Implementation of Molten Salt Properties into RELAP5-3D/ATHENA

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Outline

- Introduction
- Derivation of fluid properties
- Verification
- Implementation
- Conclusions

Introduction

- **Molten salts are being considered as coolants for the Next Generation Nuclear Plant (NGNP) in both the reactor and the heat transport loop**
  - **The salt is expected to remain liquid**
- **Consequently, four coolant salts were incorporated into ATHENA as working fluids**
  - **LiF-BeF_2 (66% - 34%) (Flibe)**
  - **$NaBF_4$-NaF (92% - 8%)**
  - **LiF-NaF-KF (46.5% - 11.5% - 42%) (Flinak)**
  - **NaF-ZrF_4 (50% - 50%)**

Introduction (cont'd)

- The salts were implemented using a simplified equation of state
  - Liquid density is a function of temperature and pressure based on correlations from ORNL
  - Liquid heat capacity is constant
  - Vapor is assumed to have the same composition as the liquid and is treated as a perfect gas
- Simplified equation of state is considered adequate for liquid properties, but two-phase, vapor, and supercritical conditions should be avoided

Liquid thermodynamic properties

- **Density is a linear function of temperature and depends slightly on pressure**
- **The isothermal compressibility is given by a correlation**

$$\rho_T = A_D (T - 273.15) + B_D$$

$$\rho = \rho_T [1 + \kappa (P - P_0)]$$

$$\kappa = A_\kappa e^{B_\kappa T}$$

Liquid thermodynamic properties (cont'd)

- **The coefficient of thermal expansion is calculated from the density and isothermal compressibility equations**

$$\beta = -\left(\frac{A_D}{\rho_T} + \frac{B_\kappa \kappa (P - P_0)}{1 + \kappa (P - P_0)} \right)$$

Liquid thermodynamic properties (cont'd)

- **The change in specific internal energy from a reference state to a given P and T is calculated as the sum of two steps**
  - **A reversible, isothermal change in pressure from the reference pressure P_0**
  - **A reversible, isobaric change in temperature from the reference temperature, T_0**

$$\Delta u_1 = Q - W = -T\int_{P_0}^{P} v\beta dP - \int_{P_0}^{P} - v\kappa P dP$$

$$\Delta u_1 \approx -T\bar{v}\bar{\beta}(P - P_0) + 0.5\bar{v}\bar{\kappa}(P^2 - {P_0}^2)$$

$$\Delta u_2 = c_P(T - T_0) - P(v - v_1)$$

Liquid thermodynamic properties (cont'd)

- The change in specific entropy is also calculated as the sum of two steps
  - A reversible, isothermal change in pressure from the reference pressure P_0
  - A reversible, isobaric change in temperature from the reference temperature, T_0

$$\Delta s_1 = -\int_{P_0}^{P} \beta v dP \approx -\bar{\beta}\bar{v}(P - P_0)$$

$$\Delta s_2 = \int_{T_0}^{T} \frac{c_P}{T} dT = c_P \ln(T/T_o)$$

Constants for liquid thermodynamic properties

Salt	Composition (mole fraction)	T_{melt} (K)	A_D (kg/m^3-K)	B_D (kg/m^3)	A_κ (1/Pa)	B_κ (1/K)	c_P (J/kg-K)
1	$LiF\text{-}BeF_2$ (0.66, 0.34)	731.15	-0.4884	2279.7	2.3E-11	0.001	2386
2	$NaBF_4\text{-}NaF$ (0.92, 0.08)	658.15	-0.7110	2252.1	9.0E-11	0.0016	1507
3	LiF-NaF-KF (0.465, 0.115, 0.42)	727.15	-0.73	2530	NA	NA	1884
4	$NaF\text{-}ZrF_4$ (0.50, 0.50)	783.15	-0.93	3790	NA	NA	1151

Saturation line properties

- **The saturation line was determined from ORNL correlations**
  - **Not available for two salts**
- **The triple point temperature was set to the melting temperature**
- **The critical point temperature was estimated from empirical relations given by Bird et al. (1960)**

$$P_{sat} = 133.32 \times 10^{(A_{sat} - B_{sat}/T)}$$

$$T_{crit} = \frac{1.15}{0.77} T_{boil} = 1.494 T_{boil}$$

Liquid transport properties

- **Dynamic viscosity and surface tension were based on correlations from ORNL**
  - **Correlations for surface tension were not available for two salts**
- **Thermal conductivity was constant**

$$\mu = A_{\mu} e^{(B_{\mu}/T)}$$

$$\sigma = A_{\sigma} (T - 273.15) + B_{\sigma}$$

Constants for liquid transport properties

Salt	Composition	A_μ (Pa-s)	B_μ (K)	k (W/m-K)	A_σ (N/m-K)	B_σ (N/m)
1	$LiF\text{-}BeF_2$	1.16E-4	3755	1.1	-1.2E-4	0.260
2	$NaBF_4\text{-}NaF$	8.77E-5	2240	0.5	-7.5E-5	0.130
3	LiF-NaF-KF	4.0E-5	4170	0.8	NA	NA
4	$NaF\text{-}ZrF_4$	7.09E-5	4168	1	NA	NA

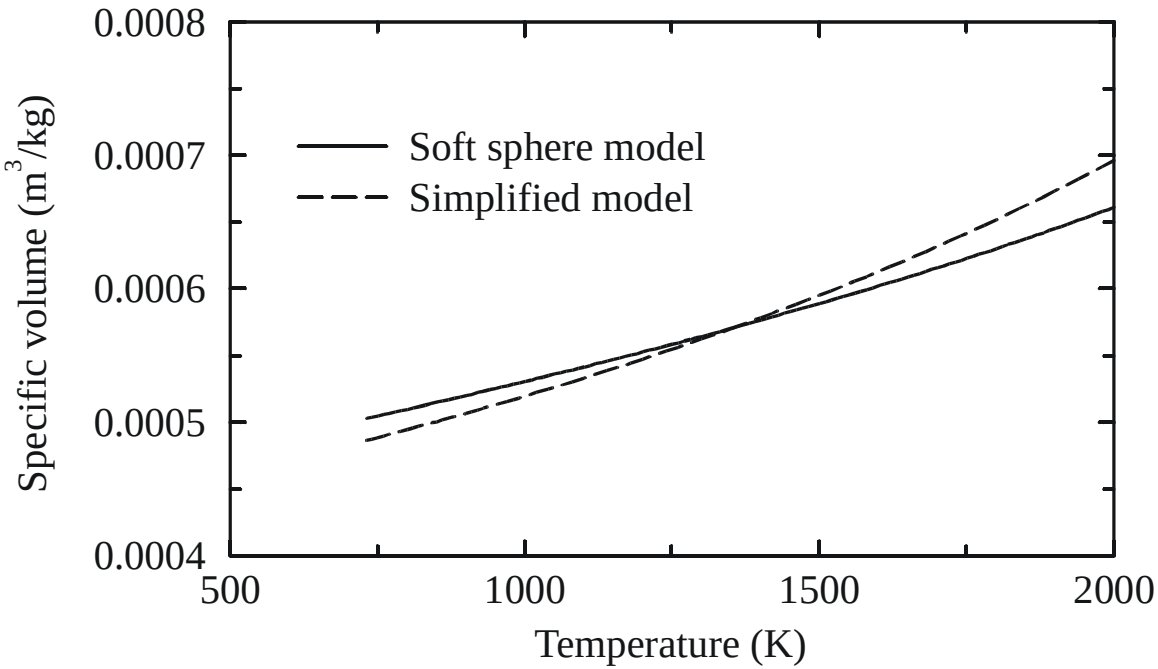
Vapor properties were estimated

- Thermodynamic properties are based on perfect gas relationships
  - Specific internal energy is a function of temperature alone
  - Constant specific heat capacity
  - Transport properties are based on Chapman-Enskog theory of gases at low density (Bird et al. 1960)
- The composition of the vapor is assumed to be the same as the liquid

The calculated fluid properties were verified

- For Flibe, the thermodynamic properties were verified against a soft-sphere model developed by Chen et al. (1992) and Moore (2000)
- The transport properties were verified by hand calculations
- The thermodynamic and transport properties for the other salts were also verified by hand calculations

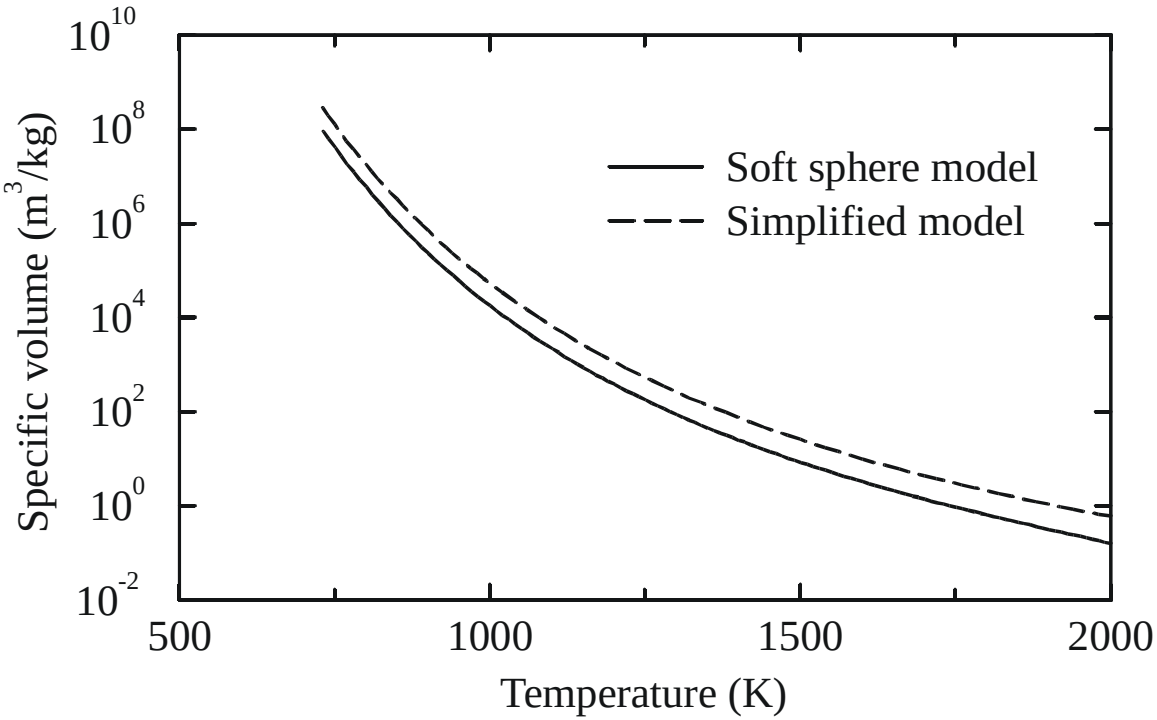
The results from the simplified and soft-sphere model agreed reasonably well for liquid



- Maximum deviations were:

v	5%
u	1%
β	37%
κ	16%
c_P	6%
s	1%

The comparisons were not as good for vapor



- Maximum deviations were a factor of 3

The molten salts were implemented into RELAP5-3D/ATHENA

- The salts can be accessed by selecting ms1, ms2, ms3, or ms4 on the Hydrodynamic System Control Cards
- The fluid properties are contained in the tpfms1, tpfms2, tpfms3, and tpfms4 files
- The molten salts were implemented using a new format, in which the transport properties are contained within the ‘tpf’ files, rather than in the old format, in which they are contained in subroutines
- This new format allows a new salt (or other fluid) to be implemented without making internal changes to the code

Conclusions

- **Four salts were implemented into RELAP5-3D/ATHENA to support analysis of the NGNP**
- **The salts were implemented using a simplified equation of state**
  - **The simplified model could be easily modified to represent any fluid where the liquid phase is of primary interest**
  - **Since all the properties are contained within the 'tpf' file, no internal modifications would be required in the code**

Conclusions (cont'd)

- Thermodynamic properties for Flibe were verified through comparisons with a detailed equation of state based on a soft-sphere model
  - The comparisons were in reasonable agreement for liquid
  - The results were not nearly as good for vapor
- The simplified model is considered acceptably accurate for analysis of the NGNP, which is expected to remain single-phase liquid
  - The model is not expected to be accurate for boiling, single-phase vapor, or supercritical applications

Conclusions (cont'd)

- **An evaluation should be performed to determine the applicability of the code's heat transfer and friction factor correlations with molten salts**
- **Additional details are provided in INEEL/EXT-05-02658**