H2ON Property Table Errors UP # 15020

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Problem Statement UP# 15020

- Code failures were reported for operation at high pressure and low temperatures for fluid h2on

- At 20.0 MPa
  - the reported kappa is negative for temperatures between 297.15 and 351.73 K.

- Negative kappa value causes RELAP5-3D to fail
  - calculation of the sound speed
  - square root of a negative number.

- Closer examination at 20 MPa shows
  - density is off by 20%
  - temperature is about 24 K higher than at 19.0 MPa and 21.0 MPa.

- Incorrect values at 21.7808 MPa as well.

- Data at 21.5 MPa and 22.0549 MPa were valid

Background

- The generating program is proprietary and is not sent out to source code customers.

- The output of the generating program is used to make the tpfh2on and tpfh2on2 files for executable code customers
  - the tpfh2on2 file is the original file used prior to 2010
  - the tpfh2on file is a larger file that has been used since 2010.

Investigation

- The h2on generating program provides incorrect values for a narrow range of high pressure and low temperature.
- Generating program was investigated to determine the root cause
  - differences between INL version and the published NIST version
  - published NIST version has errors
  - obtained corrected version of the generator from NIST
  - substantial programming differences between INL and corrected NIST generators.
- The fluid property tables were successfully generated
  - using current compiler and operating system
  - updated platform with 64 bit precision.
- Tracing the operation of the generator was time consuming
 - the bug was not found.

Solution

- Decided to manually interpolate between valid points in the ASCII tables
  - correct the a_tpfh2on and a_tpfh2on2 files by manually replacing the incorrect values with interpolated values.

- The tables were searched to find all negative kappa
  - occurred at 20.0 MPa and 21.7808MPa for tpfh2on2
  - occurred at19.0988 MPa, 19.4738 MPa, 19.8488 MPa, 20.2368 MPa, and 21.7808MPa for tpfh2on.

- An Excel spreadsheet was use to perform the interpolation
  - spreadsheet is saved in the same directory as the h2on generator
  - README file explaining the process.

Solution cont.

- Temperature, rho, kappa, beta, C_p, and S were replaced for all the bad points.

- Tables were tested using a modified version of state.i input deck
  - a verification test suite deck which tested the ability of the code to model various states from subcooled liquid to superheated vapor to supercritical for three different fluids: light water, heavy water, and helium
  - modified to test h2on only for pressures less than, equal to, and greater than the incorrect pressure values for each table
  - small Table tested 6 cases
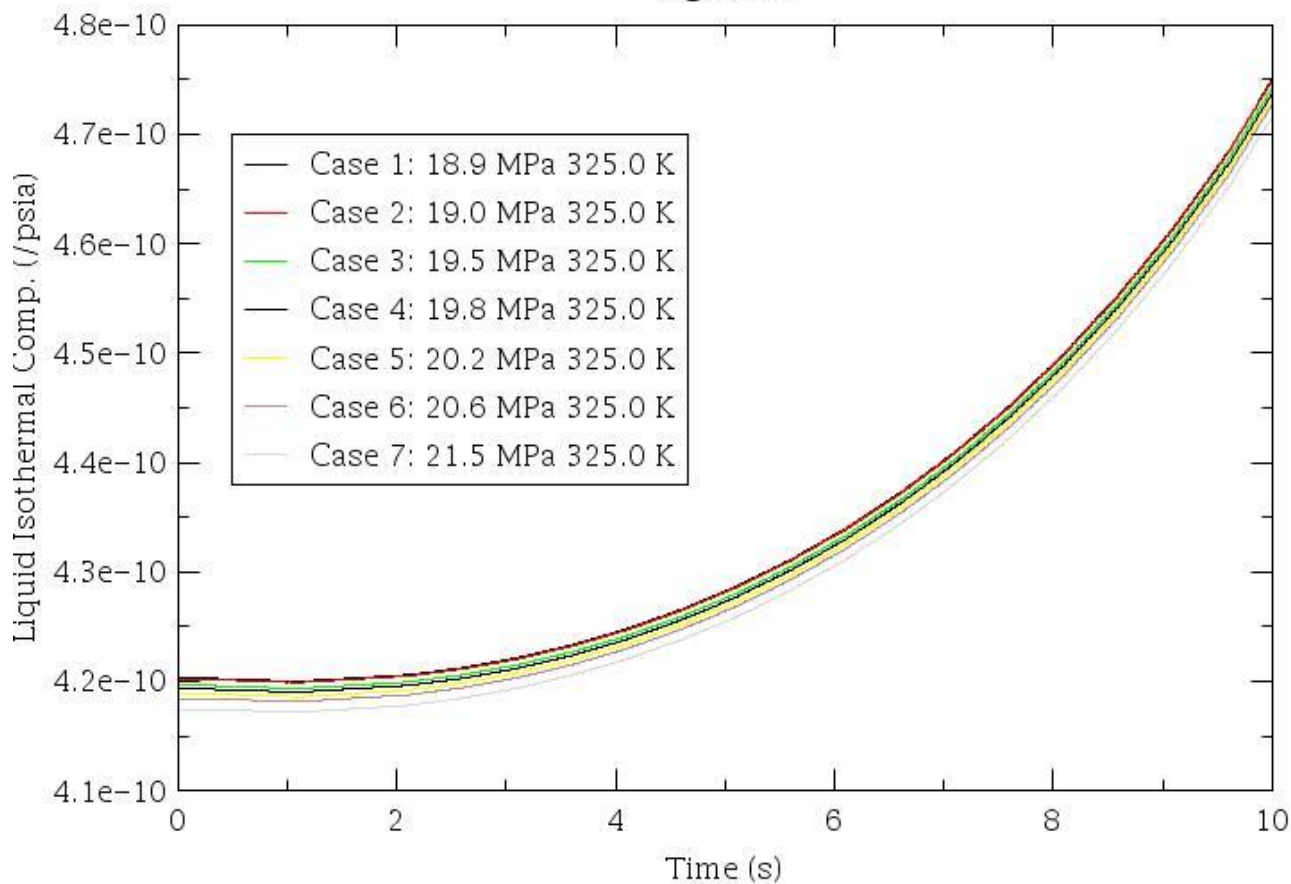 - big Table tested 9 cases.

Solution cont.

- Results showing blip in case 4 Small Table for Kappa
  - Occurs in a section we did not change.
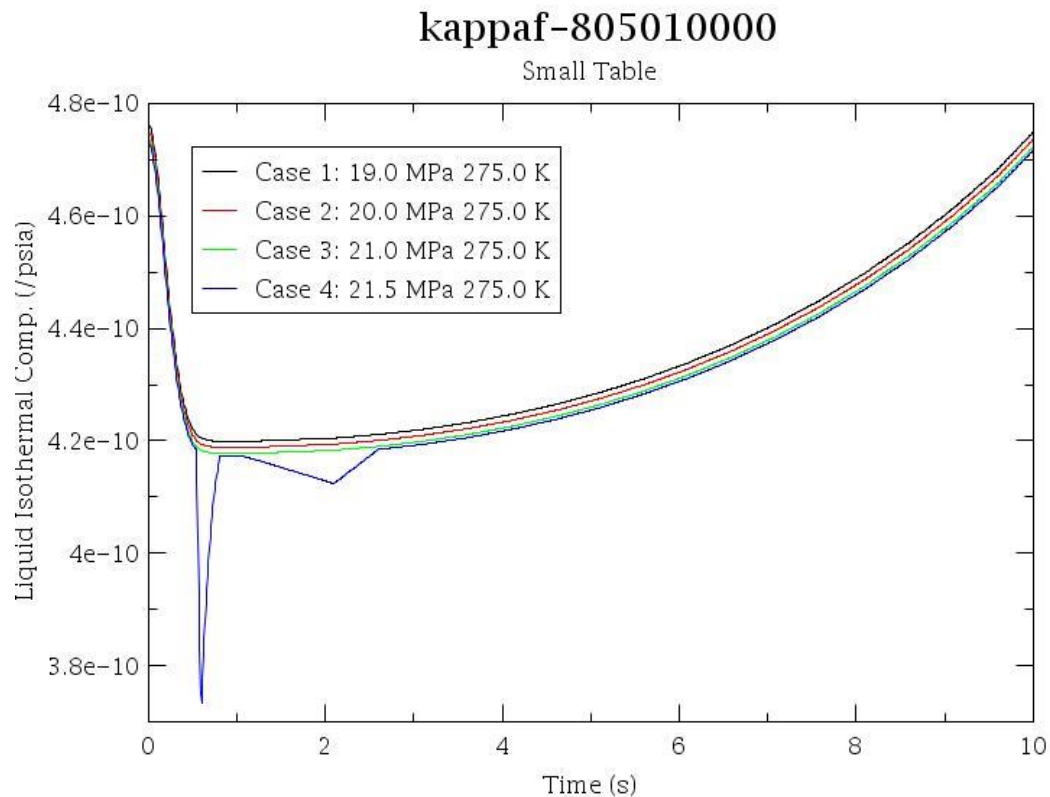
kappaf-805010000

Solution cont.

kappaf-805010000

Big Table

New Issue Discovered UP# 15023

- H2ON saturation properties are bad for points located within the pressure range 21.583E6 to 21.7808E6 Pa for both the small and large tables.

- This causes the code to either fail on input processing or to fail during execution with a negative C_g value.

- The problem **may** be that the spinodal lines at 21.7808E6 Pa are not well characterized.

- There is no valid metastable liquid or vapor data at this pressure.

- This was submitted as UP# 15023 to be investigated at a later time.

Future Effort

- NIST recommends that we use h2o95 rather than h2on.

- The current implementation of h2o95 does not provide metastable properties.

- The h2o95 generating program would have to be modified to produce metastable properties

- NIST has volunteered to help
  - provided suggestions for generator input flags
  - and changes to running the generator.

- Standby - In the queue to be investigated and hopefully implemented.