Improving the Fluid Property Evaluation for RELAP5-3D

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Background and Purpose

- Fluid properties tabulated by many organizations, including:
  - National Bureau of Standards (NBS)
  - National Institute of Standards and Technology (NIST)
  - American Society of Mechanical Engineers (ASME)
  - Nuclear Regulatory Commission (NRC)
- Besides tables generators, complex mathematical functions of many variables are generated.
  - The generators were computationally intensive compared with table lookup for older computers
- RELAP5 codes read and store needed tables of fluid property values at input then interpolate to obtain properties at a given (P,T) or (P,U)
- Purpose of this study
  - Examine different calculations of the table fluid properties and their derivatives can improve RELAP5-3D calculations

Background

- RELAP5-3D has 33 different fluid table files.
  - 9 are variation on water properties: 8 for light water, 1 for heavy
    - 1967, 1984, 1995 in original and revised form
  - Liquid metals, molten salts, supercritical CO2
  - Gases: hydrogen, helium, nitrogen, xenon
  - Refrigerants, glycerin, human blood
- All the property files start with the 3 letters “tpf” for Tabulated Properties of Fluids, or Fluid Property Tables for short.
- RELAP5-3D tables are generated in two formats:
  - ASCII and Machine independent binary XDR,

Water Property Accuracy & Mass Error

- The mathematical function, its evaluation, and interpolation all involve errors:
  - Approximation of reality, approximation of transcendental functions, numerical roundoff, and interpolation error
  - Interpolation error is the largest of these and it leads to mass error.
- In 2010, Cliff Davis studied the interpolation grid and found the regions of greatest difference between the function and interpolated values.
  - He created a new grid with more interpolation points in the areas of largest difference.
  - New grid reduced interpolation error
- A second study tested a methodology to improve fluid property derivative calculations

Mass Error and Consistency

- In RELAP5 codes, the derivatives are calculated from the nonlinear Clausius-Clapyron Equations
- $\left(\frac{\partial \rho_j}{\partial U_j}\right)_P = \frac{v_j \beta_j}{(C_{pj} - v_j \beta_j P) v_j^2}$ $\quad\quad$ $\left(\frac{\partial T_j}{\partial U_j}\right)_P = \frac{1}{C_{pj} - v_j \beta_j P}$
- $\left(\frac{\partial \rho_j}{\partial P}\right)_{U_j} = \frac{C_{pj} v_j \kappa_j - T_j (v_j \beta_j)^2}{(C_{pj} - v_j \beta_j P) v_j^2}$ $\quad\quad$ $\left(\frac{\partial T_j}{\partial P}\right)_{U_j} = \frac{P v_j \kappa_j - T_j v_j \beta_j}{C_{pj} - v_j \beta_j P}$

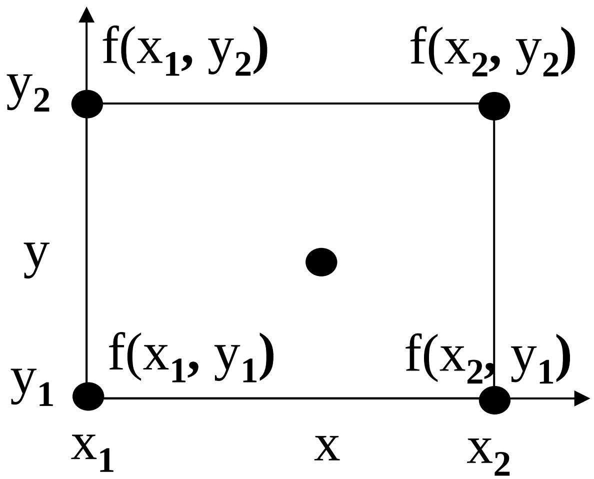
- j = f or g (for liquid or gas)
- specific volume v
- specific heat capacity C_p
- isobaric coefficient of thermal expansion β
- isothermal coefficient of compressibility κ

Goal: Less Mass Error via Better Approximation

- The numerical approximations to Governing Partial Differential Equations arise from LINEARIZATION at every step.
  - No nonlinear terms of primary variables, namely P, U_f, U_g,α_g, and X_n, are allowed
    - Linearization by putting primary variables factors at old time and leaving only one factor at new time
  - Non-primary variables are replaced by functions of primary variables. These are linearized by
    - Using old time values
    - Or replacing nonlinear terms by first order Taylor polynomials
- Since the numerical system is linear, would linear derivatives be more CONSISTENT than default Clausius-Clapyron approximation?
- Would some other form that combines the two reduce mass error?

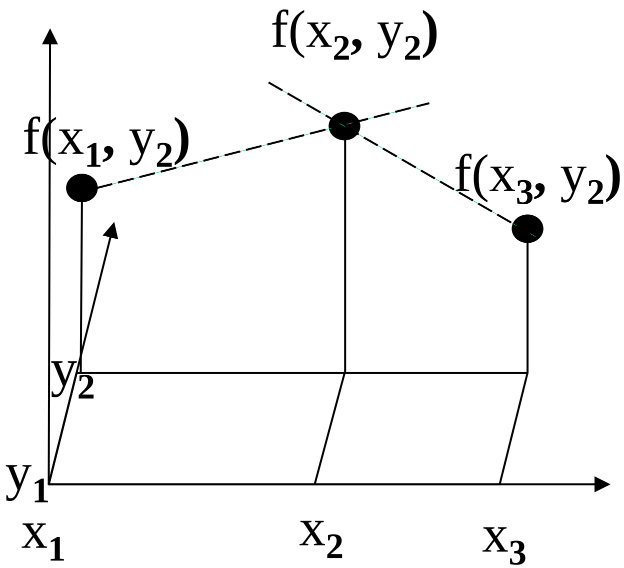
Second Study & Theory

- A second study showed promise for linear approximation
  - 1984 water properties with the detailed (U, P) mesh
  - A simple 2-vol test case showed the linear interpolant produced less mass error than the normal RELAP5-3D calculation
- Coding was written to carry out a more complete study.
- Calculate linear interpolants of the 8 derivatives based on the four corners of the bounding rectangle
- $\alpha(x) = \frac{x-x_1}{x_2-x_1}$, $\beta(y) = \frac{y-y_1}{y_2-y_1}$
- $\left(\frac{\partial f}{\partial x}\right)_{lin} = \frac{(1-\beta)[f(x_2,y_1)-f(x_1,y_1)]+\beta[f(x_2,y_2)-f(x_1,y_2)]}{x_2-x_1}$
- $\left(\frac{\partial f}{\partial y}\right)_{lin} = \frac{(1-\alpha)[f(x_1,y_2)-f(x_1,y_1)]+\alpha[f(x_2,y_2)-f(x_2,y_1)]}{y_2-y_1}$
- In example, α=0.6, β=0.4



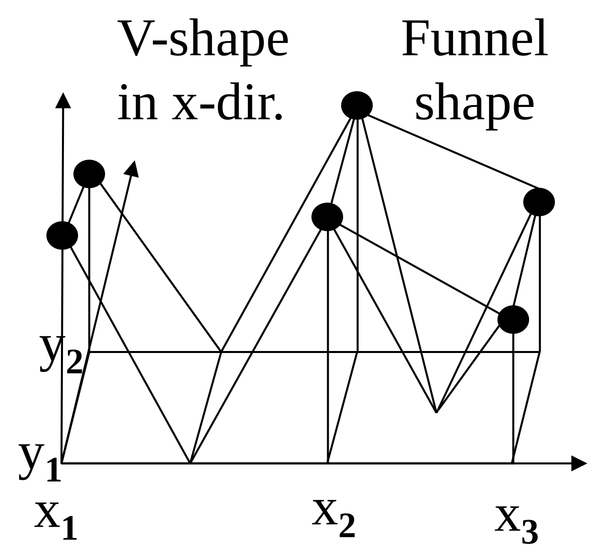
Theory – Jump Discontinuities

- reduced mass error for 2-vol test case, but not for Edward's Pipe
  - Reason: Discontinuity of the derivatives at rectangle edges
- Consider three points of the energy grid: x_1, x_2, x_3.
  - In left rectangle at $y = y_2$,
    - $\alpha(x_2) = (x_2 - x_1)/(x_2 - x_1) = 1$
  - In right rectangle at $y = y_2$,
    - $\alpha(x_2) = (x_2 - x_2)/(x_3 - x_2) = 0$
- The left and right derivative at y_2 do not match:
  - $\lim_{\epsilon \to 0} \left(\frac{\partial f}{\partial x}\right)_{lin} (x_2 - \varepsilon, y_2) = \frac{f(x_2,y_2) - f(x_1,y_2)}{x_2 - x_1}$
  - $\lim_{\epsilon \to 0} \left(\frac{\partial f}{\partial x}\right)_{lin} (x_2 + \varepsilon, y_2) = \frac{f(x_3,y_2) - f(x_2,y_2)}{x_3 - x_2}$
- Linear interpolant has **jump discontinuity**
- Default Clausius-Clapyron derivative does not



Theory – Hybrid Interpolation

- Combine the best of both - calculate a weighted average of the default Clausius-Clapyron derivatives and the linear interpolant.
- Weighted Average = $\omega^*\left(\frac{\partial f}{\partial x}\right)_{def}$ + $(1\text{-}\omega)^*\left(\frac{\partial f}{\partial x}\right)_{lin}$ similar for y-direction
  - 1.0 produces fixed Default derivatives
  - 0.0 produces fixed Linear
  - 0.5 produces fixed Hybrid
  - -1.0 triggers variable V-shaped weighting in y-dir.
  - -2.0 triggers Funnel weighting
- Other shapes were considered, but not programmed

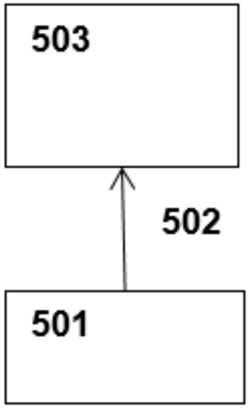


Coding Implementation

- Subroutine RMFLDS: 120-129 hydrodynamic system card adds weight as final value
  - The fluid can change from system to system, so the weighting must also.
- Subroutine LINPOLATE: new F90 routine that calculates:
  - Default or linear-interpolant derivatives
  - Matching fluid properties (Consistency)
    - T, rho, kappa, beta, Cp, k, mu, s, specific volume
  - Weighted average of linear and default
- Other modifications
  - SVPUPU, ISTATE, STPUPU – Calls to LINPOLATE for H2ON only
  - STATEP – uses weighted averages for H2ON only
- Test Cases
  - Two volume “Box” insurge and outsurge
  - Edwards Pipe Blowdown, Typical PWR, Moby Dick, Mixbub

Testing with Improved P,T Fluid Grid

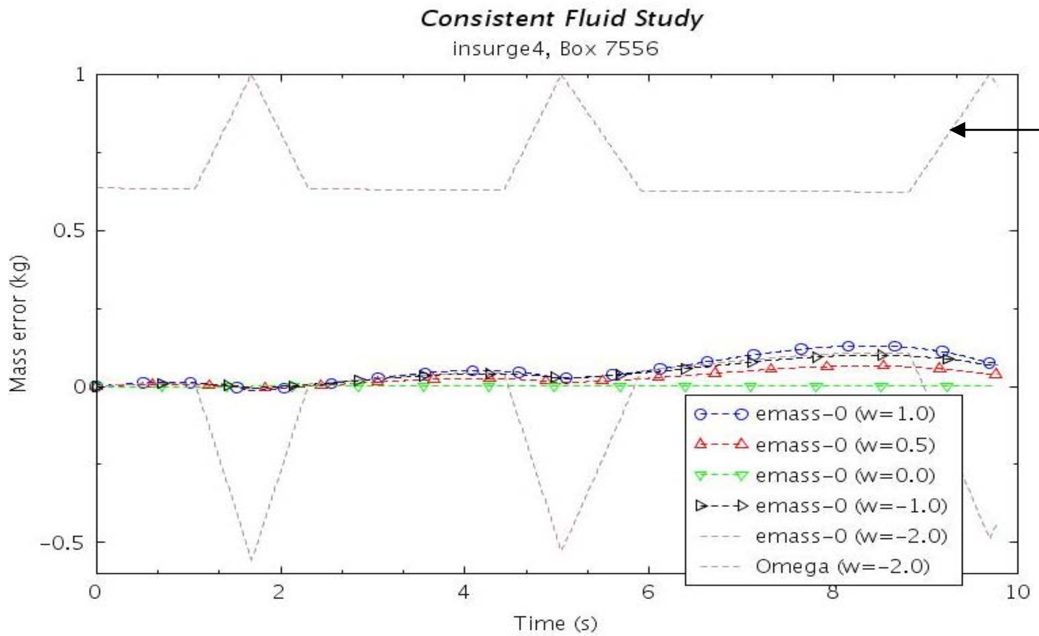
- Two volume insurge "Box" problem
  - P,T set at lowest values inside the bounding rectangle
  - P,T increased to maximum for box at 10s
  - Table shows ormalized mass errors during simple filling calculations



Box	Midpoint values		Comments
	Pressure (MPa)	Temp. (K)	
113	1.10E-03	275.33	Liquid (worst box in Region 7)[1]
341	1.50E-03	286.25	Vapor (worst box in Region 8)
1936	9.00E-02	410.0	Vapor (worst box in Region 10)
5629	7.50	377.5	Liquid (average box in Region 1)
5651	7.50	617.50	Vapor (average box in Region 2)
7400	16.00	293.75	Liquid (worst box in Region 9)[1]
7445	16.00	627.50	Vapor (worst box in Region 2)
7446	16.00	632.50	Vapor (worst box in Region 4)
7495	16.00	936.575	Vapor (high temperature)
7556	17.25	622.5	Liquid (worst box in Region 1)
7669	18.25	627.5	Liquid (worst box in Region 3)

Box 7556 Mass error, INSURGE Case

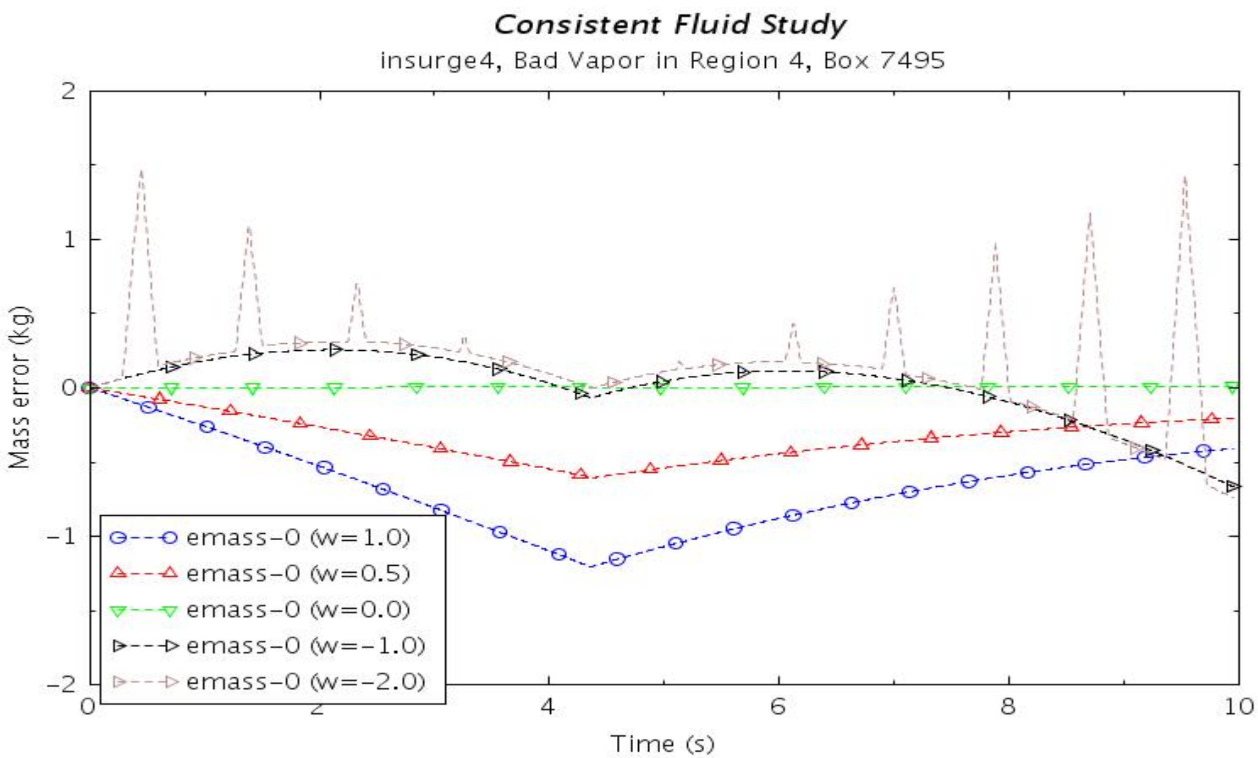
- Upper curve shows the variable ω -values generated when user selects the funnel shape (input flag $\omega = -2$).
  - The lower curve shows the mass error generate with these values
- Values $-1 \leq \omega < 1$ outperform default RELAP5-3D ($\omega = 1.0$).



ω-values from flag $\omega = -2$

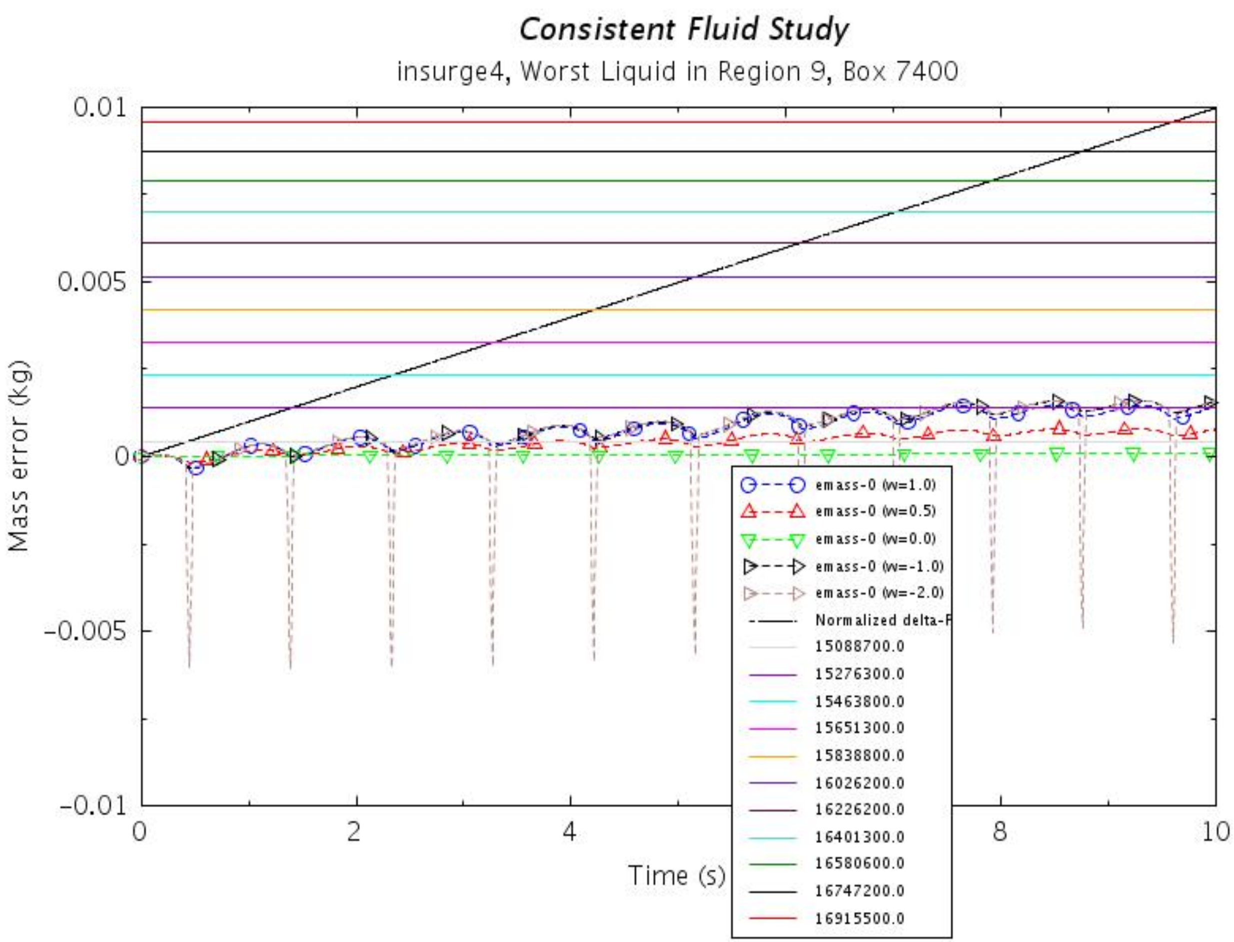
Box 7556 Mass error, INSURGE Case

- Values $-1 \leq \omega < 1$ outperform default RELAP5-3D (ω = 1.0)
- What causes the spikes for funnel-shaped ω?



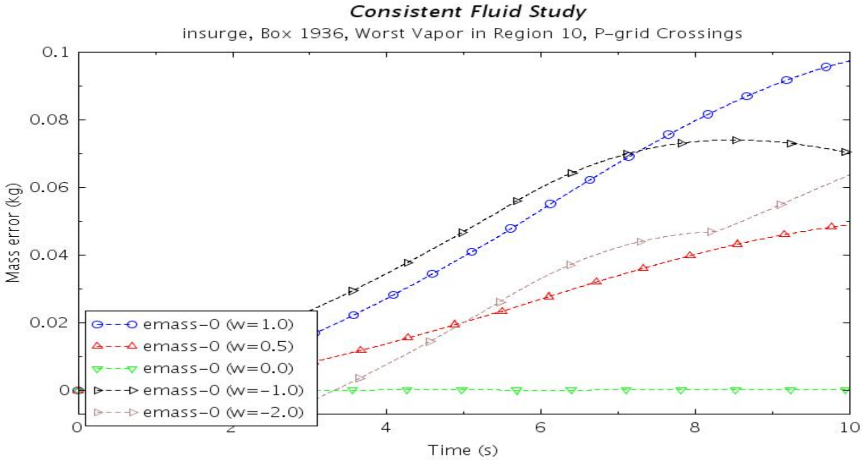
Box 7400 Mass error, INSURGE Case

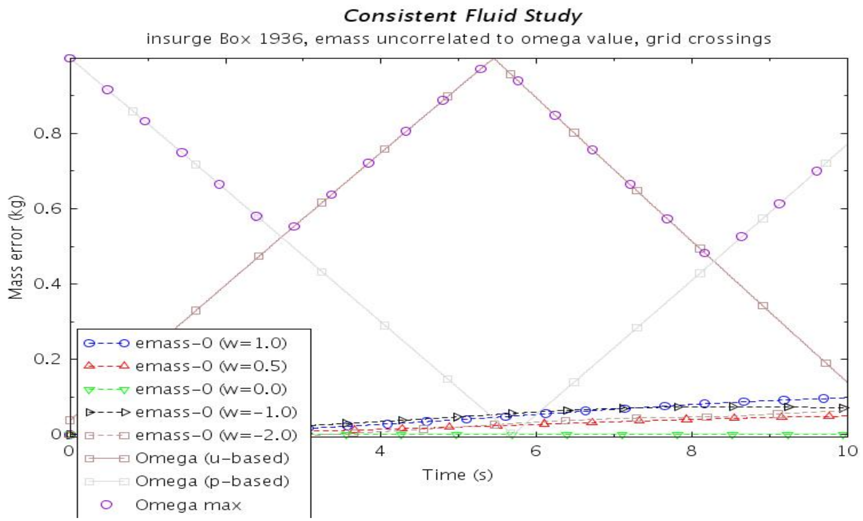
- Black and horiz. lines are **P normalized**
- $-1 \le \omega < 1$ default R5-3D (ω = 1.0)
- Local ***minima*** for ALL mass error graphs at ***pressure grid values***.
  - Also true in prior plots
- What about U grid values?



Box 1936 Mass error, INSURGE Case

- V-line gives P-based ω
- Inverted V-line shows U-based ω.
- Funnel (ω = -2) uses ω = max of V and inverted-V.
- ***Inflection point*** at the **U grid point** for $\omega = -2, -1, 0.5, 1$
- First time ω = 0.5 is worst.
- All INSURGE cases show ω = 0 has almost no mass error.





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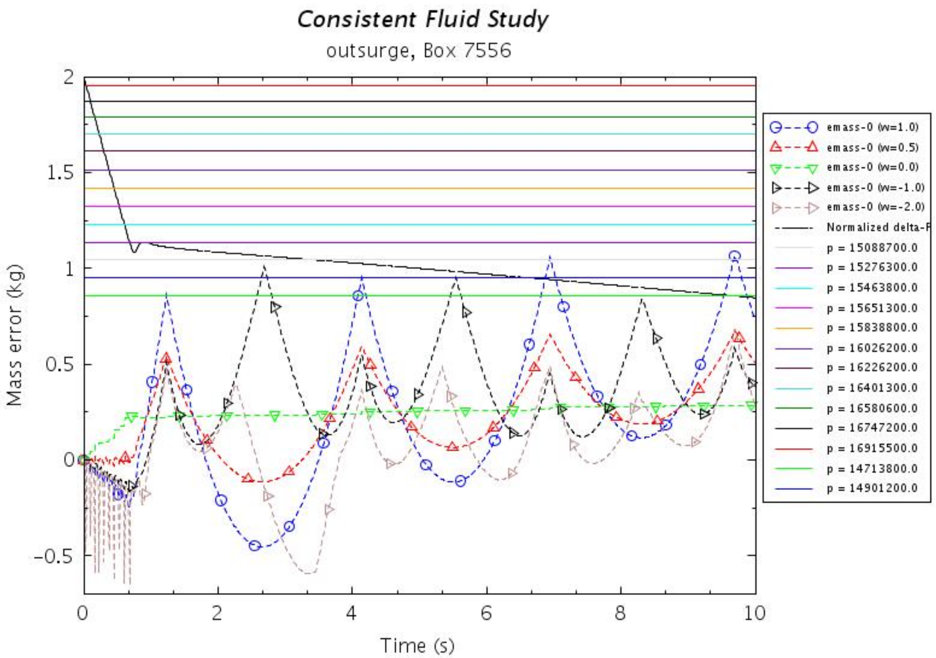
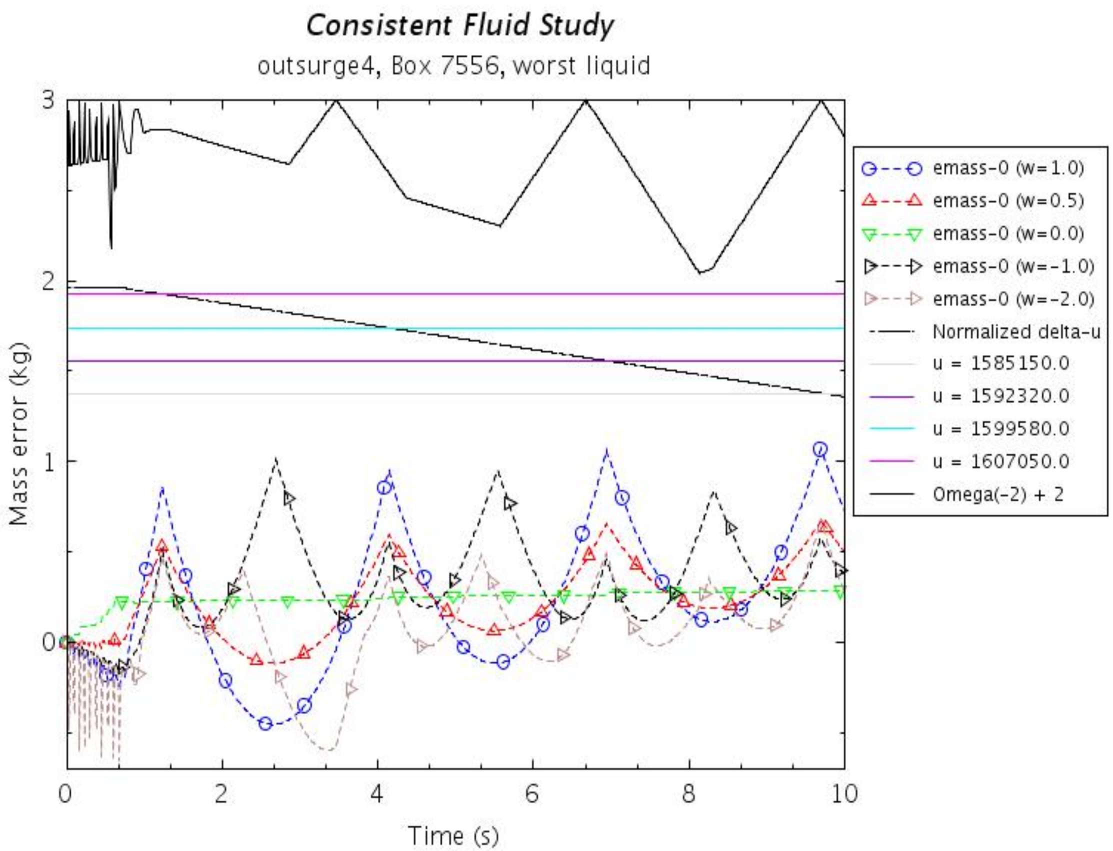
OUTSURGE Case, Box 7556 Mass error

- Identical noding diagram of the insurge and outsurge problems
- Outsurge case purpose: put the pressurizer volume through a blowdown, causing a phase boundary crossing
- Flow is reversed
- Horizontal lines show normalized U grid points
- Funnel (ω = -2) values graphed at ω + 2 for clarity
- Crossing normalized P-lines causes mass err oscillations
- Local extrema at or near P-line crossings for all ω
- ***ω*=0** mass error is **nonzero**



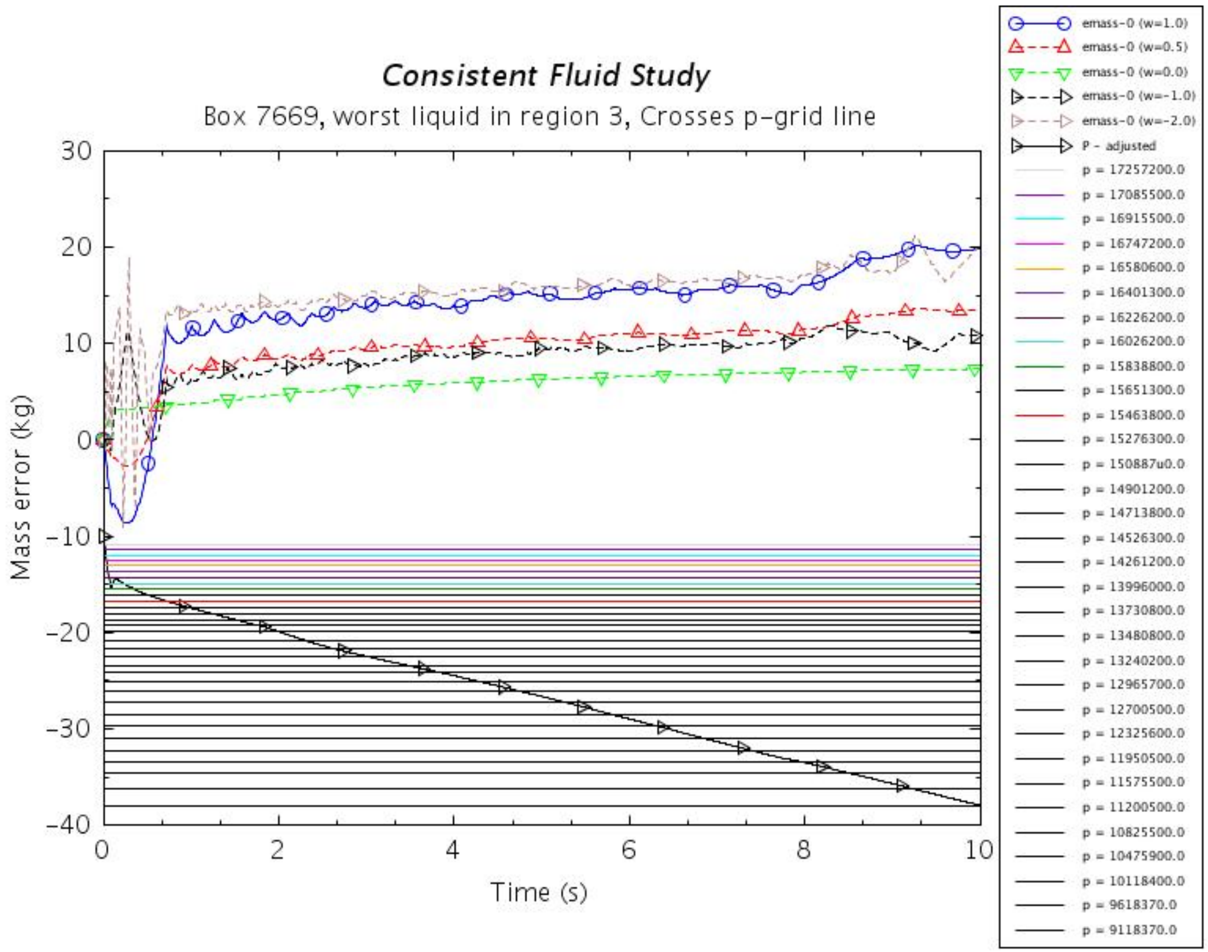
OUTSURGE Case, Box 7556 Mass error

- Local maxima at U-line crossings for all ω
- Inflection points in all graphs where funnel-ω either equals 1 or has a kink.



OUTSURGE Case, Box 7669 Mass error

- Oscillations at P-line crossings
- Again, ω=0.0 is best but has nonzero mass error

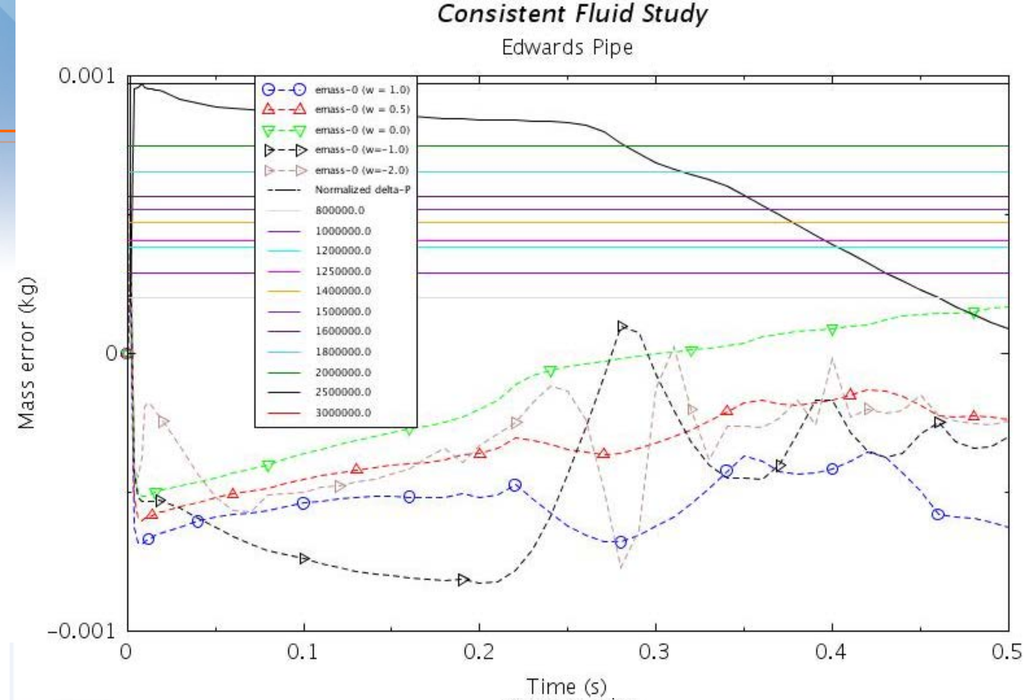


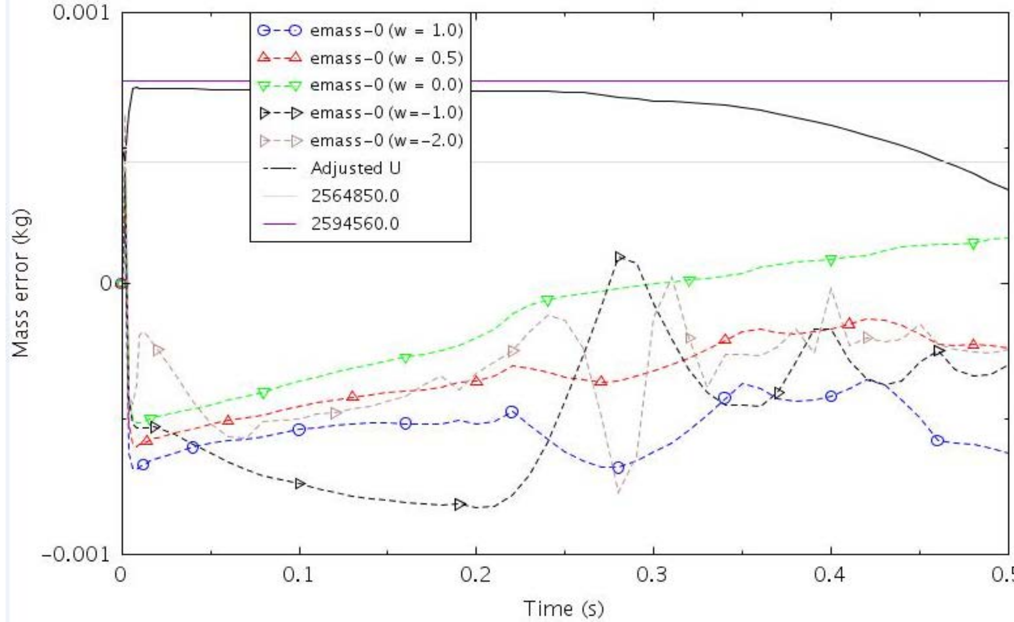
OUTSURGE Case, Box 7556 Mass error

- As with insurge, the plot of ω(-2) exhibits oscillatory behavior and has local extrema at pressure gridline crossings
- Plots of ω=1.0 and ω=0.5 have local maxima where the specific internal energy crosses gridlines
- Smallest mass error is created when ω=0.0. However, unlike with insurge, the mass error is positive in outsurge problems
- Second lowest mass error for Box 7556 comes when omega=-2
- Second lowest mass error for Box 7669 comes when omega=-1

Edward’s Mass Error

- Many local maxima and minima.
- Pressure grid point crossings and internal energy grid point crossing corresponds to an inflection point on the mass error curves
- From about 0.02s to 0.2s, where neither pressure nor energy grid points are crossed, the mass error plots are relatively smooth
- Smallest mass error for $\omega = 0$





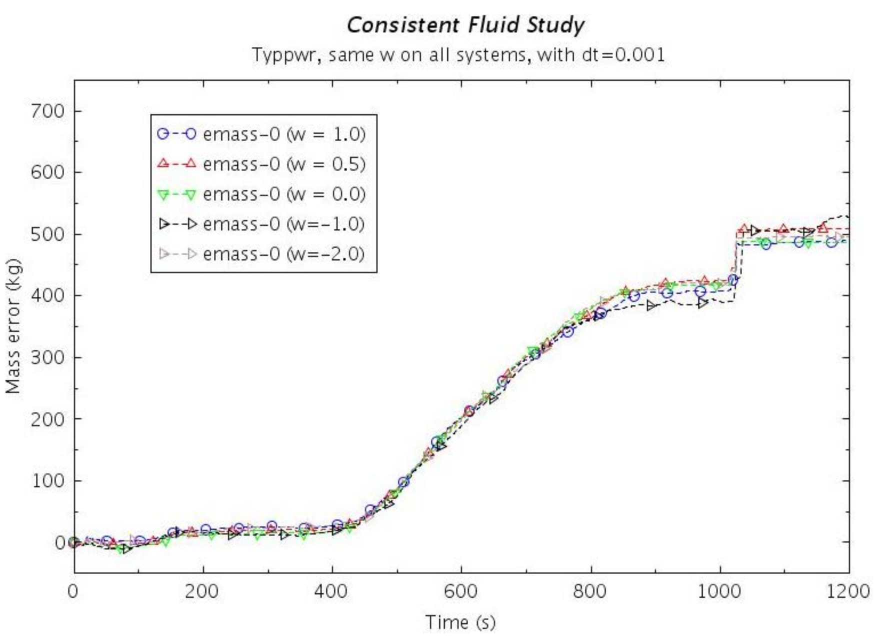
TYPPWR Test Cases

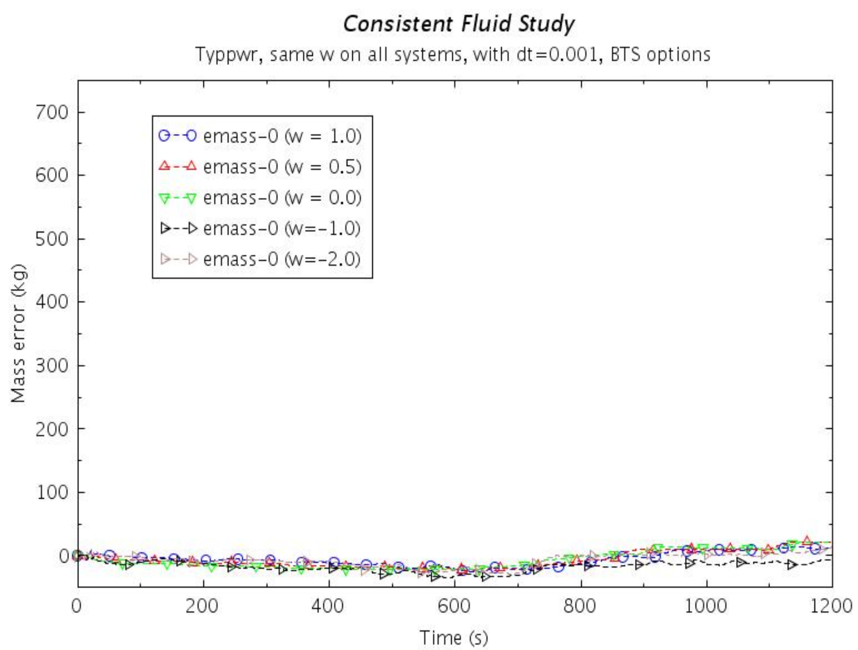
- The typical PWR model has three systems
  - Same values of $\boldsymbol{\omega}$ applied to each system
- Fifty code runs: Combinations of 5 ω-values (1.0, 0.5, 0.0, -1, -2) timestep values (Δt = 0.1, 0.05, 0.01, 0.005, 0.001) and 2 sets of card-one options: default and “Better Test Set” (BTS)
- Default and BTS produced similar results on earlier calculations

Card-1	“Better Test Set” of Options
29	Accurately solves the momentum equations at low velocities.
41	Includes energy dissipation due to form loss (code calculated abrupt area change loss and user-specified loss)
54	Changes the 2-phase to 1-phase gas transition truncation limit in EQFINL for the semi-implicit
55	Model improvements to minimize numerical sources of oscillations for low pressure 2-phase flow: • Interfacial heat transfer for annular mist, Mist pre-CHF, Mist post-CHF flow regimes, More physical Hif and Hig

TYPPWR Mass Error, Δt = 0.001

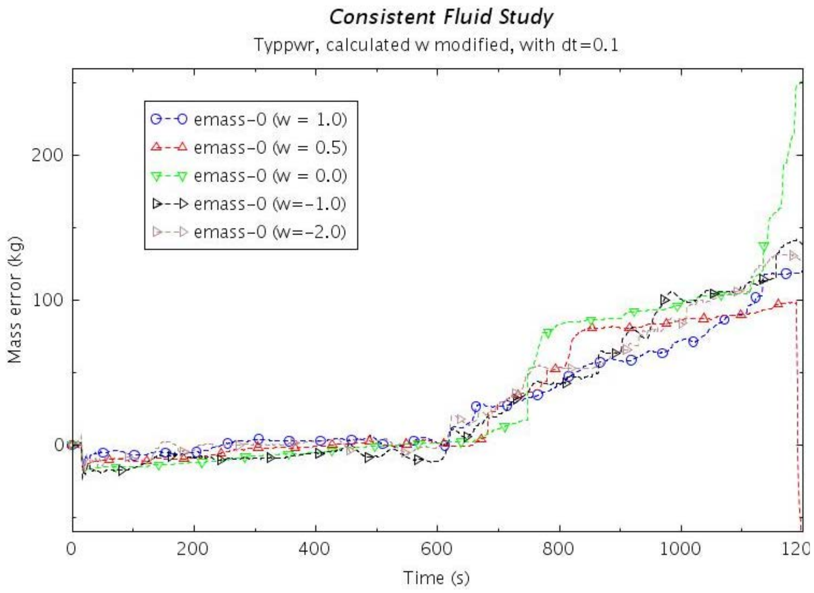
- ω=-1 has smallest mass error with BTS. ω=0.0 is best with default
- At smaller time step, BTS mass error is vastly superior to the default values of the card- options
- Why not make BTS the default?

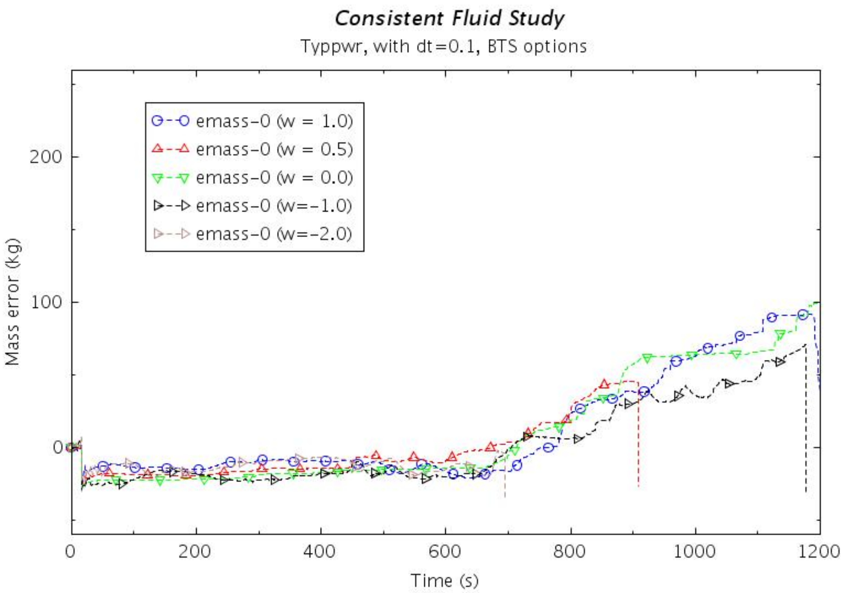




TYPPWR Mass Error, Δt = 0.1

- Except ω=1.0 and ω=0.0, all **ω-values FAIL with BTS** by 1200s
- All ω-values run with default options
- ω=0.0 has the worst mass error, more than double any other, with the default options.





TYPPWR Test Cases

- Runtime comparison
  - Orange is slowest
  - Yellow is fastest
  - Def = default
  - Ratio = failed advancements divided by total for Default options
- Ratio and runtime should correlate, but not well. Single run
- No option is best or worst for TYPPWR

ω	dt=0.5			dt=0.01		
	Ratio	Def	BTS	Ratio	Def	BTS
1.0	0.235	38.148	36.552	0.035	163.78	166.70
0.5	0.194	37.089	37.490	0.028	161.27	163.87
0.0	0.230	37.791	38.465	0.042	164.99	165.38
-1	0.174	37.033	38.344	0.045	164.85	162.29
-2	0.196	37.679	37.148	0.046	164.26	165.19

ω	dt=0.05			dt=0.001		
	Ratio	Def	BTS	Ratio	Def	BTS
1.0	0.0262	322.62	323.07	0.00871	1586.4	1586.4
0.5	0.0253	319.88	321.44	0.00743	1573.0	1573.2
0.0	0.0242	324.12	321.31	0.00804	1569.7	1564.3
-1	0.0192	320.21	322.82	0.00816	1572.2	1573.0
-2	0.0205	321.49	321.54	0.00833	1575.7	1578.1

Moby Dick Problem Conclusions

- Four types of advancement
  - 1 = semi-implicit, explicit coupling with heat transfer
  - 2 = semi-implicit, implicit coupling with heat transfer
  - 3 = nearly-implicit, explicit coupling with heat transfer
  - 4 = nearly-implicit, implicit coupling with heat transfer
- Mass error ratio
  - Default options: constant for some, not for others
  - Default options: smaller mass error for case 1.
  - BTS options: lower mass error ratios than default for other cases
- The DA graph of pressure vs. elevation shows no visible differences between the five values of omega.
- *The mass error with H2ON was typically1.5 times lower than the mass error ratio produced with default H2O*.

Conclusions

- No particular value of $\boldsymbol{\omega}$ produced consistently better results in terms of mass error, though:
  - $\boldsymbol{\omega} = -1.0$ somewhat outperformed other choices
  - $\boldsymbol{\omega} = 0.0$ performed well
- Based on these limited results, $\boldsymbol{\omega}$ did not visibly affect engineering parameters such as pressure and void fraction.
- Crossing pressure and internal energy grid lines from one time advancement to the next affects mass error
  - In simple cases, pressure crossings cause local extrema and internal energy crossing inflect the curves.
  - The effect diminishes as $\boldsymbol{\omega}$ tends toward zero, but is visible even for $\boldsymbol{\omega} = 0.0$ for some problems.

Conclusions and Recommendations

- With the BTS options, TH property failures occur with Typical PWR for all omega values at the largest DTMAX
- The default value of $\boldsymbol{\omega} = 1.0$ was seldom the best and sometimes the worst in terms of mass error and runtime
  - The user may replace it by another choice through input
- Value $\boldsymbol{\omega} = 0.0$ was:
  - Uniformly better for the simple insurge problems
  - Was generally better for the outsurge problems
  - Was sometimes worst with more complicated models
- Value $\boldsymbol{\omega} = -1.0$ seldom performed poorly and performed well or the best in a significant number of more complicated cases
- Further study is recommended
- Cubic splines to smooth crossing should improve performance