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Fluoride salt coolant properties for nuclear reactor applications: A review

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ABSTRACT
Fluoride salts are crucial to achieving the benefits of Fluoride-salt-cooled High-temperature Reactors (FHRs). Intensive studies and modeling are being performed in different countries aimed at FHR technology development. Better understanding of liquid fluoride salt coolant properties and their uncertainties are needed for design and analysis of nuclear facilities. The main objective of the present study is to perform a literature survey of the experimental data, numerical studies, reports, and other review compilations for the main thermophysical properties of liquid fluoride salts. The review recommends density, heat capacity, thermal conductivity, and viscosity properties for potential primary coolants LiF-BeF$_2$ (flibe) and NaF-ZrF$_4$ (nafzirf) and secondary coolant LiF-NaF-KF (flinak). It is found that there is a dearth of experimental data. Thus recommended property uncertainties are included, which range from 2-20%, complete with a discussion on the recommended definition of the uncertainties. The recommended properties and their uncertainties provide a reference point for incorporating uncertainty in modeling to understand its impacts and for code benchmarking and validation.

KEYWORDS: FHR, fluoride salt, thermophysical properties, flibe, nafzirf, flinak

1. Introduction

One of the critical issues for the Fluoride-salt-cooled High-temperature Reactor (FHR) is to acquire comprehensive knowledge of the fluoride salt coolant properties and their uncertainties in order to ensure reactor designs perform as expected. The use of liquid fluoride salt as a coolant for the FHR is crucial to achieving the benefits of the design. Fluoride salts have high melting temperatures at low pressure in the range of 400 to 600°C allowing for high-temperature low-pressure operation. At these high temperatures, efficiency of converting heat to electricity is improved with the ability to use an open-air-Brayton combined-cycle plant similar to that used in natural-gas fired power plants. The boiling point of these liquids is very large on the order of 500°C above peak coolant temperatures allowing for large margins (1). Unlike water, which has extensive steam tables for its properties, the thermophysical properties of salts are not well known. As a result, determination of the fluoride salt coolant properties and their uncertainties would be necessary for design and analysis for nuclear applications like the FHR.

Hence, it is essential to summarize the coolant property research to date to present a comprehensive picture of research on fluoride salt coolant properties. Additionally, having reference coolant properties and associated uncertainties allows for incorporating uncertainty in modeling to understand its impacts and for performing code benchmarking and validation without introducing another source of uncertainty from selection of coolant properties.

The first work studying salt coolants for nuclear reactors comes from Oak Ridge National Laboratory (ORNL), specifically the Aircraft Nuclear Propulsion (ANP) project in the 1950s and early 1960s and the Molten Reactor Experiment (MSRE) project in the 1960s and 1970s. During the 1970s and 1980s, interest in salt coolants suited for nuclear applications waned. However, in the 2000s, a resurgence of interest in using fluoride salts as nuclear coolants yielded assessments of candidate coolant thermophysical properties. Several reviews or summaries of the existing literature emerged. First, Williams et al. (2006) assessed molten salt performance, which included determining properties for molten salts, for the Advanced High Temperature Reactor and coolant loop between the Next Generation Nuclear Plant and the Nuclear Hydrogen Initiative hydrogen-production plant (2,3). Benes and Konings (2009) present properties for fluoride salts for molten salt reactors including flibe and flinak (4). Holcomb and Cetiner (2010) look at the technologies involved in liquid salt heat transport including an assessment of heat transfer loop performance which includes an overview of salt properties (5). Serrano-Lopez (2013) reviews a wide range of molten salts for energy applications including flibe and flinak (6). Sohal (2010) also reviews molten salts for energy applications including properties of flibe and flinak (7). Lastly, Yoder (2014) reviews heat transfer data for liquid salts including flinak and compares existing heat transfer correlations (8). A handful of studies presented updates, and in recent years, a couple molecular dynamics simulations have looked at molten salts.

This paper reviews the experimental and theoretical property data for candidate fluoride salt coolants for the FHR to provide an easy reference point for recommended coolant properties and associated uncertainties for use in nuclear application analyses. The review traces coolant properties to experimental data when available and importantly emphasizes including property uncertainties estimated to be at 95% confidence level, which is an important consideration for thermal-hydraulic licensing analysis (9).

2.   Determination of Candidate Coolants

The salts currently under consideration for the FHR include $LiF-BeF_2$ (flibe) and $NaF-ZrF_4$ (nafzirf) as potential primary loop coolants and LiF-NaF-KF (flinak) as a secondary loop coolant. Flibe is the primary candidate for the primary loop coolant. It has the lowest neutron cross section, is chemically stable with low corrosion rates in high-nickel alloy systems, and is weakly radioactive with the primary activation product tritium resulting in very low radiation levels in the primary loop. Flibe does have some disadvantages, which include toxicity of beryllium and the need to enrich lithium to at least 99.995% Li-7 to maintain a low nuclear cross section (1). For neutronic design analysis, the baseline salt used is nafzirf because it has less attractive neutronic and thermophysical properties. The benefits of nafzirf over flibe include no direct tritium production and lower cost. By designing a reactor to operate using nafzirf, it is assumed that the reactor will operate better using flibe as the coolant. Thus, one can consider the coolants flibe and nafzirf to be bounding primary salt coolants for reactor design (10). For the secondary loop, the neutronic properties are not a concern. Ignoring any salts with beryllium, flinak has the best figures of merit for turbulent forced convection and for turbulent and laminar natural convection (2). Thus, flinak is the leading candidate due to its low melting point, its high heat capacity, and its chemical stability at high temperatures.

3. Investigation of Coolant Properties

3.1. LiF-BeF₂ (Flibe)

The preferred FHR primary coolant choice and primary candidate for a commercial FHR is peritectic LiF-BeF₂ (flibe), with a 2 to 1 ratio (66-34 mol%) of LiF to BeF₂. The primary coolant operating temperature range for the FHR is approximately 600-700°C (873-973 K). The melting temperature is 459°C, and it boils at over 1430°C (3–6,11–14).

3.1.1. Density

The literature available on density is more prolific, and typically has a smaller uncertainty than other properties. Most density correlations are based on three sets of experimental data from Blanke et al. (15), Cantor (16), and Janz et al. (17), which are plotted in Figure 1 as data points. Several correlations for the density of flibe have been proposed and are enumerated in Table 1. Each correlation is plotted in Figure 1 where any data markers only at the end points of correlation lines correspond to the temperature range limits and are not experimental data points. The majority of the data converge to the experimental data presented by Cantor (16) and Janz et al. (17), with their reported density correlation converted to units of kg/m³ as a function of temperature in Kelvin of ρ = 2413 - 0.488*T[K]. The best report of uncertainty that includes more than just precision is 2% from Cantor et al. in 1968 (18).
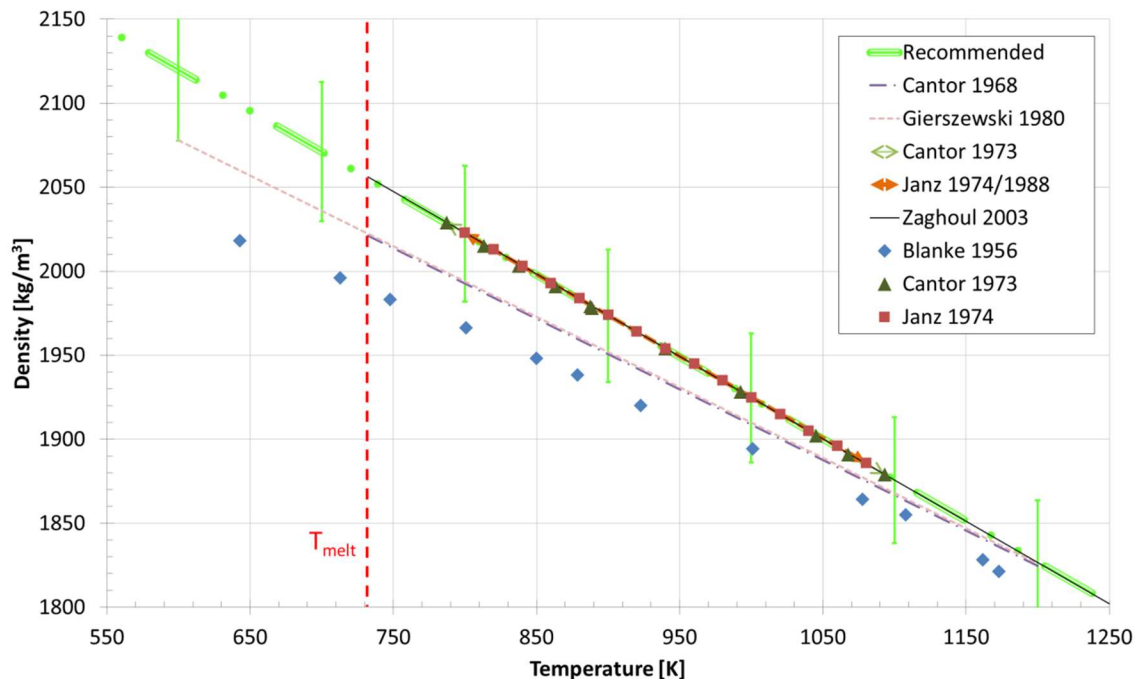

Figure 1. Flibe Density

Note: Any data markers only at the end points of correlation lines correspond to the temperature range limits and are not experimental data points. Experimental data points represented with data markers only.

Table 1. Flibe Density Correlations

LiF [mol%]	BeF$_2$ [mol%]	Correlation [kg/m^3]	Temp. [K]	Uncertainty	References
67	33	2329 – 0.42*T[K]		2%	Cantor 1968 (18,19)
67	33	2330. – 0.42*T[K]	600-1200	4%	Gierszewski 1980 (20)
67	33	2413 – 0.488*T[K]	800-1080		Janz 1974/1988 (3,14,17,21,22)
67	33	2413 – 0.4884*T[K]	800-1080		Cantor 1973 (4,6,7,11,16)†
67	33	2415.6 – 0.49072*T[K]	732.2-4498.8		Zaghloul 2003 (7,14,22)

Note: All correlations are converted to units of kg/m^3 for density and temperatures in Kelvin.
† Reported here with correction of Benes and Konings (4)

3.1.2. Heat Capacity

The experimental data reported for heat capacity is summarized in Table 2 along with heat capacity data reported by others reviewing the literature. Review of listed data suggests that a temperature independent heat capacity of 2386±3% J/kg-K for the liquid temperature range envelopes all the data surveyed.

Table 2. Flibe Heat Capacity

c_p [cal/g-K]*	c_p [J/kg-K]†	Temp. [K]	Uncertainty	Notes	References
0.56	2343	liquid		measurement	(18,23)
	2347	745.2-900		measurement	(23)‡
0.566	2369	liquid		predicted	(3,5,14)§
	2380	600-1200	20%	reported	(20)
0.57	2386	liquid	3%	reported	(6,11,12,18,24)
	2390	liquid			(4)
0.577±0.008	2414	liquid		measurement	(3–5,7,14,18,25)

* Values in units of cal/g-K to J/kg-K converted using 4184 as the conversion ratio.
† Values in units of J/kg-K are good to three significant figures; variation in more significant figures is due to conversion and rounding errors. Any values given with both units were originally given in cal/g-K and converted to J/kg-K.
‡ Originally data given as 232.09 J/mol-K with 1 mole = 98.884 g (23)
§ Value given by Sohal et al. (7)was incorrectly transcribed from Williams et al. (3).

3.1.3. Thermal Conductivity

Thermal conductivity measurements typically have the greatest error in heat transfer analysis because the fluid property is difficult to measure. Analytical expressions for thermal conductivity are presented by Rao-Turnbull (temperature independent) in (3,26) and Khokhlov et al. (temperature dependent) (27). The Rao-Turnbull correlation is

$$k = 1.19\left(\frac{T_m^{1/2}\rho^{2/3}}{(M/n)^{7/6}}\right)$$

where k is thermal conductivity in W/m-K, T_m is the melting temperature in K, ρ is the density in cm^3/mole, M is the average weight of the salt in g/mol, and n is the discrete ions per salt formula. The Khokhlov correlation is

$$k = 0.0005 \cdot T + \frac{32.0}{M} - 0.34$$

where k is thermal conductivity in W/m-K, T is the temperature in K, and M is the average molecular weight in g/mol (27).

Only a few sources of thermal conductivity experimental data are reported. Measured thermal conductivity data given for specific temperature(s) are listed in Table 3 along with predicted thermal conductivity reported in the literature. Experimental data at various temperatures reported in ORNL-4344 by Cooke in 1968 (25) and ORNL-4396 by Cooke in 1969 (28) is plotted in Figure 2. Although thermal conductivity changes slightly with varying temperature, the measurement uncertainties are greater than the temperature dependence variation (18). Also, in measuring thermal diffusivity, Kato demonstrates that the data scatter best fits a constant value (13). Thus, the temperature dependence of thermal conductivity is neglected. From the data collected, the recommended value for the thermal conductivity of flibe is 1.1 W/m-K with an uncertainty of ±10%. This value agrees with the most extensive measurements of thermal diffusivity by Kato et al. (13) and thermal conductivity measurements by ORNL as seen Figure 2.
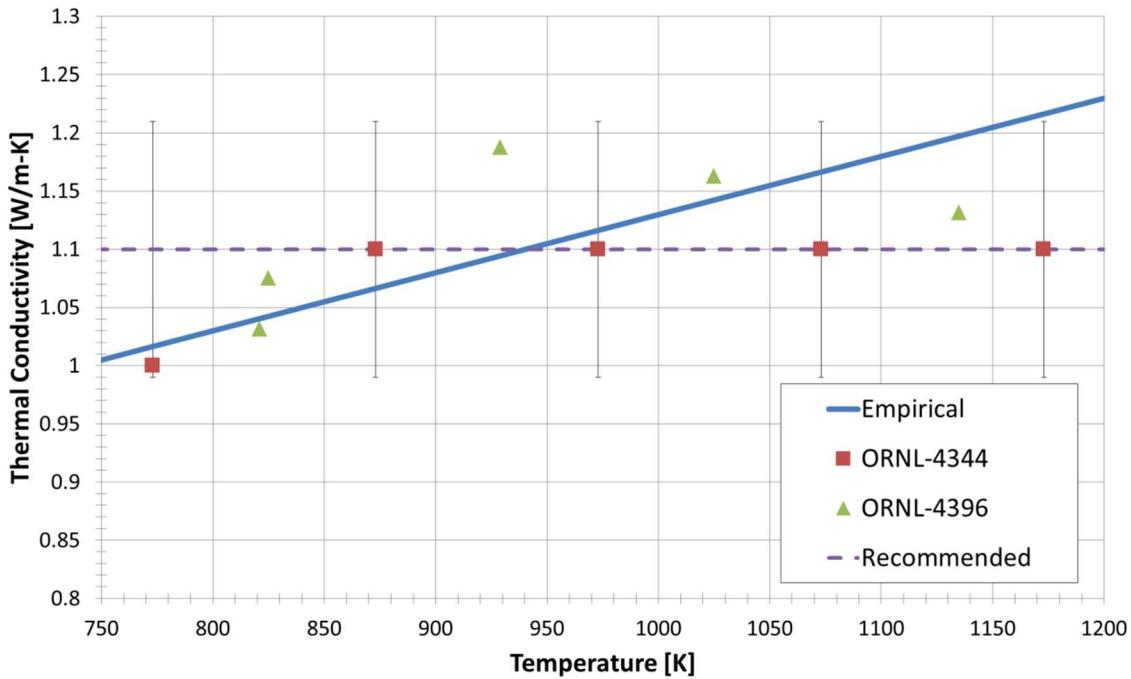

Figure 2. Flibe Thermal Conductivity

Table 3. Flibe Thermal Conductivity

Temp. [K]	k [W/m-K]	Note	References
873	0.79	(analytical: Rao-Turnbull)	(3,5)
	0.8	(analytical: Rao-Turnbull)	(25)
600-1200	1.0	with 20% error	(20)
	1.0	(measured) ±10% uncertainty	(3–5,12,14,18,25)
873	1.066	(analytical: Khokhlov)	(3,5,7,14)
	1.07	(measured)	(25)
	1.1	10-50% uncertainty	(11,19)
459-610	1.1	calculated from Kato et al.'s measurement of α=8.9E-4 m/hr	(4,13)

3.1.4. Viscosity

Molten salts are Newtonian fluids which follow an Arrhenius equation, exponential decrease in viscosity with reciprocal temperature. Due to this behavior, viscosity varies the most with temperature compared to other thermophysical properties. For the components of the binary salt flibe, LiF has a relatively low viscosity on the order of 10^{-3} Pa-s whereas the viscosity of BeF_2 is very high on the order of 10^5 Pa-s (29). The large difference in viscosity between LiF and BeF_2 has led to more viscosity experiments with different varying compositions of flibe. Only reports of viscosity close to the 67-33 mol% composition of interest are included here.

Experimental data points were presented by Abe et al. (29), Blanke et al. (15), Cohen et al. (30,31), and Janz et al. (17) in both tabular and graphical forms. Correlations for viscosity reported in the literature based on experimental data from Cantor et al. 1968 (18), Cantor et al. 1969 (32), Abe et al. (29) or literature reviews from Janz et al. 1974 (17), Janz 1988 (21), Dewan (12), Gierszewski et al. (20), Grimes et al. (33), Cohen et al. (30,31), Davis (11), Williams et al. (3), Benes and Konings (4), Holcomb and Cetiner (5), Sohal et al. (7), and Serrano-Lopez et al. (6) are listed in Table 4. Both the experimental data points and the correlations are plotted in Figure 3 and plotted with the natural log of viscosity in Figure 4. The correlation by Cantor (18) of $\mu = 0.116e^{3755/T[K]}$ in cP, which is most reported in the literature, is recommended with the associated uncertainty of 20%.

Table 4. Flibe Viscosity Correlations

LiF [mol%]	BeF$_2$ [mol%]	Correlation [cP]	Temp. [K]	Uncertainty	References
64	36	$0.0594e^{4605/T[K]}$	740-860	4%	(12,17,21,32)
67.2	32.8	$0.07803e^{4022/T[K]}$	812.5-1573	1.3%	(29)
66	34	$0.116e^{3755/T[K]}$	873-1073	15-20%	(3–7,11,14,18)
66	34	$0.116e^{3760/T[K]}$	600-1200		(20)
66	34	$0.118e^{3624/T[K]}$	773-1073	10-20%	(30,31,33)
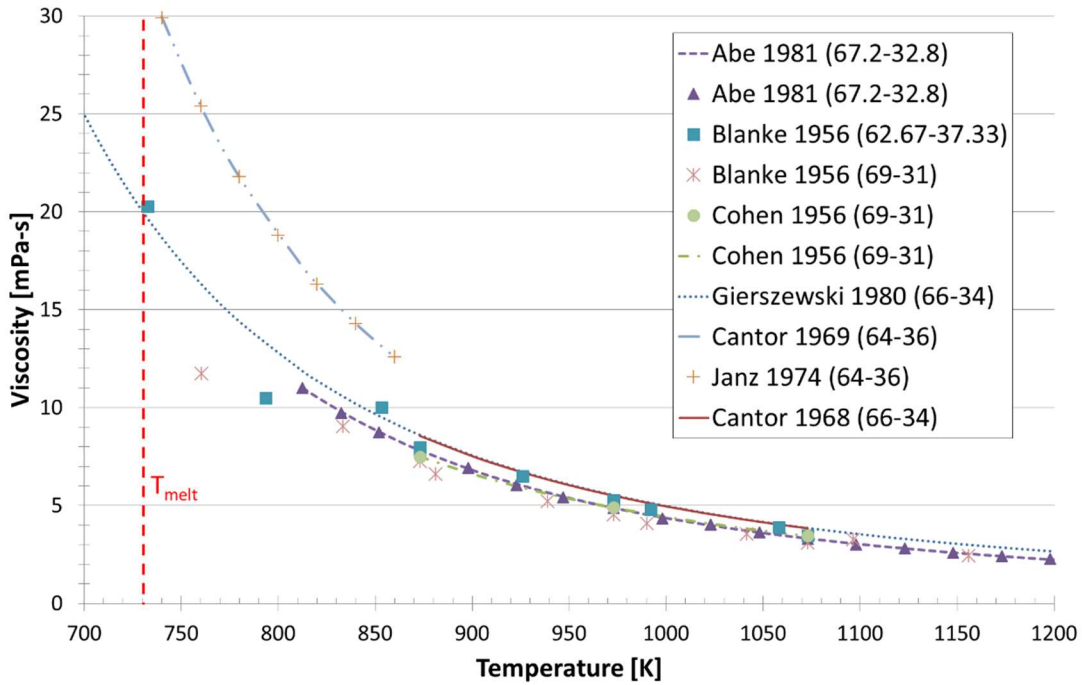
Figure 3. Flibe Viscosity
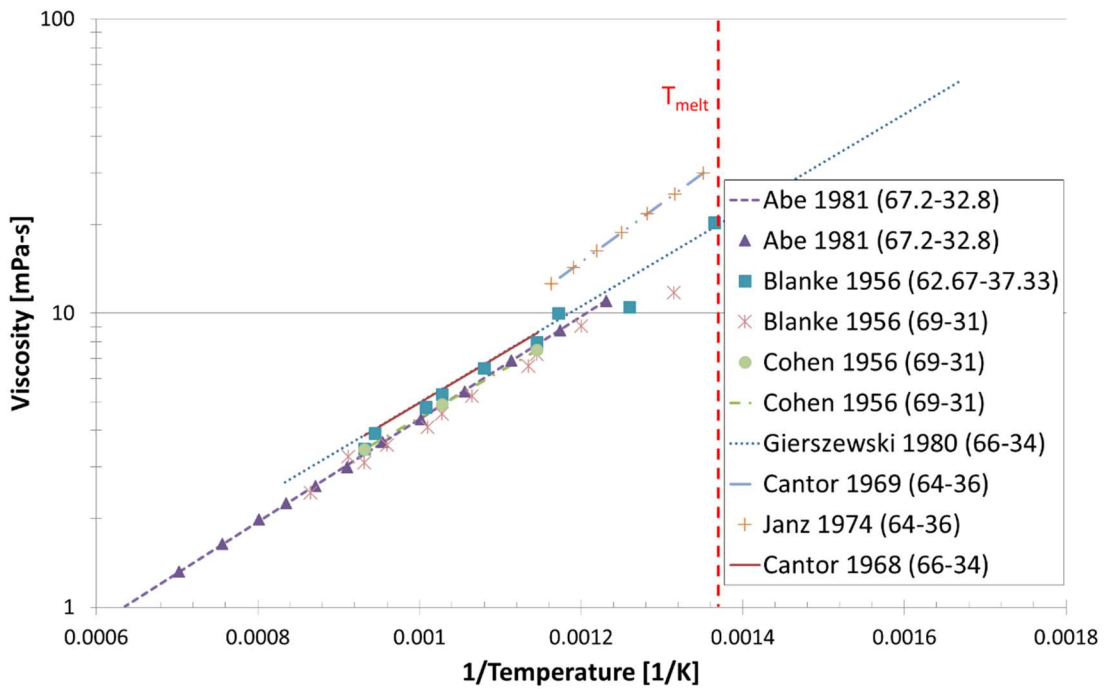
Figure 4. Flibe Viscosity Log Plot

3.2. NaF-ZrF₄ (Nafzirf)

3.2. NaF-ZrF$_4$ (Nafzirf)

The candidate primary coolant for a Fluoride-Salt-Cooled High-Temperature Test Reactor (FHTR) is nafzirf, a sodium zirconium fluoride salt with a 59.5-40.5 mol% composition of NaF and ZrF$_4$, respectively. The melting temperature is 500°C, and it boils at over 1350°C. However, it must be noted that ZrF$_4$ does not boil but instead forms ''snow'' that does not condense back to a liquid. ''Snow traps'' must be used to mitigate this problem. Compared to flibe, the melting point of nafzirf is a little higher and the boiling a little lower. Additionally, the heat capacity and thermal conductivity is about half that of flibe. The properties of nafzirf are thus not as ideal as flibe; however, nafzirf has the potential to be less expensive and not need isotopic separation, and does not directly produce tritium.

There are other compositions of nafzirf which have been considered as coolants. A list of these compositions and their melting points is listed in Table 5. This section will review all nafzirf compositions and make a recommendation on properties to use for the candidate composition 59.5-40.5 mol%.

Table 5. Nafzirf Mixtures Melting Temperatures

NaF [mol%]	ZrF$_4$ [mol%]	Temp. [°C]	Temp. [K]	References
42.2	58.8	570	842	(30,34,35)
48	52	510-515	783-788	(30,34,35)
50	50	510	783	(30,34–36)
52	48	500-515	773-788	(30,34,35)
53	47	500-520	773-793	(30,34,35)
54.1	45.9	520	793	(30,37)
57	43	490-530	763-803	(30,34,35,38)
59.5	40.5	500	773	(3,14)
66.7	33.3	625-680	898-953	(30,34,35)
81	19	750	1023	(30,35)

3.2.1. Density

The density of nafzirf has been reported for various compositions in Table 6. The correlations presented by Powers et al. in 1963 are experimentally determined with 5% uncertainty for the 50-50, 53-47, and 57-43 mol% compositions (37). The 42.2-57.8, 48-52, 52.48, and 81-19 mol% compositions are predicted correlations with 5% uncertainty. Other compositions are calculated or estimated. For example, Williams et al. calculated the density correlation with additive molar volumes (3). No other density data is presented with reference to its uncertainty.

Four experimental density data points were provided by Cohen and Jones at 600, 700, 800, and 900°C for the 50-50 mol% composition as 3.23, 3.14, 3.04, and 2.93 g/cc, respectively, with no measure of uncertainty reported (34). Any other experimental data was reported in the published literature as its corresponding fitted temperature dependent correlation.

The recommended density correlation is calculated using the additive molar volume method for 59.5-40.5 mol% and converted to units of kg/m³ for temperature in Kelvin as $\rho = 3827 - 0.889 \cdot T[K]$ with 5% uncertainty.

Table 6. Nafzirf Density

NaF [mol%]	ZrF_4 [mol%]	Density [g/cc]	Uncertainty	References
42.2	58.8	3.86 - 0.00092·T[°C]	5%	(30,34,37)
48	52	3.79 - 0.00090·T[°C]	5%	(30,34,37)
50	50	3.75 - 0.00090·T[°C]		(34)
		3.79 - 0.00093·T[°C]	5%*	(11,30,36,37)
52	48	3.72 - 0.00089·T[°C]	5%	(30,34,37)
53	47	3.71 - 0.00089·T[°C]	5%*	(30,34,37)
54.1	45.9	3.70 - 0.00089·T[°C]		(30)
57	43	3.65 - 0.00088·T[°C]	5%*	(3,30,34,37)
		3.935 - 0.000918·T[°C]		(38)
59.5	40.5	3.584 - 0.000889·T[°C]		(2)
		3.65 - 0.00088·T[°C]		(3,14)
66.7	33.3	3.49 - 0.00086·T[°C]		(30,34)
81	19	3.22 - 0.00081·T[°C]	5%	(30,37)

* experimentally determined

3.2.2. Heat Capacity

The heat capacity of nafzirf has been reviewed for both solid and liquid temperatures. Cohen et al. and Powers and Blalock measured 0.196 cal/g or 0.820 J/g-K for the 50-50 mol% composition at 300°C with a 10-15% uncertainty (30,35). All values were originally reported in units of cal-g/K and were converted using the conversion factor is 4.187 J/kg-K per cal/g-K. Cohen et al. also predicted the heat capacity for other compositions of nafzirf (30). Heat capacities for 300°C are presented in Table 7.

More extensive research has been conducted on liquid nafzirf. Measurements have been made for 50-50, 53-47, and 57-43 mol% compositions. All compositions under study have reported predicted values except the 59.5-40.4 composition. Additionally, predicted values using the modified Dulong-Petit method of

$$c_p = \frac{8 \sum_{i=1}^{n} N_i p_i}{\sum_{i=1}^{m} N_i M_i}$$

where N_i is the mole fraction, p_i is the number of atoms in a molecule, and M_i is the molecular weight of component i (24,39), and using the simple empirical analytical form

$$c_p = (0.2916 \pm 0.04040) + \frac{(0.00802 \pm 0.216 \times 10^{-3}) \times 10^4}{M}$$

where c_p is heat capacity in J/g-K and M is molar mass is g/mol, which is given by Khokhlov et al. (27), are calculated for all compositions under study. The measured, reported, and predicted values from Dulong-Petit and Khokhlov are given in Table 8. The recommended heat capacity for the 59.5-40.5 mol% liquid nafzirf is 1.172 J/g-K with 10% uncertainty. This value is within the uncertainty of heat capacity predicted by Khokhlov.

Table 7. Nafzirf Heat Capacity at 300°C

NaF [mol%]	ZrF$_4$ [mol%]	Measured [J/g-K]	Predicted [J/g-K]	References
42.2	58.8		0.795±20%	(30)
48	52		0.795±20%	(30)
50	50	0.820±15%		(30,35,36)
52	48		0.837±20%	(30)
53	47		0.837±20%	(30)
54.1	45.9		0.837±20%	(30)
57	43		0.837±20%	(30)
59.5	40.5			
66.7	33.3		0.879±20%	(30)
81	19		0.963±20%	(30)

Table 8. Nafzirf Heat Capacity at 700°C

NaF [mol%]	ZrF$_4$ [mol%]	Measured [J/g-K]	Predicted [J/g-K]	Dulong-Petit [J/g-K]	Khokhlov [J/g-K]	Measured/Predicted References
42.2	58.8		1.130±20%, 1.089±20%	1.094	0.993±0.059	(30,35)
48	52		1.130±20%	1.113	1.040±0.061	(30,35)
50	50	1.151±15%	1.172	1.121	1.058±0.061	(11,30,35,37)
52	48		1.130±20%	1.129	1.077±0.062	(30,35)
53	47	1.130±10%	1.130±20%	1.133	1.087±0.062	(30,35,37)
54.1	45.9		1.172±20%	1.137	1.098±0.062	(30,35)
57	43	1.172±10%	1.172±20%†	1.150	1.128±0.063	(3,30,35)
59.5	40.5	1.172±10%*		1.162	1.157±0.064	(3,14)
66.7	33.3		1.214±20%	1.200	1.250±0.066	(30,35)
81	19			1.309	1.511±0.073	

* Value is reported for 59.9-40.5 mol; however, the reference the value lists the heat capacity value for the 57-43 mol% composition.

† Salanne et al. reports 1.066 J/kg-K (38)

3.2.3. Thermal Conductivity

A search for reporting of experimental data for thermal conductivity did not yield any results. However, for the 59.5-40.5 mol% composition, Williams et al. reported values of 0.36 W/m-K using the Rao-Turnbull correlation and 0.49 W/m-K using the Khokhlov correlation (3,27). Table 9 reports the values for both correlations for the compositions under study. Comparing the reported values by Williams et al.

and Table 9, it is assumed that Williams et al. may have reported values for the 57-43 mol% composition as values for the 59.5-40.5 mol% composition. The recommended thermal conductivity of nafzirf for 59.5-40.5 mol% composition is 0.49 W/m-K with 15% uncertainty. The uncertainty of this correlation is based on experiments by Ignat'ev et al. who found good agreement between the Khokhlov correlation with experimental data for salts containing LiF, NaF, and BeF_2 with an estimated uncertainty, mainly due to inaccuracy in calibration, of 15% (40).

Table 9. Nafzirf Thermal Conductivity

NaF [mol%]	ZrF_4 [mol%]	Rao-Turnbull [W/m-K]	Khokhlov [W/m-K]
42.2	58.8	0.30	0.43
48	52	0.31	0.45
50	50	0.31	0.45
52	48	0.34	0.46
53	47	0.35	0.46
54.1	45.9	0.36	0.47
57	43	0.39	0.48
59.5	40.5	0.43	0.49
66.7	33.3	0.60	0.53
81	19	0.96	0.63

3.2.4. Viscosity

Experimental viscosity data values for nafzirf with a 10% uncertainty were given by Cohen et al. in 1956 for 50-50 and 53-47 mol% compositions at 873, 973, and 1073 K (30) and were also reported later by Cohen and Jones in 1957 (31) and Janz et al. in 1974 (17). In 1993, Grande et al. reported experimental data for 50-50 mol% composition in a figure (41). Table 10 lists the values given by Cohen and Janz and the values extrapolated from the figure in Grande. The experimental data are plotted in Figure 5.

Table 10. Nafzirf Experimental Viscosity Data

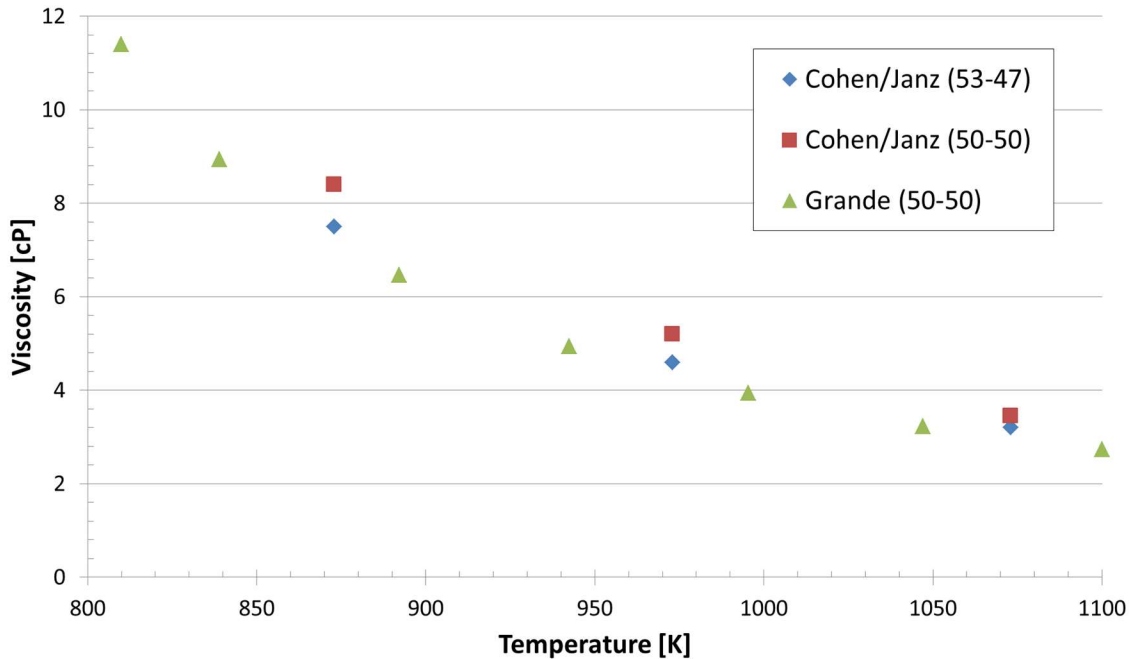| Temp. [K]	Grande (50-50 mol%)	Cohen/Janz (50-50 mol%)	Cohen/Janz (53-47 mol%)
810	11.4		
839	8.93		
873		8.4	7.5
892	6.47		
942	4.94		
973		5.2	4.6
995	3.94		
1047	3.23		
1073		3.45	3.2
1100	2.73		

Figure 5. Nafzirf Experimental Viscosity Data

The viscosity of nafzirf has been reported for various compositions in Table 11. The correlations presented by Powers et al. in 1963 are experimentally determined with 10% uncertainty for the 50-50, 53-47, and 57-43 mol% compositions, and predicted with 20% uncertainty for the 48-52, 52-48, and 54.1-45.9 mol% compositions (37). The 48-52, 52-48, and 54.1-45.9 mol% compositions are predicted correlations with 20% uncertainty. No other viscosity data is presented with reference to its uncertainty. The recommended viscosity for the 59.5-40.5 mol% composition is listed in Table 11, and the recommended uncertainty is conservatively 20%.

Table 11. Nafzirf Viscosity

NaF [mol%]	ZrF$_4$ [mol%]	Correlation [cP]		Uncertainty	References
100	0	0.1197	exp(3183/T[K])		(42)
48	52	0.098	exp(3895/T[K])	20%	(37)
50	50	0.0709	exp(4168/T[K])	10%*	(11,30,31,37)
		0.02993	exp(3901/T[K])		(42)
52	48	0.0785	exp(4020/T[K])	20%	(37)
53	47	0.078	exp(3984/T[K])	10%*	(37)
		0.07667	exp(3997/T[K])		(42)
54.1	45.9	0.078	exp(3984/T[K])	20%	(37)
57	43	0.078	exp(3984/T[K])	10%*	(37)
		0.0767	exp(3977/T[K])		(3,14)
59.5	40.5	0.0767	exp(3977/T[K])		(2)†

* experimentally determined

† Williams (2) reports the viscosity correlation from Williams et al. (3) which gives the correlation for 57-43 mol% not 59.5-40.5 mol%.

3.3. LiF-NaF-KF (Flinak)

The secondary coolant choice is a eutectic mixture of sodium, potassium and lithium fluoride with a 46.5-11.5-42.0 mol% composition of LiF, NaF, and KF, respectively. The melting temperature is 454°C, and it boils at over 1570°C. It must be noted that the melting point of 454°C is based on phase-rule type (cooling) curves, and Janz and Tomkins cite 462°C as a more exact recommended value based on the heat of fusion (43). The 462°C melting temperature was also recommended by Rogers (44). However, the more accepted melting temperature remains 454°C. Nevertheless, for conservative operation, the recommended melting temperature is 462°C.

3.3.1. Density

Despite numerous sources, four correlations for the density of flinak, which are listed in Table 12 and plotted in Figure 6, are presented in the literature. They are for the temperature range of approximately 940 to 1170 K. The recommended correlation is $\rho = 2579 - 0.624 \cdot T[K]$ in kg/m^3 with 2% uncertainty originally proposed by Janz and Tompkins (45) in 1981 and later proposed by Chrenkova et al. (46) in 2003 and Cibulkova et al. (47) in 2006.
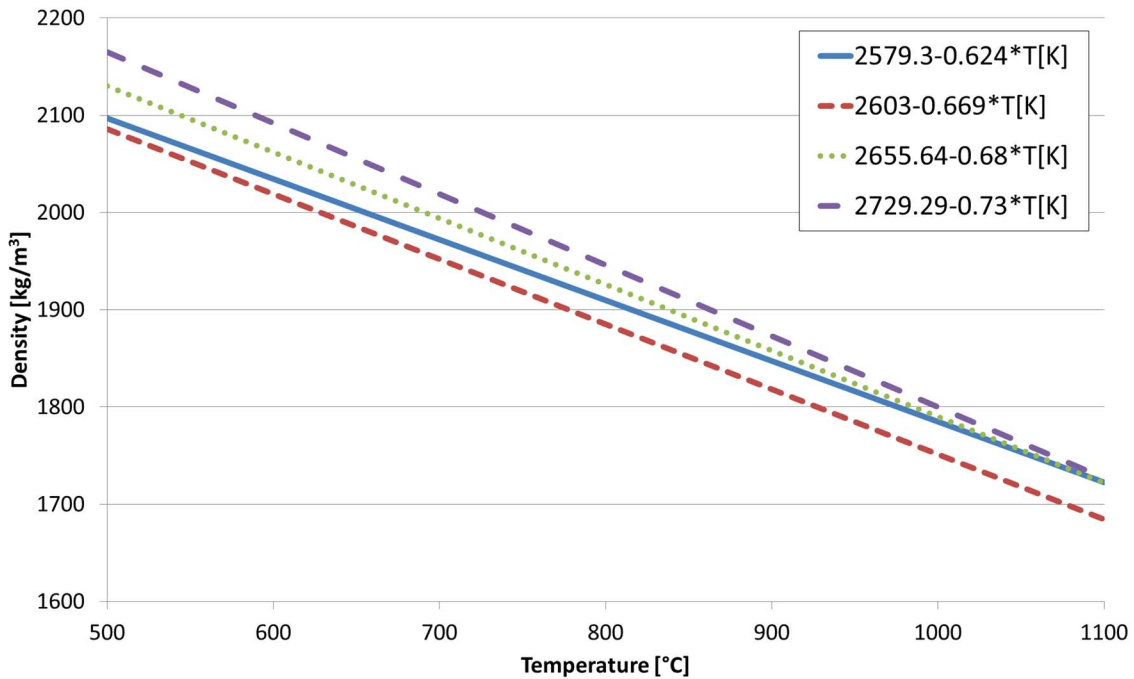

Figure 6. Flinak Density

Table 12. Flinak Density

Correlation [kg/m^3]	Uncertainty	References
$2579.3 - 0.624 \cdot T[K]$	2%	(4,6,14,21,45–47)
$2603 - 0.669 \cdot T[K]$		(38)
$2655.64 - 0.68 \cdot T[K]$		(34)[c]
$2729.29 - 0.73 \cdot T[K]$	5%	(2,3,5,8,11,14,30,33,34,37,48–50)[e]

[c] Correlation from Cohen and Jones (34) is calculated
[e] Correlation from Cohen and Jones (34) is experimentally determined

3.3.2. Heat Capacity

Only Powers reported heat capacity data for various temperatures, which was acquired from three laboratories: National Bureau of Standards (NBS), Naval Research Lab (NRL), and Oak Ridge National Lab (ORNL). Additional data for various temperatures is presented from correlations presented by Khokhlov et al. (51), Rogers et al. (44), and Williams et al. (3)

$$c_p[\text{J/g-K}] = 0.66 + 1.37\text{E-3} \cdot T \pm 0.013 \qquad \text{Khokhlov}$$

$$c_p[\text{cal/mol-K}] = \begin{array}{ll} 12.8218 - 9.651\text{E-3} \cdot T + 1.513\text{E-5} \cdot T^2 & \text{(solid)} \\ 9.636 + 10.487\text{E-3} \cdot T & \text{(liquid)} \end{array} \qquad \text{Rogers}$$

$$c_p[\text{cal/g-K}] = 0.2333 + 2.54\text{E-4} \cdot T \qquad \text{Williams}$$

respectively, where c_p is heat capacity and T is temperature in Kelvin. Temperature dependent data is list in Table 14. Others have reported measured and predicted heat capacity values as listed in Table 13a. Predicted values were derived from calculating the heat capacity with the ideal and Dulong-Petit methods and also using molecular dynamic simulation. Any data not designated as an experiment, measurement, or a predicted value is listed in Table 13b labeled as reported heat capacity. The recommended heat capacity for the liquid temperature range is 1884 J/kg-K with a conservative 10% uncertainty.

Table 13. Flinak Heat Capacity [J/kg-K]

Measured	Predicted	Uncertainty	References	Reported	Uncertainty	References
1381.7		10%	(30)	1674.8	4%	(45)
1880.0	1660.0 (Ideal)		(4)	1880.0		(6,50)
1882.8	1619.2 (Dulong-Petit)		(5)	1882.8		(7)
1883.0			(52)	1884	10%	(11)
1884.2	1620.4 (Dulong-Petit)	10%	(3,14)	1884.15		(33)
1884.2		10%	(30,37)	1890.0	5%	(48,49)
2009.8	1620.4 (Dulong-Petit)		(2)	1905.97		(53)
	1769.0 (Simulation)		(38)	2010.0		(5,8)
				2090.0		(54)

(a)   (b)

Table 14. Flinak Temperature Dependent Heat Capacity [J/kg-K]

Temp. [°C]	NBS (35)	NRL (35)	ORNL (35)	Khokhlov (51)	Rogers (44)	Williams (3)
100		1164	1214	1171	1151	1374
200		1227	1298	1308	1183	1480
300		1290	1382	1445	1246	1586
400		1348	1465	1582	1339	1693
500	1863	1913	1884	1719	1803	1799
600	1821	1842	1884	1856	1910	1905
700	1787	1796	1884	1993	2016	2012
800	1746	1758	1884	2130	2123	2118
900	1708	1721	1884	2267	2229	2224

3.3.3. Thermal Conductivity

Table 15 lists all the reported, estimated, or measured data points for thermal conductivity. There is a wide range from 0.6 to 4.5 W/m-K. The uncertainty is not well documented and may be as high as 10-25%. Some experimental data and correlations are for temperature dependent thermal conductivity. The change in thermal conductivity with temperature is small; however, most experimental data reported at more than one temperature shows that thermal conductivity changes with temperature. Older data reported by Grele and Gedeon (54), Hoffman and Lones (49), Grimes et al. (33), Powers et al. (37), and Janz and Tompkins (45) have very high thermal conductivity. This is presumably because other heat transfer modes were present, and as such they are considered anomalous. Thermal conductivity presented by Smirnov et al. as

$$k[\text{W/m-K}] = 0.36 + 0.00056 \cdot T$$

in which the difference between calculated and observed magnitudes do not exceed 5% and the total relative error is less than 4% (55), and by Kato et al. (13), and Khokhlov et al. (27) and Yoder (8) as

$$k[\text{W/m-K}] = 0.435 + 0.0005 \cdot T$$

has been reviewed by Benes and Konings and Serrano-Lopez et al. (4,6). There is excellent agreement between Kato et al. and Smirnov et al. (4,6), and good agreement with the Khokhlov correlation of slightly higher thermal conductivity as well. Thus, the recommended correlation is that of Smirnov et al. with an uncertainty of 10%.

Table 15. Flinak Thermal Conductivity

Estimated	Measured	Temp. [K]	References
	0.6	773	(2,3,5,14,26,56)
0.8		773	(4,11)
	0.8		(4,13)
0.83	0.82	790	(51)
0.84	0.81	800	(27)
0.85			(6)
0.92		973	(14)
0.94	0.92	1000	(27)
0.98	0.96	1080	(51)
1.2			(25)
1.30			(48,50)
3.63	4.50		(33)
4.48			(37)
4.50			(30,33,49,50,54)
	4.50		(4)

Table 16. Flinak Temperature Dependent Thermal Conductivity

Temp. [°C]	Temp. [K]	Smirnov	Khokhlov
454	727	0.77	0.80
500	773	0.79	0.82
517	790	0.80	0.83
527	800	0.81	0.84
550	823	0.82	0.85
600	873	0.85	0.87
650	923	0.88	0.90
700	973	0.90	0.92
727	1000	0.93	0.94
750	1023	0.93	0.95
800	1073	0.96	0.97

3.3.4. *Viscosity*

Most of the viscosity data is from the Oak Ridge National Laboratory Aircraft Nuclear Propulsion project during 1950-1956. A compilation of certain physical properties which have been determined experimentally or predicted from correlations of experimental data for fluoride salt mixtures is presented by Cohen et al. (30) and Powers et al. (37) with 10% uncertainty. Later Janz and Tompkins (45) measured viscosity of flinak with uncertainty of only 2%. In reviewing the literature, the correlations presented by these two studies have been repeatedly reported for flinak and are listed in Table 17 with all correlations presented in literature. Only Cohen et al. reported experimental data points. These four data points and all correlations are presented in Figure 7. The recommended viscosity correlation is the

experimentally determined $\mu = 0.04e^{4170/T[K]}$ in cP with 10% uncertainty from Cohen et al. and Powers et al. that is more heavily cited and more conservative.

Table 17. Flinak Viscosity

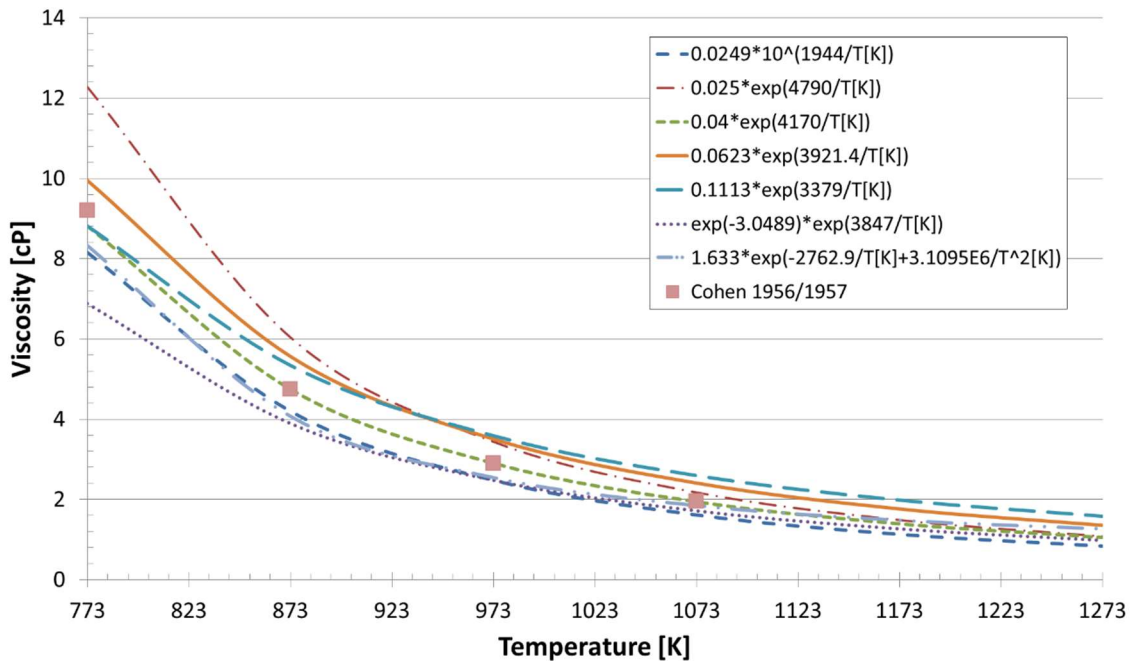| Correlation [cP]	Temp. [K]	Uncertainty	References
0.0249 exp(4476/T[K])	773-1173	2%	(21,45)
0.249 x 10$^{1944/T[K]}$			(4,6,46)
0.025 exp(4790/T[K])			(49,50,54)
0.04 exp(4170/T[K])	773-1073	10%	(2,3,5,8,11,14,30,31,33,37,50)
0.0623 exp(3921.4/T[K])			(57)
0.1113 exp(3379/T[K])			(48,50)
exp(-3.0489) exp (3847/T[K])			(47)
$1.633 \exp\left(\frac{-2762.9}{T[K]} + \frac{3.1095E6}{T^2[K]}\right)$	773-993	2%	(58)

Figure 7. Flinak Viscosity

4.   Results and Discussion

Table 18 lists the thermophysical properties for density, viscosity, thermal conductivity, and heat capacity recommended for use in any thermal hydraulic analyses and their associated uncertainties. Given reported uncertainties only list a percent uncertainty without explanation, it is necessary to define these uncertainties with a confidence level. Standard uncertainty may be thought of as equivalent to one standard deviation, while expanded uncertainty applies a coverage factor to standard uncertainty so results may be given a confidence level. For 95% confidence, the scaling factor is two for normal

distributions and corresponds to two standard deviations. Because the uncertainties reported in the literature are not well documented, there was no indication whether the uncertainty reported was standard or expanded. Typically, any measurements that fall outside two standard deviations are considered statistically significant and not just due to chance. Measurements greater than two standard deviation from the mean would then be considered due to some phenomena not expected, and thus not what the experiment intended to measure. As such, it is assumed that the thermophysical property data uncertainty expressed as percent uncertainty has a coverage factor of two and thus has a level of confidence of 95% (two standard deviations).

Table 18. Recommend Thermophysical Properties and 95% Level Confidence Uncertainties

Coolant	Liquid Range	Property	Units	Uncertainty
Flibe	$T_m = 459°C$ $T_b = 1430°C$	$\rho = 2413 - 0.488*T[K]$	kg/m^3	2%
		$\mu = 1.16E\text{-}4*exp(3755/T[K])$	Pa-s	20%
		$c_p = 2386$	J/kg-K	3%
		$k = 1.1$	W/m-K	10%
Nafzirf	$T_m = 500°C$ $T_b = 1350°C$	$\rho = 3827 - 0.889*T[K]$	kg/m^3	5%
		$\mu = 7.67E\text{-}5*exp(3977/T[K])$	Pa-s	20%
		$c_p = 1172$	J/kg-K	10%
		$k = 0.49$	W/m-K	15%
Flinak	$T_m = 462°C$ $T_b = 1570°C$	$\rho = 2579 - 0.624*T[K]$	kg/m^3	2%
		$\mu = 4.0E\text{-}5*exp(4170/T[K])$	Pa-s	10%
		$c_p = 1884$	J/kg-K	10%
		$k = 0.36 + 0.00056*T[K]$	W/m-K	10%

5. Conclusions

Tremendous potential of liquid fluoride salts and growing research efforts around FHR technology has generated increased interest in fluoride coolant properties. However, the knowledge base is still far from complete, and most studies do not address uncertainty or address it incompletely. Hence, it is important to summarize the research and present recommended coolant properties and associated uncertainties for performing analyses for nuclear applications. Based on the literature surveyed from some of the first experimental data in the 1950s to molecular dynamics simulations in the 21st century, the recommended coolant properties for flibe, nafzirf, and flinak for nuclear reactors has been determined. Additionally, uncertainty for each property is recommended. However, the lack of data and reported uncertainties is a concern for analyzing FHR technology. More experimental data is necessary to properly quantify property uncertainty and validate coolant properties. Meanwhile, the current

recommended properties and associated uncertainties can be used as a reference for code benchmarking and validation and for modeling to understand the impacts of property uncertainty.

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