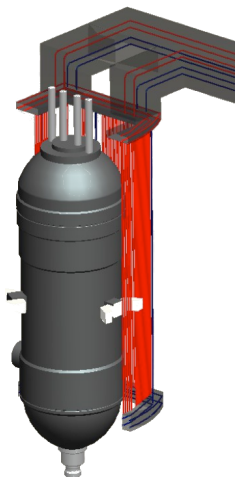
Stability

Applications?

- Thermosiphon
- Power cycle loops
- And...



Reactor Cavity Cooling System

**Purpose:**

Naturally-driven cooling of reactor under accident conditions

Accident conditions:

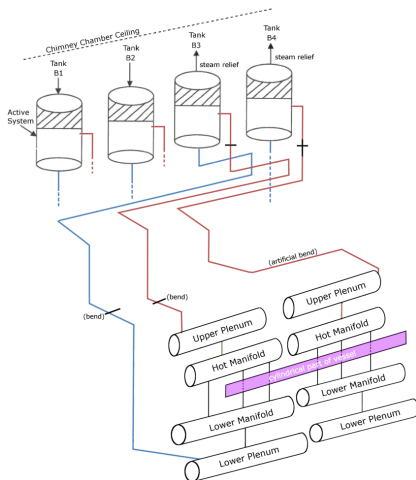
Loss of onsite, offsite power (station blackout)



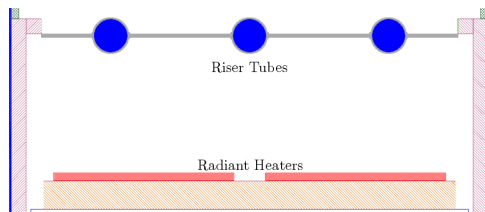
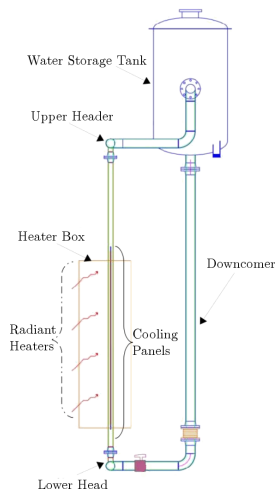
Reactor Cavity Cooling System: Big picture

Selected specifications:

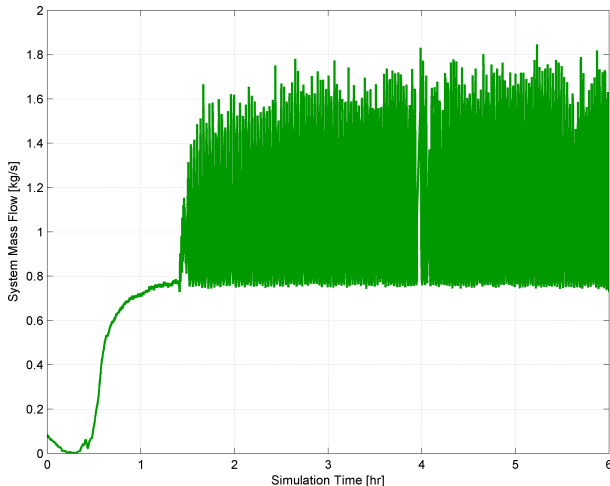
- Trains: 2
- Lines/Tanks: 8
- Elevation change: 35 meters
- Path length: 200 meters
- Heated length: 20 meters
- Risers: 200+
- Heat transfer:
 - Radiation: 80%
 - Convection: 20%



RCCS Experiment



Experimental data: flow oscillations during boiling



Been done before?

Two-phase, natural circulation stability in the literature exists (see thesis). But...

- Analytical work limited to simple equations-of-state
- Large volumes with piece-wise properties (non-dimensional numbers abound)
- System code usage hindered by simple discretization scheme and confounded by complicated models



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General Conservation Law (CLaw)

Conservation laws balance a vector of conserved variables \mathbf{q} over a control volume.

Nonlinear form:

$$\frac{\partial q_i}{\partial t} + \frac{\partial f_i(q_i; x_i, t)}{\partial x_i} = s_i(q_i, z, t) \quad (1)$$

Quasilinear form:

$$\frac{\partial q_i}{\partial t} + \frac{\partial f_i(q_i; z, t)}{\partial q_i} \frac{\partial q_i(x_i, t)}{\partial z} = s_i(q_i, x_i, t) \quad (2)$$

Characteristic speeds:

$$\Lambda = \text{Eig} \left[\frac{\partial f_i(q_i; z, t)}{\partial q_i} \right] \quad (3)$$



Conservation of Mass

Integral form:

$$\partial_t \int_{\Omega} \rho \, d\Omega = \int_{\Gamma} -u_j \rho n_j \, d\Gamma + \int_{\Omega} s^{\rho} \, d\Omega \quad (4)$$

Differential form:

$$\partial_t \rho + \partial_j (u_j \rho) = s^{\rho} \quad (5)$$



Conservation of Momentum

Integral form:

$$\partial_t \int_{\Omega} \rho u_i d\Omega = \int_{\Gamma} (-u_j \rho u_i) n_j d\Gamma + \int_{\Gamma} (-\delta_{ij} P + \tau_{ij}) n_j d\Gamma + \int_{\Omega} \rho g_i + s^u d\Omega \quad (6)$$

Differential form:

$$\partial_t(\rho u_i) + \partial_j(u_j \rho u_i) = -\partial_i P + \partial_i \tau_{ij} + \rho g_i + s^u \quad (7)$$



Conservation of Energy

Integral form:

$$\partial_t \int_{\Omega} \rho e \, d\Omega = \int_{\Gamma} [-(\rho e + P)u_j + u_i \tau_{ij} - q_j] n_j \, d\Gamma + \int_{\Omega} \rho g_j u_j + s^e \, d\Omega \quad (8)$$

Differential form:

$$\partial_t(\rho e) + \partial_j[(\rho e + P)u_j] = \partial_j(u_i \tau_{ij} - q_j) + \rho g_j u_j + s^e \quad (9)$$



Conservation of Bulk Momentum

Only want to track one momentum per cell.

Dot the Conservation of Momentum equation with bulk flow direction z_i :

$$\partial_t \int_{\Omega} \rho u_i z_i \, d\Omega = \int_{\Gamma} (-u_j \rho u_i) n_j z_i \, d\Gamma + \int_{\Gamma} (-\delta_{ij} P + \tau_{ij}) n_j z_i \, d\Gamma + \int_{\Omega} \rho g_i z_i + s_z^u \, d\Omega \quad (10)$$

Let $u_z = u_i z_i$:

$$\partial_t \int_{\Omega} \rho u_z \, d\Omega = \int_{\Gamma} (-u_j \rho u_z) n_j \, d\Gamma + \int_{\Gamma} (-\delta_{ij} P + \tau_{ij}) n_j z_i \, d\Gamma + \int_{\Omega} \rho g_i z_i + s_z^u \, d\Omega \quad (11)$$



Conservation of Bulk Momentum

Only want to track one momentum per cell.

Dot the Conservation of Momentum equation with bulk flow direction z_i :

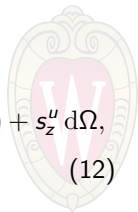
$$\partial_t \int_{\Omega} \rho u_i z_i \, d\Omega = \int_{\Gamma} (-u_j \rho u_i) n_j z_i \, d\Gamma + \int_{\Gamma} (-\delta_{ij} P + \tau_{ij}) n_j z_i \, d\Gamma + \int_{\Omega} \rho g_i z_i + s_z^u \, d\Omega \quad (10)$$

Let $u_z = u_i z_i$:

$$\partial_t \int_{\Omega} \rho u_z \, d\Omega = \int_{\Gamma} (-u_j \rho u_z) n_j \, d\Gamma + \int_{\Gamma} (-\delta_{ij} P + \tau_{ij}) n_j z_i \, d\Gamma + \int_{\Omega} \rho g_i z_i + s_z^u \, d\Omega \quad (11)$$

Channel flow conservation:

$$\frac{d}{dt} \int_{\Omega} \rho u_z \, d\Omega = \int_{\Gamma_1 + \Gamma_2} \pm (P + u_z \rho u_z) \, d\Gamma + \int_{\Gamma_w} \tau_{ij} z_i n_j \, d\Gamma + \int_{\Omega} \rho g \cos(\theta) + s_z^u \, d\Omega, \quad (12)$$



Other Assumptions

- Heat conduction and viscous heating is negligible compared to enthalpy flow
- Fluid-fluid friction is negligible compared to fluid-wall friction and form losses
- Time-rate of change of potential and kinetic energy is negligible to the thermal energy change



Results to equations

$$\rho e \approx \rho i \quad (13)$$

$$q_j \approx 0 \quad (14)$$

$$u_i \tau_{ij} \approx 0 \quad (15)$$

$$\tau_{ij} z_i n_j \approx \frac{1}{2} f_{\text{darcy}} \frac{L_{\text{char}}}{D_h} \text{Abs}(\rho u_z) u_z \quad (16)$$



Equation of State

- IAPWS-95 non-ideal equation of state for water
- Magnificently huge curve fit of Helmholtz free energy potential
- Natural variables are ρ and T
- Back calculate T from ρ and i (plot)



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Purpose

Derive quasi-two-dimensional thermohydraulic equations to enable adequate modeling of a branched system.

Consider only conservation of mass, momentum, and energy.



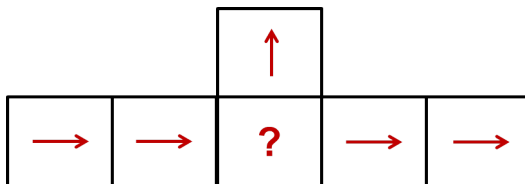
Methodology

- Consider a collection of control volumes and momentum cells.
- Information is exchanged through surface fluxes.
- Control volumes and momentum cells cover same physical space; but are off-set.



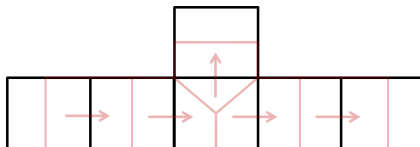
Coincident Spatial Grid

All equations solved on same grid:

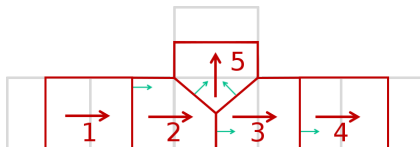


Staggered Spatial Grid

Mass and energy grid:



Momentum grid:



Semi-Discretized Control Volume Equations

Mass and energy for control k :

$$\frac{d}{dt} \int_{\Omega} \rho_k d\Omega = s_k^{\rho} V_k + \sum_{n=1}^N u_n \rho_{d,n} A_n \quad (17)$$

$$\frac{d}{dt} \int_{\Omega} \rho i d\Omega = s_k^e V_k + \sum_{n=1}^N u_n \rho h_{d,n} A_n \quad (18)$$



Semi-Discretized Momentum Cell Equation

Momentum for momentum cell k :

$$\frac{d}{dt} \int_{\Omega} \rho u_k d\Omega = (\rho_k g_k + s_k^u) V_k - \sum_{n=1}^N (P_n z_n + u_{1,n} \rho u_{d,n}) A_n - \frac{1}{2} f_{D,k} \frac{L_{\text{char},k}}{D_{\text{eff},k}} \text{Abs}(\rho u_k) u_k A_k \quad (19)$$



Time Stepping

Semi-discrete equations are now of the form:

$$\partial_t q_i = D_i(q_i) \quad (20)$$

Various choices of stepping over a time step p :

$$q_i^p - q_i^{p-1} = \Delta t D_i(q_i^{p-1}) \quad (21)$$

$$q_i^p - q_i^{p-1} = \Delta t D_i(q_i^p) \quad (22)$$

$$q_i^p - q_i^{p-1} = \frac{1}{2} \Delta t \left[D_i(q_i^{p-1}) + D_i(q_i^p) \right] \quad (23)$$



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Full discretized equations

Consider the Implicit Euler full discretization:

$$q_i^p - q_i^{p-1} = \Delta t D_i(q_i^p) \quad (24)$$

How do you find q_i^p to satisfy that equations assuming D_i is nonlinear?



Newton-Raphson: Procedure

Put the equation into “residual” form

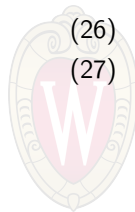
$$r(q_i^P) = q_i^P - q_i^{P-1} - \Delta t D_i(q_i^P) \quad (25)$$

and search for the vector q_i^P that makes $r(q_i^P)$ equal to 0 (or close enough).

Common search technique is Newton-Raphson method:

$$\text{Solve } \partial_{q_i} r(q_i^P) \Delta q_i^P = -r(q_i^P) \quad (26)$$

$$q_i^P = q_i^P + \Delta q_i^P \quad (27)$$



Newton-Raphson: Problems

- Calculating the Jacobian $\partial_{q_i} r(q_i^P)$ can be time and memory intensive.
- Solving the linear system is likewise difficult



JFNK

JFNK: Jacobian-Free Newton-Krylov method.



Krylov method

A particular way of solving the linear system $Ax = b$:

- 1 Compute a search direction z_n :

$$z_n = \begin{cases} r_{n-1} & \text{if } r_{n-1} < r_{n-2} \\ v_{n-1} & \text{otherwise} \end{cases} \quad (28)$$

- 2 Update a QR factorization:

$$[A z_1, A z_2, \dots, A z_n] = V_n R_n \quad (29)$$

- 3 Update residual:

$$r_n = r_{n-1} - v_n^T r_{n-1} v_n \quad (30)$$

- 4 Solve the system

$$R_n w_n = [v_1^T r_1, \dots, v_n^T r_{n-1}]^T; \quad x_n = x_0 + [z_1, \dots, z_n] w_n \quad (31)$$



Approximate Jacobian

Important part to notice

$$[A z_1, A z_2, \dots, A z_n] \quad (32)$$

The only new computation every iteration is Az_n (matrix-vector product).

Jacobian-Free method uses the following finite difference relation:

$$\partial_{q_i} r(q_i^p) z_n \approx \frac{r(q_i^p + \varepsilon z_n) - r(q_i^p)}{\varepsilon} \quad (33)$$

Instead of creating the Jacobian, approximate its existence using this formula (Jacobian-free) in a Krylov Method.



Jacobian-Free Newton-Krylov

A particular way of solving the linear system $Ax = b$:

- 1 Compute a search direction z_n :

$$z_n = \begin{cases} r_{n-1} & \text{if } r_{n-1} < r_{n-2} \\ v_{n-1} & \text{otherwise} \end{cases} \quad (34)$$

- 2 Update a QR factorization:

$$[A z_1, A z_2, \dots, A z_n] = V_n R_n \quad (35)$$

- 3 Update residual:

$$r_n = r_{n-1} - v_n^T r_{n-1} v_n \quad (36)$$

- 4 Solve the system

$$R_n w_n = [v_1^T r_1, \dots, v_n^T r_{n-1}]^T; \quad x_n = x_0 + [z_1, \dots, z_n] w_n \quad (37)$$



Jacobian-Free Newton-Krylov

A particular way of solving the linear system $Ax = b$:

- 1 Compute a search direction z_n :

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- 2 Update a QR factorization:

$$\left[z_1, \frac{r(q_i^p + \varepsilon z_2) - r(q_i^p)}{\varepsilon}, \dots, \frac{r(q_i^p + \varepsilon z_n) - r(q_i^p)}{\varepsilon} \right] = V_n R_n \quad (35)$$

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$$R_n w_n = [v_1^T r_1, \dots, v_n^T r_{n-1}]^T; \quad x_n = x_0 + [z_1, \dots, z_n] w_n \quad (37)$$



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Perturbation equations

Assumed that the true solution is a summation of a steady-state and a transient

$$q_i(x_i, t) = q_i^{\text{ss}}(x_i) + \delta q_i(x_i, t). \quad (38)$$



Perturbation equations

Assumed that the true solution is a summation of a steady-state and a transient

$$q_i(x_i, t) = q_i^{\text{ss}}(x_i) + \delta q_i(x_i, t). \quad (38)$$

General nonlinear perturbation equation (diagrams):

$$\frac{\partial \delta q_i}{\partial t} + \frac{\partial}{\partial x_j} [f_{ij}(q_i^{\text{ss}} + \delta q_i)] = s_i(q_i^{\text{ss}} + \delta q_i) \quad (39)$$



Perturbation equations

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General nonlinear perturbation equation (diagrams):

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Taylor expansion about perturbation (neglecting H.O.T.) yields general linear perturbation equation:

$$\frac{\partial \delta q_i}{\partial t} + \frac{\partial}{\partial x_j} \left[\frac{\partial f_{ij}}{\partial q_k^{\text{ss}}} \delta q_k \right] = \frac{\partial s_i}{\partial q_k^{\text{ss}}} \delta q_k \quad (40)$$



Solution method of general linear equations

Perturbations still part of spatially varying PDE.

Discretizing like full transient equations will yield spurious, positive eigenvalues from mass/energy advection.

Solution: integration over entire system and isolate global time-evolution on left-hand side:

$$\partial_t \delta q_i(t) = \frac{1}{\int_{\Omega} d\Omega} \left[\int_{\Omega} \frac{\partial s_i}{\partial q_k^{ss}} d\Omega - \int_{\Gamma} \frac{\partial f_{ij}}{\partial q_k^{ss}} n_j d\Gamma \right] \delta q_k(t) \quad (41)$$



Solution method of thermohydraulic system

Apply to mass, energy, momentum system:

$$\frac{d}{dt} \begin{bmatrix} \delta\rho \\ \delta\rho i \\ \delta\rho u_z \end{bmatrix} = -\partial_j \left(\begin{bmatrix} \partial_{q_k}(\rho u_j) \\ \partial_{q_k}[(\rho i + P)u_j] \\ \partial_{q_k}(u_j \rho u_z + P\delta_{ij}z_i - \tau_{ij}z_i) \end{bmatrix} \delta q_k \right) + \left(\begin{bmatrix} \partial_{q_k}(s^\rho) \\ \partial_{q_k}(s^e) \\ \partial_{q_k}(\rho g_z + s_z^u) \end{bmatrix} \delta q_k \right) \quad (42)$$



Solution method of thermohydraulic system

Integrating to the skin of the system and eliminating terms that vanish:

$$\frac{d}{dt} \begin{bmatrix} \delta\rho \\ \delta\rho i \\ \delta\rho u_z \end{bmatrix} = \frac{1}{V_{\text{sys}}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \alpha_\rho & \alpha_{\rho i} & \alpha_{\rho u_z} \end{bmatrix} \begin{bmatrix} \delta\rho \\ \delta\rho i \\ \delta\rho u_z \end{bmatrix}, \quad (42)$$

where $\alpha_* = - \int_\Gamma \partial_* \Delta P_{\text{dar}} d\Gamma$



Solution method of thermohydraulic system

Integrating to the skin of the system and eliminating terms that vanish:

$$\frac{d}{dt} \begin{bmatrix} \delta\rho \\ \delta\rho i \\ \delta\rho u_z \end{bmatrix} = \frac{1}{V_{\text{sys}}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \alpha_\rho & \alpha_{\rho i} & \alpha_{\rho u_z} \end{bmatrix} \begin{bmatrix} \delta\rho \\ \delta\rho i \\ \delta\rho u_z \end{bmatrix}, \quad (42)$$

where $\alpha_* = - \int_\Gamma \partial_* \Delta P_{\text{dar}} d\Gamma$

With the solution

$$\begin{bmatrix} \delta\rho(t) \\ \delta\rho i(t) \\ \delta\rho u_z(t) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{\alpha_\rho}{\alpha_{\rho u_z}} (e^{\tilde{\alpha}t} - 1) & \frac{\alpha_{\rho i}}{\alpha_{\rho u_z}} (e^{\tilde{\alpha}t} - 1) & e^{\tilde{\alpha}t} \end{bmatrix} \begin{bmatrix} \delta\rho(0) \\ \delta\rho i(0) \\ \delta\rho u_z(0) \end{bmatrix}, \quad (43)$$

where $\tilde{\alpha} = \alpha_{\rho u_z} / V_{\text{sys}}$.



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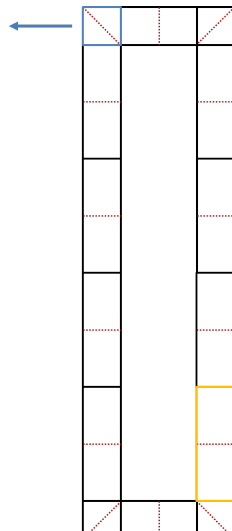
Methodology

- 1 All closed-loop systems exhibit a singular steady-state solution.
- 2 Solution: perform a transient calculation that provided diagonal regularity and run transient to a stationary-state using all previous equations and tools.
- 3 Once the steady-state is attained, computer the eigenvalues and examine.



Primary Test Loop

- 1 14 control volume / momentum cells
- 2 1.4 meters high, 0.4 meters wide (3.5 aspect ratio)
- 3 0.1 meter hydraulic diameter



Single Phase Results



Two-Phase Results



Two-Riser Results

Two Riser Results?



Questions

“The key to wisdom is this: constant and frequent questioning. For by doubting we are led to question, and by questioning we arrive at the truth.”

— Peter Abelard



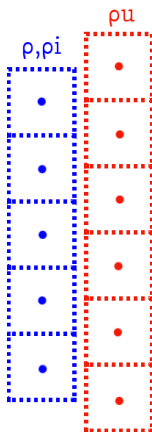
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7 Supplements

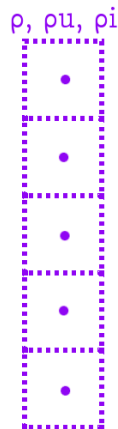


Staggered/Collocated

Staggered mesh:

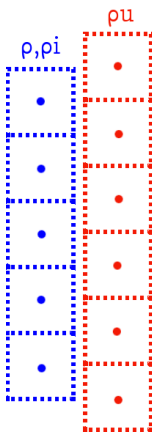


Collocated mesh:

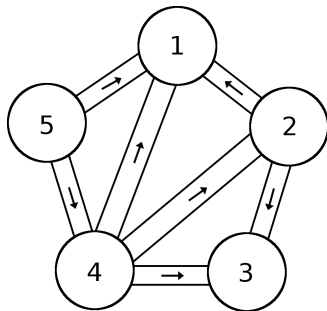


Rigorous vs. Non-Rigorous

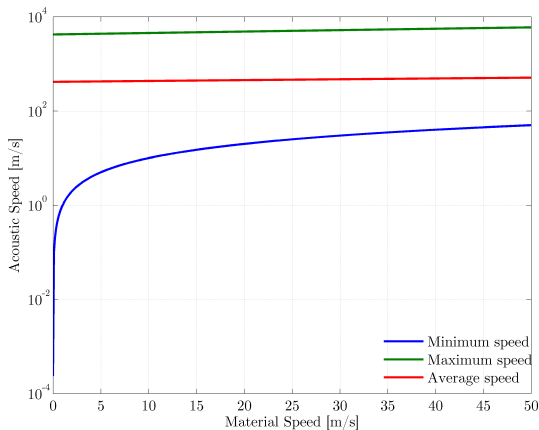
Rigorous staggered mesh (CFD):



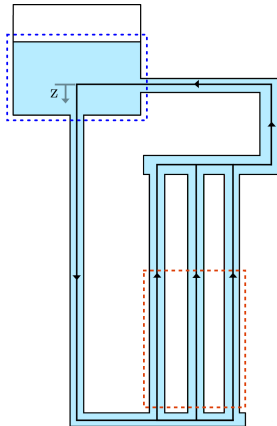
Non-rigorous staggered mesh
(System codes):



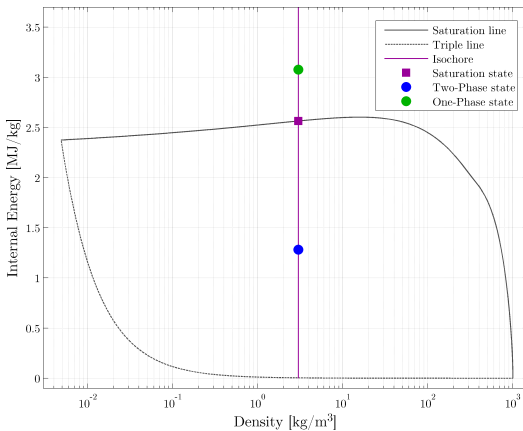
Acoustic Speeds



Non-simple, closed loop

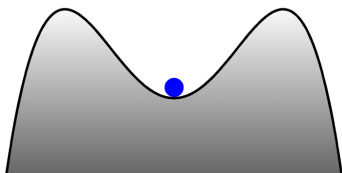


i - ρ Diagram

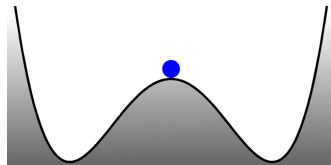


Stability Diagrams

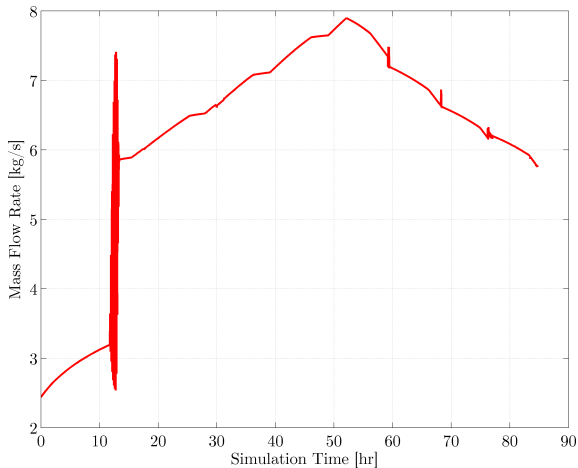
Linearly stable, nonlinearly unstable:



Linearly unstable, nonlinearly stable:



System Mass flow: 4 days



Multiphase Model

$$\frac{\partial}{\partial t} \begin{bmatrix} \alpha \rho_\phi \\ \alpha \rho u_\phi \\ \alpha \rho i_\phi \end{bmatrix} + \frac{\partial}{\partial z} \begin{bmatrix} \alpha \rho u_\phi \\ u_\phi \alpha \rho u_\phi + P(\rho_\phi, i_\phi) \\ u_\phi [\alpha \rho i_\phi + P(\rho_\phi, i_\phi)] \end{bmatrix} = \quad (44)$$

$$\begin{bmatrix} \mathbb{M}_\phi \\ \alpha \rho_\phi g(z) - \frac{K_{\text{eff},\phi}(\mathbf{q})}{2} u_\phi |\alpha \rho u_\phi| + \mathbb{P}_\phi \\ \dot{Q}_{\text{add},\phi}(\mathbf{q}, z, t) + \mathbb{E}_\phi \end{bmatrix}$$

