# *Development of New H2O95N Fluid Properties*

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RELAP5-3D International Users Seminar

Date: May 3, 2018

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# Project Introduction

- Develop a hybrid fluid property table (H2O95N)
  - NBS/NRC Steam Tables from 1984 (H2ON)
  - NIST/ASME Steam Tables from 1995 (H2O95)
- Independent parameters
  - Pressure (P)
  - Specific internal energy (U)
- Extend into the metastable regions like H2ON
- Properties generated using H2O95 fluid table

# Method

- Compiling and updating the H2O95 fluid property generator
- Adapting portions of the H2ON fluid property generator
- Extend the accuracy based generation methodology to work with H2O95, H2ON, and H2O95N
- Modify the polate utility for testing purposes
- Modify the developmental assessment (DA) scripts to compare the new fluid to both H2ON and H2O95

# H2O95 Table Generator Updates

- The RELAP5-3D H2O95 steam table was created from an ASCII file
- The NIST/ASME STEAM properties database
- Tested
  - Spot checking
  - state.i verification case

# *H2O95N Table Generator*

- Rebrand H2O95 generator as H2O95N
- The NIST (H2ON) generators use T and ρ as independent parameters
  - Convert pressure and internal energy to temperature and density
  - Used conversion subroutine from the H2ON generator
  - Used property subroutine from H2O95 generator
  - Preserve the H2O95 fluids characteristics
- Extended the new generator from three to six states
  - 0 = noncnvgd => *0 value in table*
  - 1 = liquid
  - 2 = metastable liquid
  - 3 = metastable vapor
  - 4 = vapor
  - 5 = unstable => *0 value in table*

# H2ON Table Generator Bug

- A bug was identified in the conversion subroutine
  - Initial guess for the T, ρ values corresponds to given P, U
  - Newton's method converges on the correct T, ρ combination
  - Pressures greater than 16 MPa and low temperatures converged to temperatures close to the critical point and low densities
- Corrected by modifying the method of calculating the change in density
- Fixed issues addressed by manual correction implemented in user problem #15020 "Error in h2on generator at high pressure and low temperature"
- Correction implemented and tested with the H2ON generator
  - Modifications and new fluid table submitted to the code custodian
  - Included in the next release of RELAP5-3D

# H2O95N Fluid Property Added to RELAP5-3D

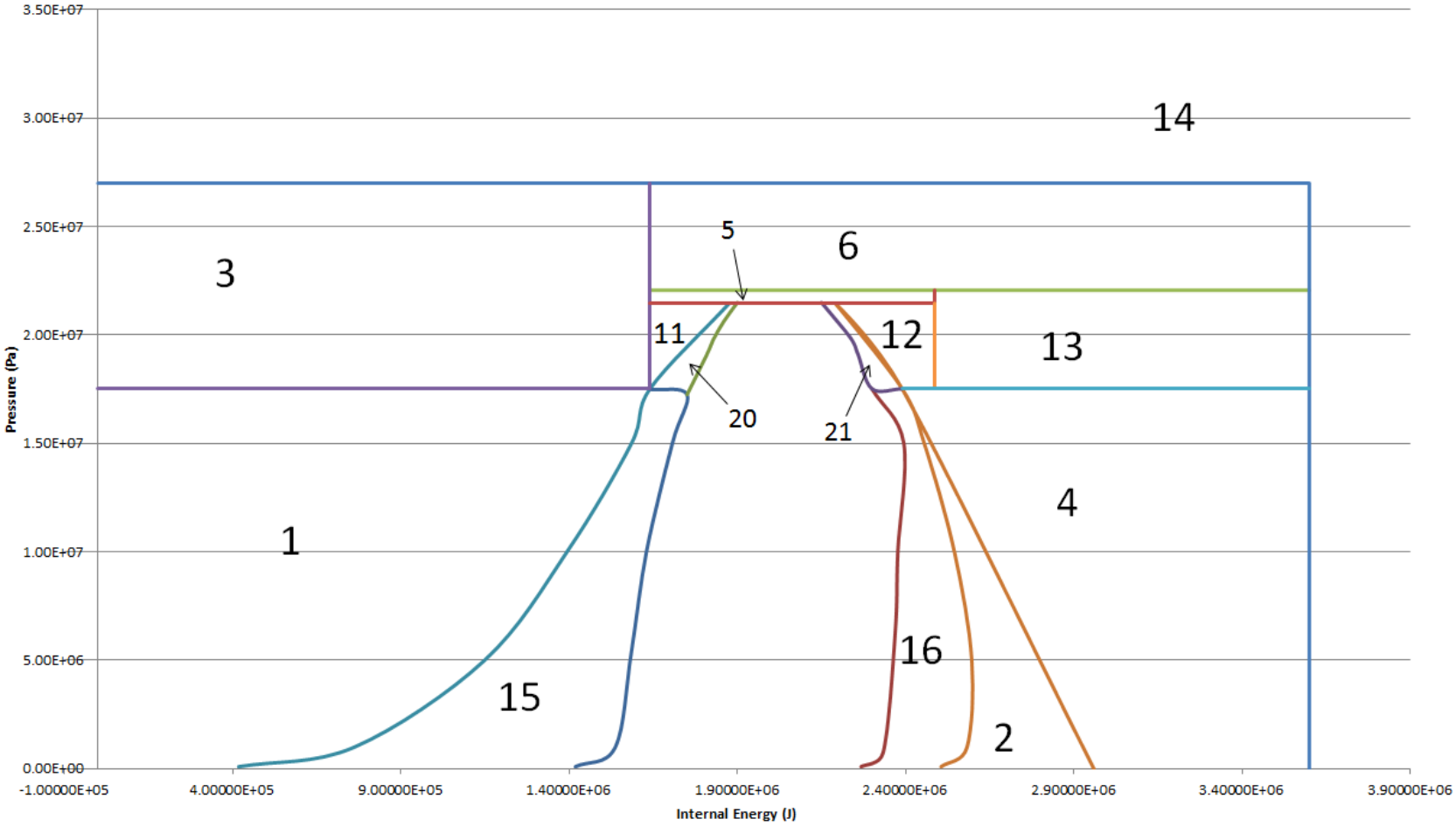
- Modify RELAP5-3D to recognize ‘h2o95n’ input
  - Test with H2ON fluid file (called H2O95N)
- Compared typ12002.i, typ1200n2.i, typKryNemSS.i, and typpwrr2.i
  - H2ON vs H2O95N (copy of H2ON)
  - Differences in output were
    - Designation fluid (i.e. H2ON, H2O95N),
    - Date
    - CPU times
- Modified input files
  - (typ1200295n.i, typ1200n295n.i,typKryNemSS95n.i, typpwrr295n.i)
  - Added to installation suite
  - Submitted to the code custodian
  - Included in next release of RELAP5-3D

# Define Grid

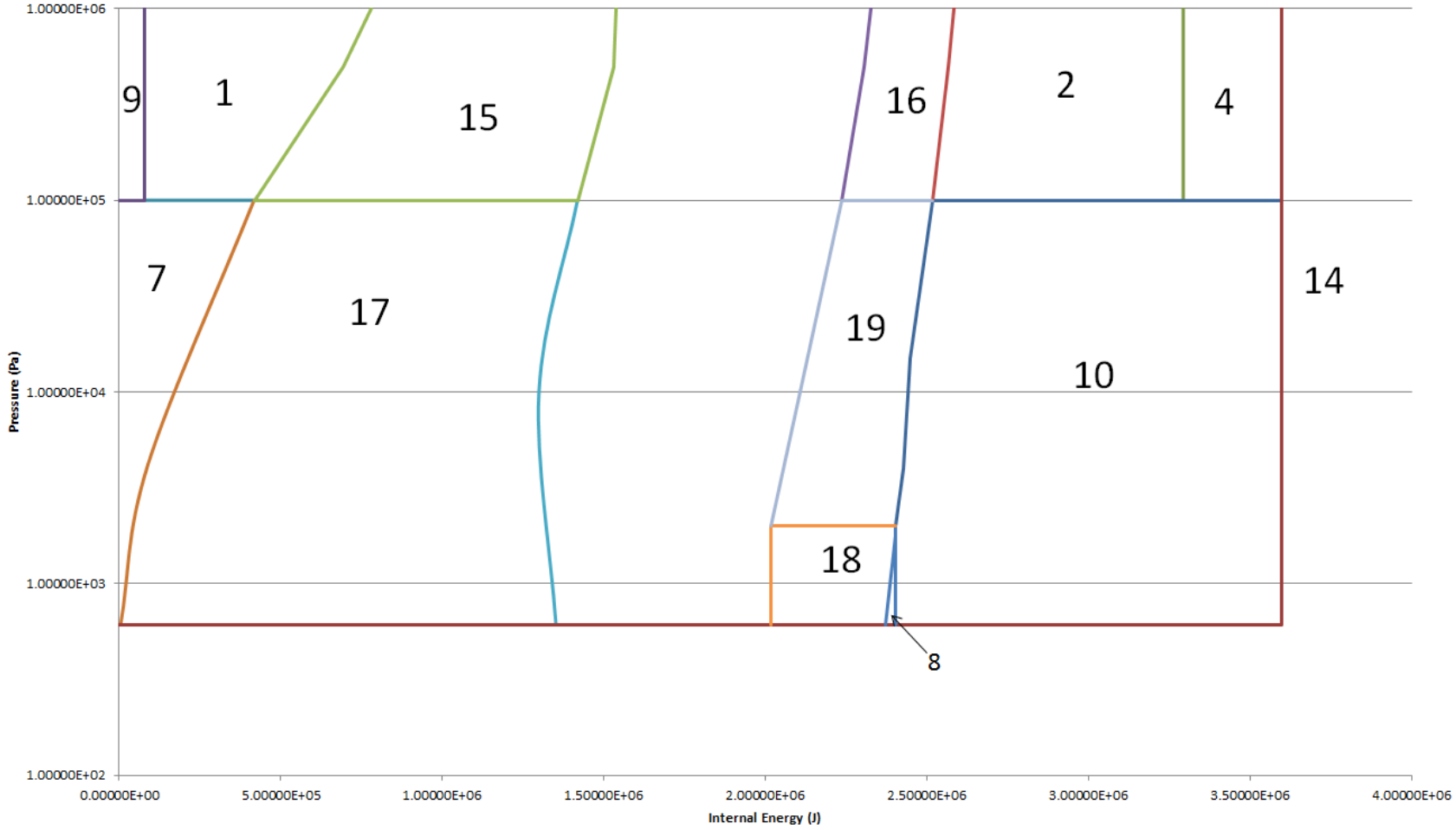
- Pressure and Temperature OR
- Pressure and Internal Energy
- Grid Cells = Boxes

| | | | |
|---|---|---|---|
| PI,T1 | P1,T2 | P1,T3 | P1,T4 |
| P2,T1 | P2,T2 | P2,T3 | |
| P3,T1 | P3,T2 | P3,T3 | |

# Define High Pressure Regions



# Define Low Pressure Regions



# Update Accuracy Based Methodology

- Specifies level of accuracy for thermodynamic properties
- Methodology produces an input pressure and temperature mesh
  - Uses pressure and temperature input
  - Generates the fluid property tables
  - Generates a table of properties at midpoints in the grid
  - Generates a table of properties at midpoints using the RELAP5-3D interpolators
  - Calculates errors from midpoint tables
  - Provides a summary and statistics for midpoint tables
  - Creates a pressure and temperature mesh (new generator input)
  - Written specifically for H2O
- Modified to work with H2O95N
  - Use the transport properties and the H2O95 fluid generators
  - Modify the input to P, U rather than P, T
  - Include the metastable states

# Update Polated Driver Program

- Plots the H2O95N fluid properties over range of thermodynamic states
- Polated uses normalized pressures and relative temperatures
  - P based on the triple point and critical values
  - Saturation temperatures
  - Normalized similar to the pressures
- Modified to use actual values of thermodynamic input data
- Unusable for metastable regions with PU input
  - Developed Polatem
  - Uses P and U as input values
  - Works for metastable states

# Testing

- **Accuracy based property generation** tool
  - Compare the generated versus interpolated values
  - Identified significant discrepancies
  - Worst box in each region selected based on density (ρ)
- **Polated utility**
  - Generate plots of the relative error
  - Compare analytical and numerical derivatives
  - H2ON, H2O95, and H2O95N for each region's worst box
  - Primary variables (β, κ, μ, ρ, $c_p$, h, k, S, and T) in each region's worst box
  - Plot using pressure and temperature or internal energy at the midpoint of the worst box and two adjacent boxes
- **Developmental Assessment** use light water for working fluid
  - Modified input to use H2O95N, H2ON, and H2O95
  - Compared H2O95N to H2ON and H2O95N to H2O95

# Results Verification Test Suite

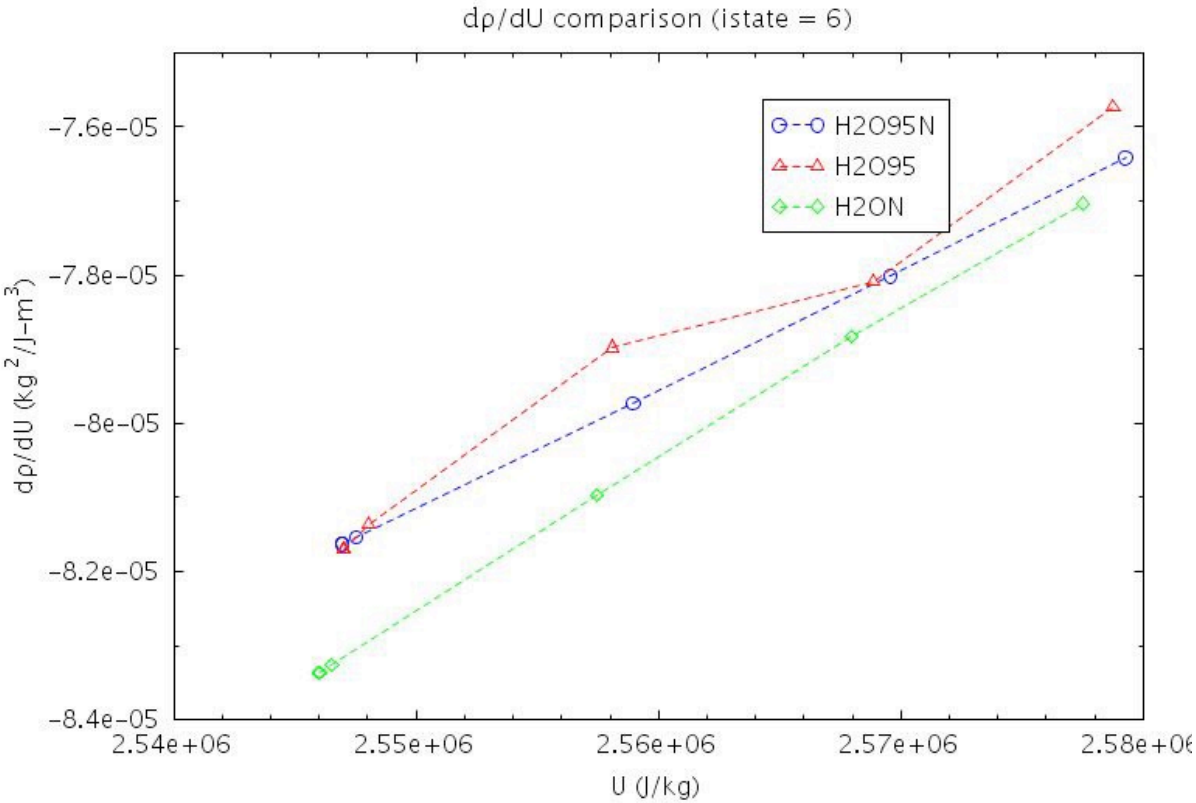
- Test changes made to implement the new H2O95N fluid
  - To confirm that nothing outside of the fluid scope was affected
  - The verification suite on original 4.3.4t and modified 4.3.4t
  - Resulting verification directories and their contents were compared
  - Differences detected in the time stamps and CPU clock cycles

# Results Polated Utility

- Accuracy based generation method used to compare H2ON, H2O95, and H2O95N
- Method used to generate statistics on the worst boxes for each region using the H2O95N fluid
- Pressure and temperature values for that box and adjacent boxes were determined from output
- Polated used to generate comparison plots of primary variables and principal derivatives
- Results showed that the new fluid performs as well as H2ON and is smoother than H2O95 in the derivatives in region 2 (normal vapor)

# Region 2 Normal Vapor dρ/dU

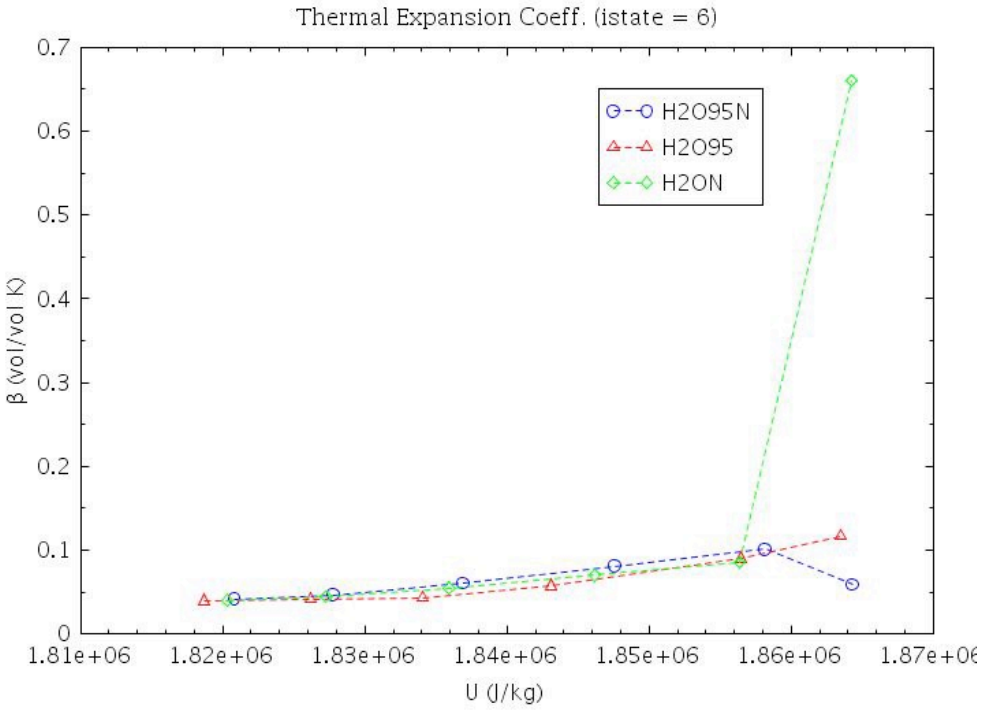
P = 9.86E+06 (Pa)  T ~ 580 (K)



# Results in Other Regions

- Plots for the other liquid and vapor regions (regions 1, 3 through 14) were compared and show the new fluid performs as well as H2ON and H2O95

- **Region 11**, Liquid near critical point provides examples of the H2O95N properties that are better behaved than H2ON



# *Some Exceptions*

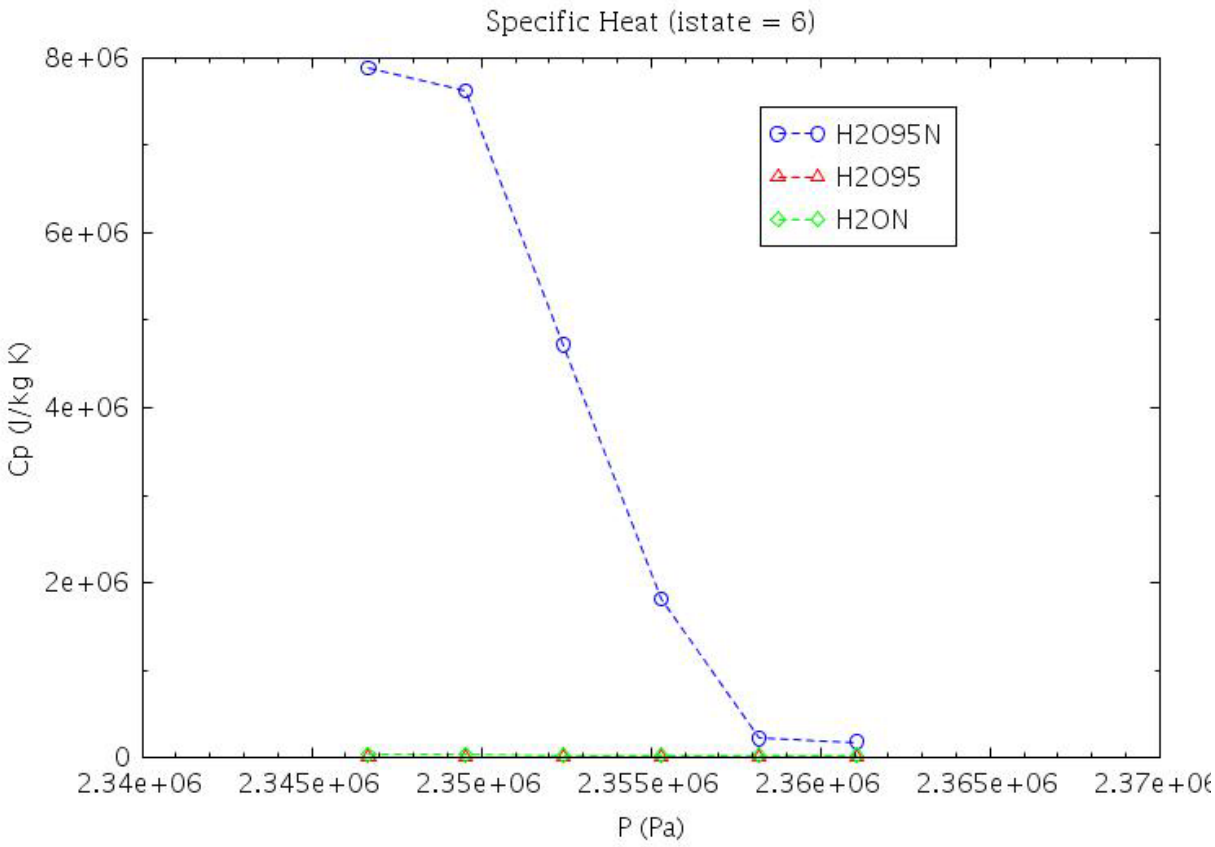
- **Region 5,** near the critical point
  - contains the worst box from the accuracy generator
  - next to a unstable/nonconvergent box
  - after inspection poor performance cause is in the NIST generator
  - derivatives sensitive to slight changes
  - results are unreliable at best
- **Region 6**, above the critical pressure
  - density from H2ON and H2O95N increases with internal energy
  - caused by interpolation problem with H2ON and H2O95N
  - Reported as user problem #16030
- **Region 10,** low pressure vapor
  - Relative error between the analytical and numerical derivatives of dT/dP is very large for H2ON and H2O95N
  - An issue with the analytical derivative for dT/dP returned by polate
  - Discrepancy is noted for further investigation

# Results Polatem Utility

- **Regions 15 – 21** are metastable regions
- Worst box of H2O95N provided results generally consistent with H2ON
- Thermal conductivity and viscosity
  - Based on H2O95 tables with some metastable values
  - Does not extend as far as H2ON into metastable regions
  - Values based on extrapolation of properties from liquid or vapor
  - Bound by minimum values
  - Also based on P and T
  - Conversion to P and U affects results
- Regions 15, 17, 18, and 19
  - H2O95 interpolators fail to return properties
  - Only able to compare H2ON and H2O95N

# Region 16 “Normal MetaVapor” Cp

- Slight shift between H2ON and H2O95N where generator transitions from unconverged or unstable to a metastable condition can result in large differences



# Accuracy Based Generation Results

- Comparison shows errors are in reasonable agreement
- Results not expected to be equivalent
  - differences in property generators
  - differences introduced by the use of internal energy rather than temperature
- Region 1 average errors generally agree with those from H2O; in some cases, the maximum errors tend to be higher for the new fluid
- Region 2 errors are similar and in most cases better than H2O

# Developmental Assessment Results

- New fluid compared to H2ON and H2O95
  - separate effects
  - integral effects
- Phenomenological cases fluid effect in most cases judged negligible

# Developmental Assessment Results cont..

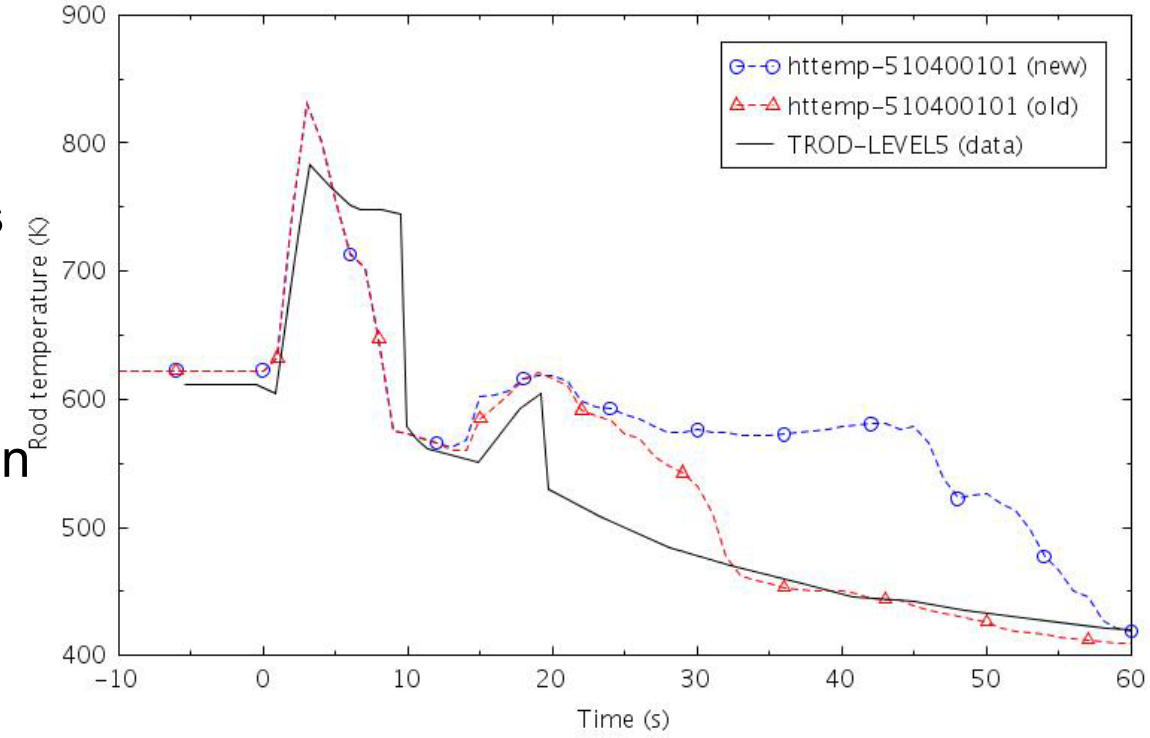
- MB-2 1712 full power steady state calculation (mb2_1712.i) failed to run with H2O95N
  - Initial conditions were grossly inconsistent,
  - Cause severe pressure oscillations on primary side of U-tubes
  - Resulted in huge amounts (> 100K) of liquid superheat early in the transient with both fluids
  - Choking was turned off at exit of U-tubes
  - Steady-state temperature profiles with both fluids nearly the same
- Moby Dick nitrogen/water test no. 3141 failed to execute for H2O95N
  - Inconsistent initial conditions
  - Inconsistent pressure in the gas supply time-dependent volume with steady-state pressure in the system
  - Corrected by decreasing an initial pressure and air supply pressure
  - The axial pressure profiles with both fluids were nearly identical

# Developmental Assessment Results cont..

- Models failed to complete when using the H2O95 fluid
  - UPTF test number 6 run 131
    - (uptf131_2lp.i and uptf131_2lp_pipe.i)
  - Dukler-Smith air water test 130-1000 lb/hr
    - (dukler100.i,dukler250.i,dukler500.i,dukler1000.i)
  - Input processing errors not flagged for H2O, H2ON, or H2O95N
  - LOFT L2-5 1D and 3D (l2-5_1D.i and l2-5_3D.i)
  - LOBI (LOBI-A1-4R.i) all failed with NaN's occurring in the output
- Submitted user trouble report #16032 which has been resolved
- Issue was incorrectly set variable indices

# Developmental Assessment Results cont..

- LOBI results significant difference in heater rod temperature between H2ON and H2O95N
- Same parameter in previous DA reports show similar differences between code versions, although at different elevations
- Similar results were seen with the LOFT L2-1D



# Conclusions

- H2O95N hybrid fluid property table based on H2ON and H2O95
  - Independent parameters PU
  - Extends into the metastable regions similar to the H2ON
- Updated the H2O95 fluid property generator
  - Resulted in new H2O95 fluid property table for RELAP5-3D
- Improved H2ON fluid property table for use with RELAP5-3D
- Accuracy based generation extended to H2O95, H2ON, and H2O95N
- The polate utility modified to allow use of absolute and relative values of pressure, temperature, and internal energy
  - Minor script errors identified and corrected
- Potential error in the RELAP5-3D interpolation routines UTR #16030
- Polatem developed based on polated to test metastable regions
- Several areas for follow on work were identified