

## **TCS Molten Salts Database (TCSALT)**

**Validation and Calculation Examples Collection**



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## About the Database Examples

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The *Validation and Calculation Examples Collection* that is available for many databases demonstrates both the *validity* of the database itself as well as demonstrates some of its *calculation* capabilities when combined with Thermo-Calc software and its Add-on Modules and features. For each database, the type and number of available examples varies. In some cases an example can belong to both a validation and calculation type.

### Validation vs Calculation Examples

*Validation* examples include experimental data in the plot or diagram to show how close to the predicted data sets the Thermo-Calc calculations are. It is applicable to the most recent version of the software and relevant database(s) unless otherwise specified.

*Calculation* examples are generally intended to simply demonstrate a use case of the database. This might be showing a binary or ternary system calculated in a phase diagram, or demonstrate how the database and relevant software features would be applied to a heat treatment application, process metallurgy, soldering process, and so forth.



Where relevant, references related to each example set are included at the end of the individual topic. You can also find additional references specific to the database itself when using the database within Thermo-Calc.

### Learn More



*Database Technical Information and Examples*: Included in the help is all the information about the databases. There are also separate *Technical Information* and *Validation and Calculation Examples Collection* PDFs for the **current version** of the database available for download from the Thermo-Calc [website](#). There are many other resources and examples also available.



If you are interested in sharing your own examples using Thermo-Calc products in unique or surprising ways, or if you want to share your results from a peer reviewed paper, send an email to [info@thermocalc.com](mailto:info@thermocalc.com).

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## TCS Molten Salts Database (TCSALT) Resources

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Database technical content and examples are available in different formats (html help files or PDFs).

Go to these locations to access the same content:

- **Locally Installed Help:** When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the **Databases** folder to browse the contents.
- **Web Help:** Go to the [Documentation](#) page to link to the most recent version of the web help. Then search or navigate to the **Databases** folder to browse the contents.
- **Website resources:** The individual database technical information and examples are also available in PDF format from the website. Download the *current version* of the PDFs for each database.

### About the CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.



Learn more on our website about the [CALPHAD Method](#) and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our [website](#) or our [YouTube playlist](#).

### Learn More



Go to the [Molten Salt Databases](#) page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information*. Also explore further applications of Thermo-Calc to molten salts on this page.

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Read more on our website about applications for [Sustainability](#). The webpage highlights several examples demonstrating how Thermo-Calc has been applied to address key sustainability challenges.



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

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## TCSALT Validation Examples

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## TCSALT Validation of NaCl-KCl-NaF-KF System

The NaCl-KCl-NaF-KF molten salt mixture is a reciprocal system and a core system in the TCS Molten Salts Database (TCSALT). It is designed to combine the low cost of chloride salts with the favorable heat transfer properties of fluorides. Example applications can be in electrochemical processing, thermal energy storage, and molten salt reactors.

 For a calculation example of this same system, see [TCSALT NaCl-KCl-NaF-KF Example](#)

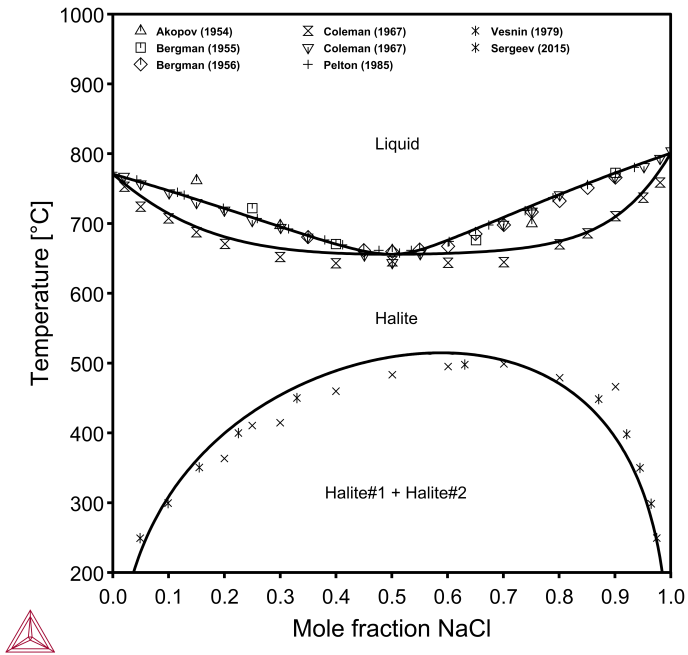


Figure 1: Calculated KCl-NaCl section compared to experimental data in [2015Ser].

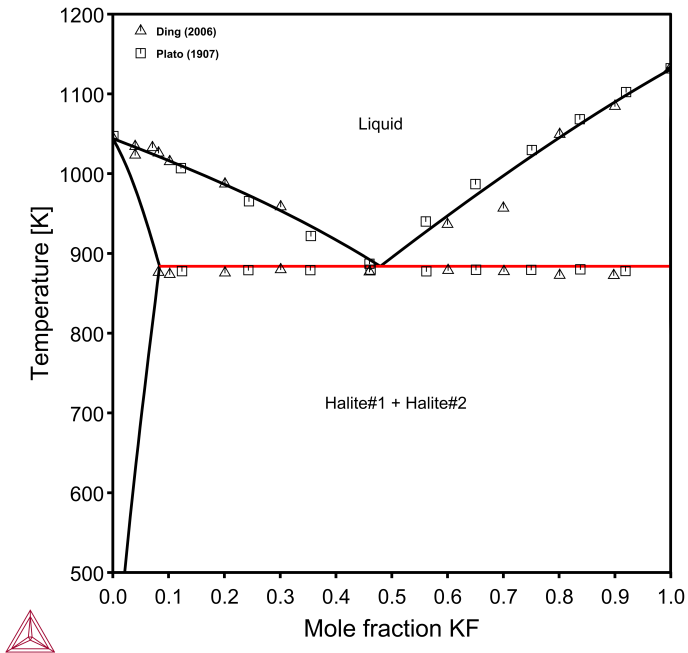


Figure 2: Calculated KCl-KF section compared to experimental data in [2021Oik].

## References

- [2015Ser] D. Sergeev, E. Yazhenskikh, D. Kobertz, K. Hack, M. Müller, Phase equilibria in the reciprocal NaCl–KCl–NaNO<sub>3</sub>–KNO<sub>3</sub> system. *Calphad* 51, 111–124 (2015).
- [2021Oik] K. Oikawa, N. Ueshima, Thermodynamic analysis of KCl-KF-AlCl<sub>3</sub>-AlF<sub>3</sub> system. *J. Japan Inst. Light Met.* 71, 32–38 (2021).

## TCSALT Validation for $\text{MgCl}_2$ -NaCl

Molten alkali-alkaline earth halide solutions are of much technological importance in, for example, the production of Mg and Na. A large amount of experimental thermodynamic and phase diagram data exists for these systems. NaCl, KCl,  $\text{MgCl}_2$ , NaF, and KF are used extensively as fluxing agents for liquid aluminum treatment. For example, the electrolytes used for Mg production are based mainly on NaCl,  $\text{CaCl}_2$ , and  $\text{MgCl}_2$  salts, which can also be used as fluxes for Mg casting.

These examples using the TCS Molten Salts Database (TCSALT) are showing calculations for the  $\text{MgCl}_2$ -NaCl system along with some validation of the results compared to experimental data.

? For additional calculation examples, see [TCSALT Calculations with Mg and Ca](#)

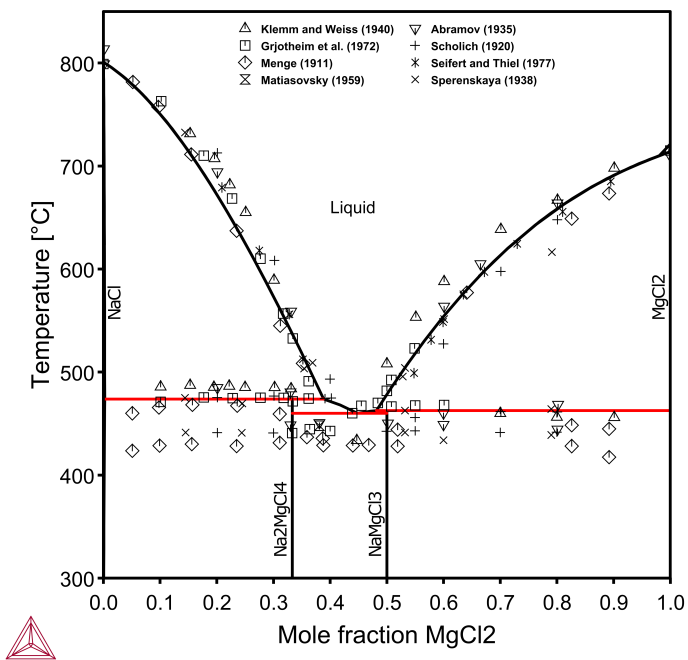


Figure 3: Calculated  $\text{NaCl}$ - $\text{MgCl}_2$  phase diagram with experimental data in [2001Pel].

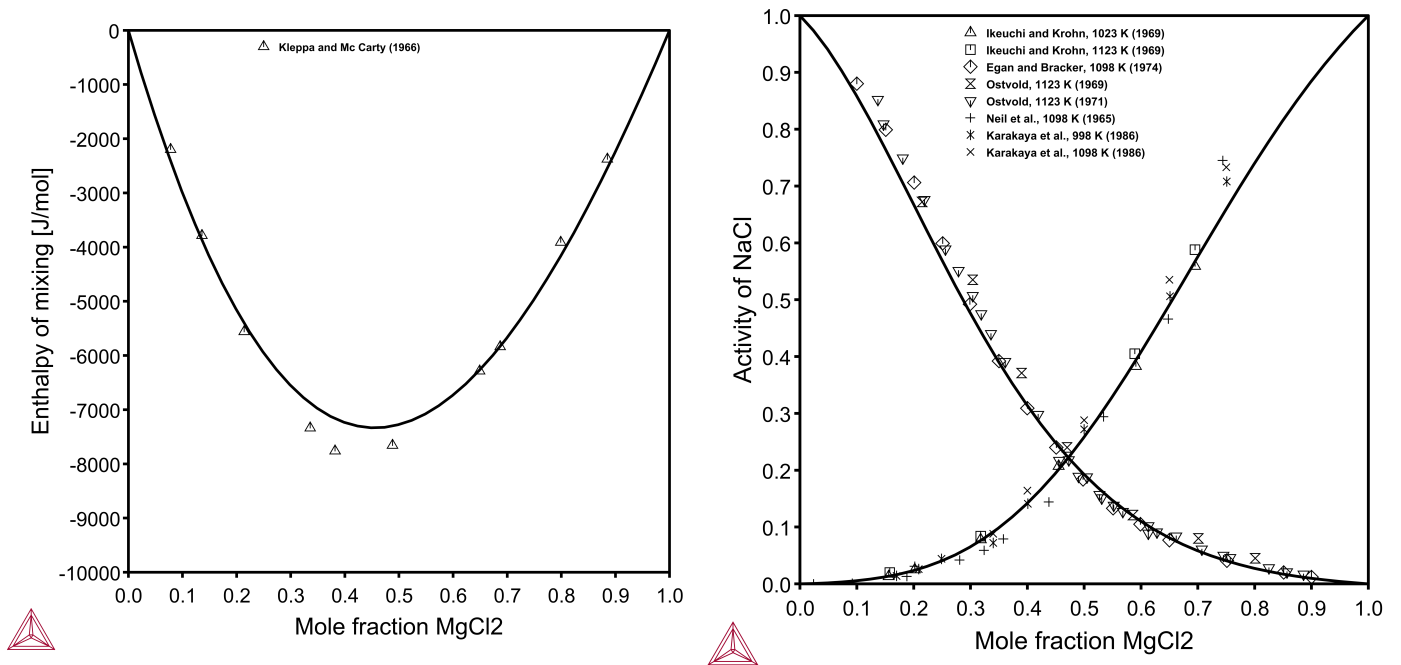


Figure 4: Calculated enthalpy (left) and activity of NaCl and MgCl<sub>2</sub> (liquid standard state) in liquid NaCl-MgCl<sub>2</sub> solution with experimental data in [2001Pe].

## CaCl<sub>2</sub>-MgCl<sub>2</sub>

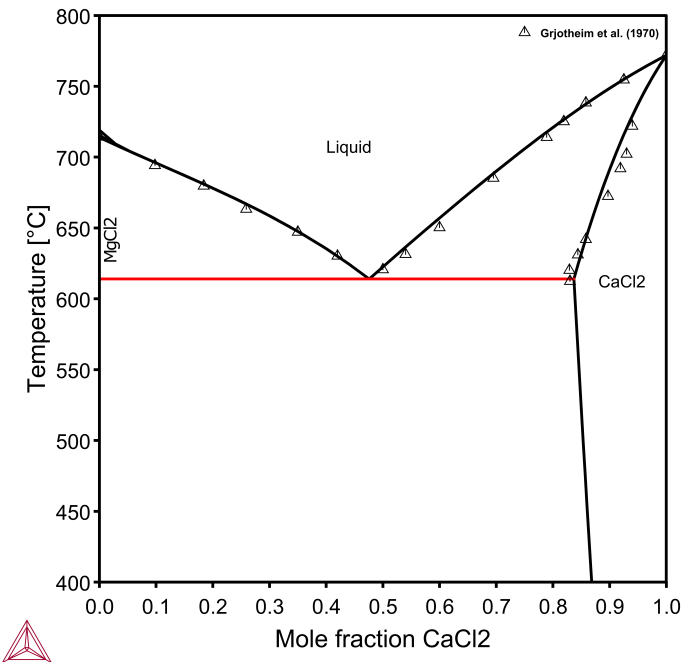


Figure 5: Calculated CaCl<sub>2</sub>-MgCl<sub>2</sub> section compared to experimental data from [1970Grj].

## References

- [1970Grj] K. Grjotheim, J. L. Holm, J. Malmo, B. Jerslev, C. E. Schäffer, E. Sunde, N. A. Sørensen, The Phase Diagram of the System  $\text{MgCl}_2\text{-CaCl}_2$ , and Thermodynamic Properties of Molten Mixtures in this System. *Acta Chem. Scand.* 24, 77–86 (1970).
- [2001Pel] A. D. Pelton, P. Chartrand, Thermodynamic evaluation and optimization of the  $\text{LiCl-NaCl-KCl-RbCl-CsCl-MgCl}_2\text{-CaCl}_2$  system using the modified quasi-chemical model. *Metall. Mater. Trans. A* 32, 1361–1383 (2001).
-

## TCSALT Validations for Aluminum (Al) Systems

Chloroaluminate melts are of considerable industrial interest. They may be used as electrolytes to produce aluminum. NaF, CaF<sub>2</sub>, LiF, and MgF<sub>2</sub> are important components in the Hall-Heroult electrolysis cells for Al production.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

 For additional examples, see [TCSALT Examples Related to Aluminum Production](#).

### AlCl<sub>3</sub>-MCl/AlF<sub>3</sub>-MF (M=K, Li, Na)

Systems with Al show a very strong short range ordering, which is modeled using complex ions in the liquid model: AlCl<sub>4</sub>-1, AlF<sub>4</sub>-1, and AlF<sub>6</sub>-3.

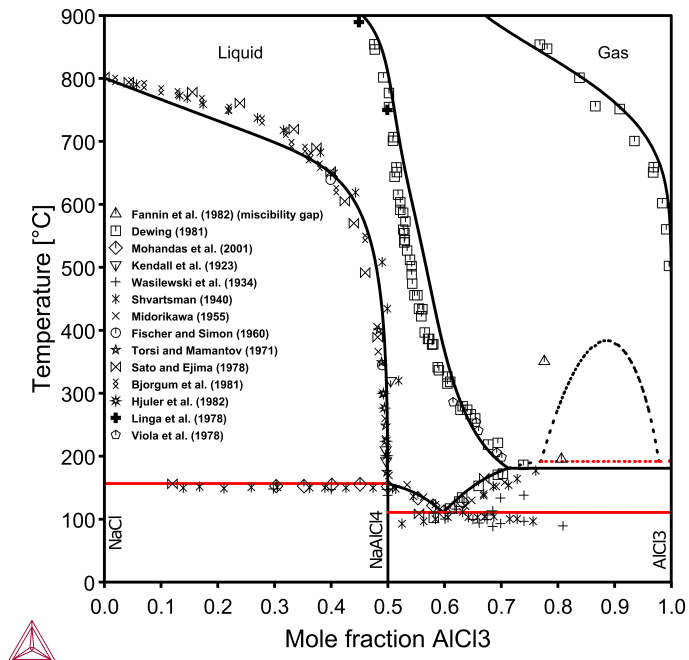


Figure 6: Calculated NaCl-AlCl<sub>3</sub> section (gas phase included) with experimental data from [2004Rob]. Dotted lines: calculated metastable liquid miscibility gap.

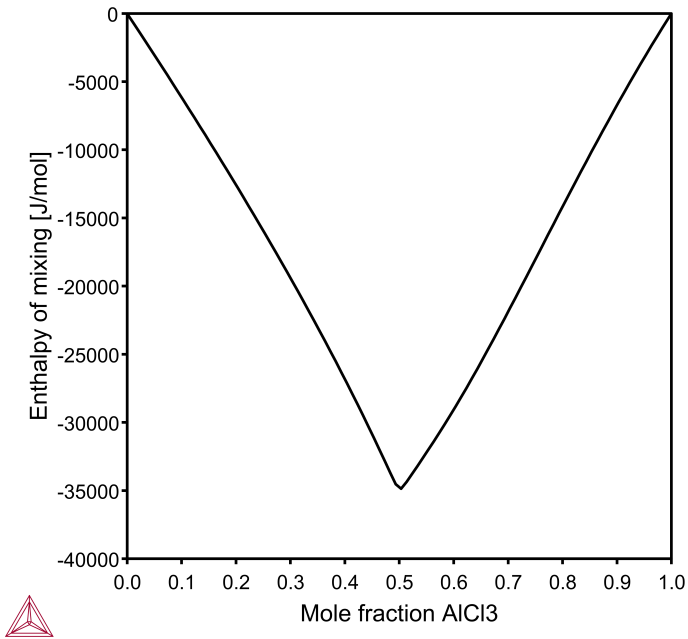


Figure 7: Calculated enthalpy of mixing of liquid  $AlCl_3$ - $NaCl$  solution at 800 K.

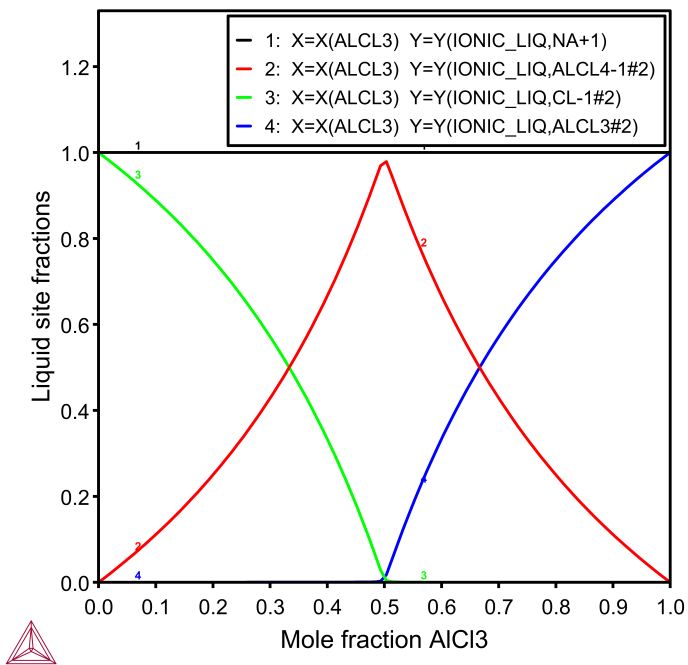


Figure 8: Calculated site fractions of liquid  $AlCl_3$ - $NaCl$  solution at 800 K.

### AlCl<sub>3</sub>-KCl-NaCl

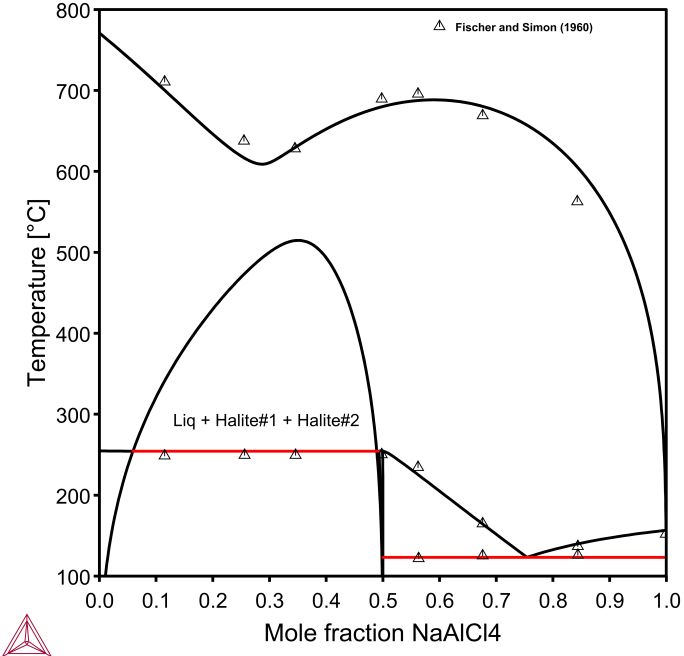


Figure 9: Calculated KCl-NaAlCl<sub>4</sub> phase diagram with experimental data from [1960Fis].

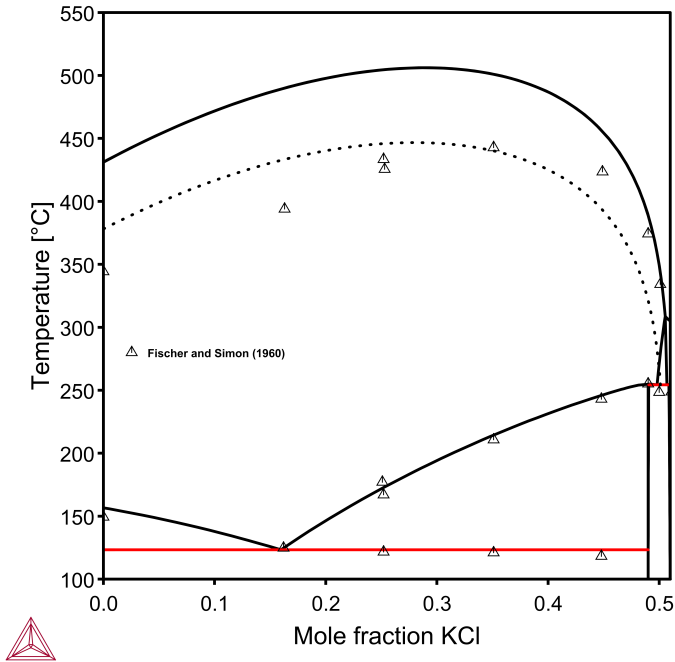


Figure 10: Calculated AlCl<sub>3</sub>-NaCl-KCl section at a constant 49% AlCl<sub>3</sub> with experimental data from [1960Fis]. The liquidus calculated at 49.54% AlCl<sub>3</sub> is shown as a dotted line.

### AlCl<sub>3</sub>-AlF<sub>3</sub>-KCl-KF

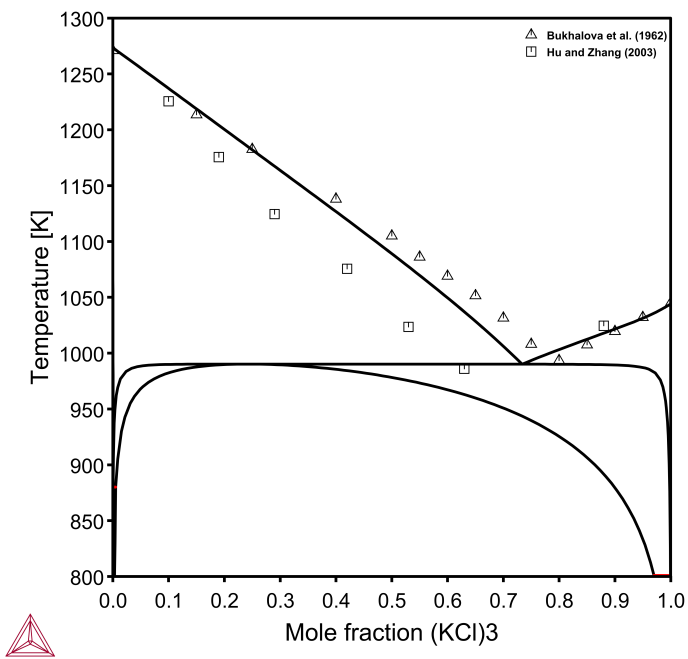



Figure 11: Calculated pseudo-binary system for K<sub>3</sub>AlF<sub>6</sub>-3KCl system with experimental data [1962Buk; 2003Hu].

## References

- [1960Fis] W. Fischer, A. Simon, Über thermische Eigenschaften von Halogeniden. 15. Über das Schmelzdiagramm des Systems:  $\text{AlCl}_3 - \text{NaCl} - \text{KCl}$  (mit Beobachtungen bei der Elektrolyse von Natrium-aluminium-chlorid-Schmelzen). Zeitschrift für Anorg. und Allg. Chemie 306, 1–12 (1960).
- [2004Rob] C. Robelin, P. Chartrand, A. D. Pelton, Thermodynamic evaluation and optimization of the (NaCl + KCl +  $\text{AlCl}_3$ ) system. J. Chem. Thermodyn. 36, 683–699 (2004).
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## TCSALT Validation of Lithium (Li) Systems

Li can be substituted for Na/K. These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

 For additional calculation examples, see [TCSALT Examples of Lithium \(Li\) Systems](#)

### LiCl-MgCl<sub>2</sub>

Large uncertainties remain on the subliquidus equilibria, but it is clear that extensive solid solutions are present. MgCl<sub>2</sub> dissolves in solid LiCl, with the formation of cationic vacancies. For very dilute solutions, the Mg<sup>2+</sup> ions and vacancies are distributed independently on the lattice sites, giving rise to a large entropy term and stabilizing the solid solution relative to the liquid. This could account for the reported maximum in the liquidus near 1.6 pct MgCl<sub>2</sub>.

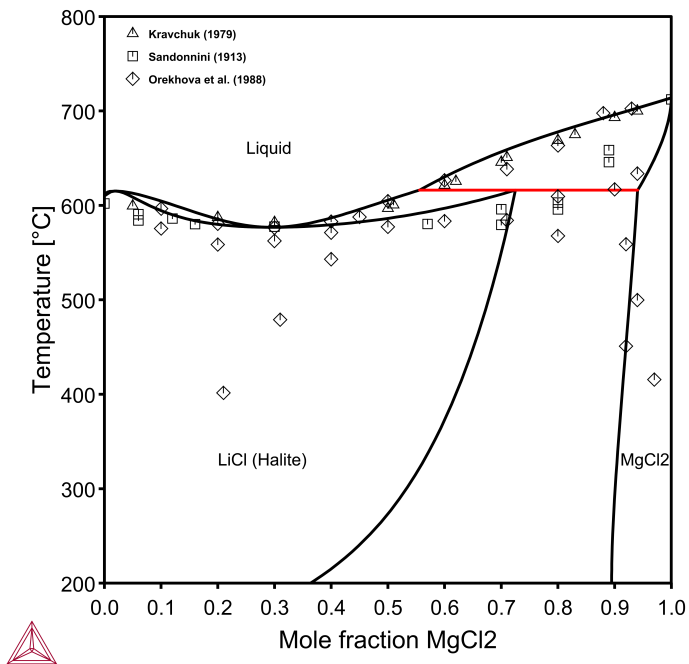


Figure 12: Calculated LiCl-MgCl<sub>2</sub> section with experimental data in [2001Pel].

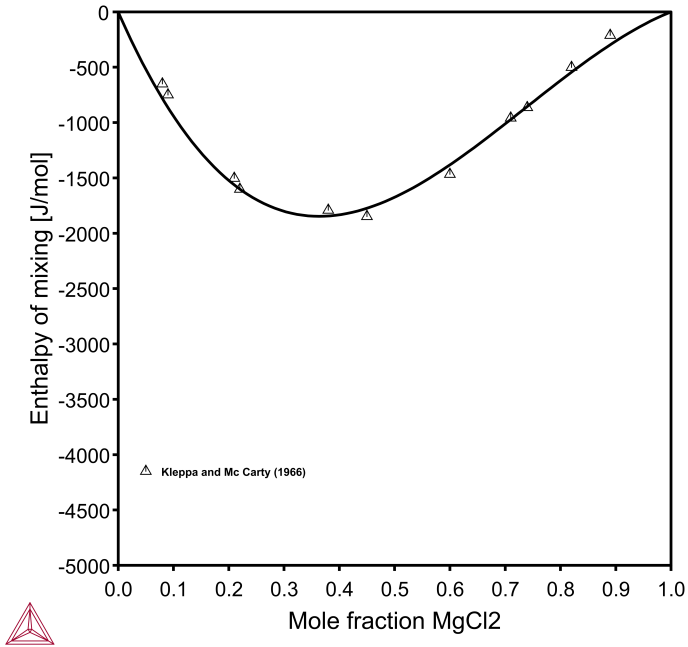


Figure 13: Calculated enthalpy of mixing of LiCl-MgCl<sub>2</sub> at 1003 K compared to experimental data in [2001Pe].

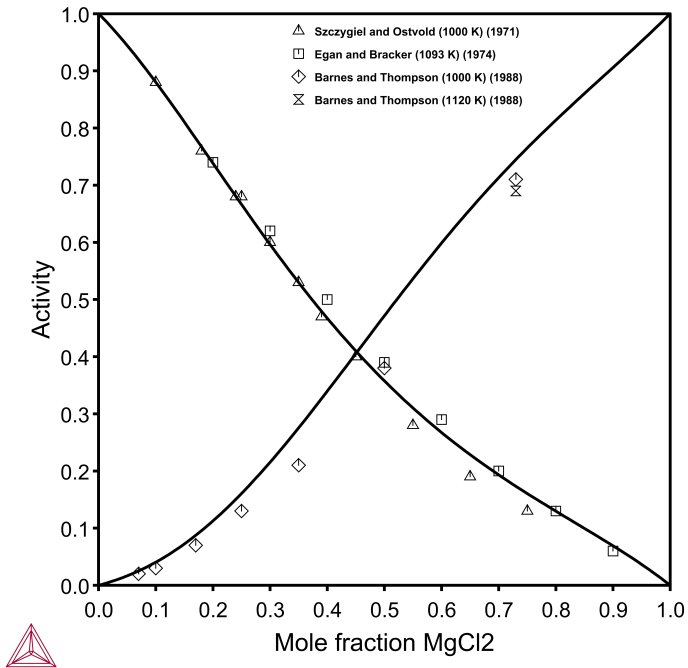


Figure 14: Calculated activities of LiCl-MgCl<sub>2</sub> in the liquid at 1023 K (liquid reference state) compared to experimental data in [2001Pe].

## KCl-LiCl-MgCl<sub>2</sub>

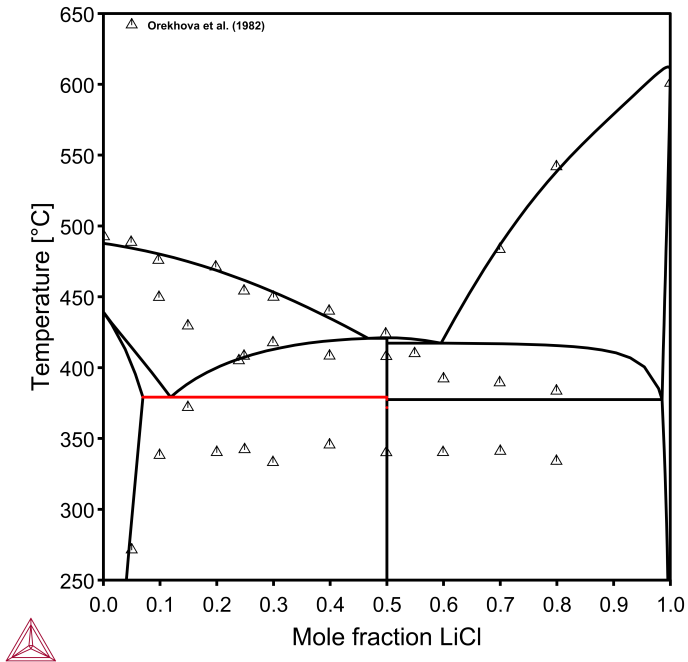


Figure 15: Calculated KMgCl<sub>3</sub>-LiCl section compared to experimental data in [1982Ore].

## References

- [1982Ore] A.I. Orekhova, N.P. Podlesnyak, L.Kh. Kvznetsova, N.A. Krasil'nikova, T.A. Puzanova, *Izv. Vyssh. Ucheb. Zaved., Tsv. Metall.* 4 (1982) 26-29
- [2001Pel] A. D. Pelton, P. Chartrand, Thermodynamic evaluation and optimization of the LiCl-NaCl-KCl-RbCl-CsCl-MgCl<sub>2</sub>-CaCl<sub>2</sub> system using the modified quasi-chemical model. *Metall. Mater. Trans. A* 32, 1361–1383 (2001).

## TCSALT Validation of KF-LiF-SrF<sub>2</sub> System

 For additional examples, see [TCSALT Strontium \(Sr\): LiCl-SrCl<sub>2</sub>-LiF-SrF<sub>2</sub>](#)

Seven sections of the KF-LiF-SrF<sub>2</sub> ternary system were measured by the visual-polythermal method using the TCS Molten Salts Database (TCSALT). The data points and calculated liquidus temperatures for some sections are compared to experimental data from [1960Buk].

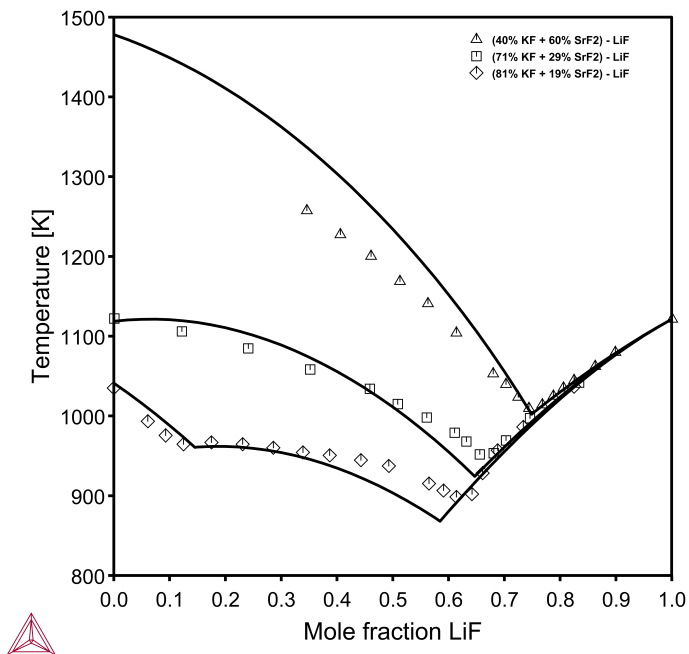


Figure 16: Calculated and experimental (40% KF + 60% SrF<sub>2</sub>)-LiF, (71% KF + 29% SrF<sub>2</sub>)-LiF and (81% KF + 19% SrF<sub>2</sub>)-LiF liquidus. Experimental data from [1960Buk].

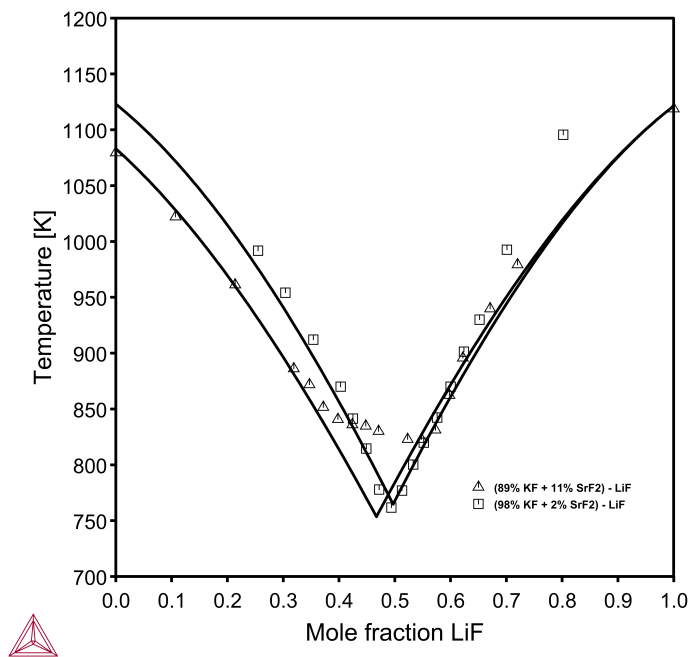


Figure 17: Calculated and experimental (89% KF + 11% SrF<sub>2</sub>)-LiF and (98% KF + 2% SrF<sub>2</sub>)-LiF liquidus [need references]. Experimental data from [1960Buk].

## Reference

[1960Buk] V. T. Berezhnaya, G. A. Bukhalova, Russ. J. Inorg. Chem. 5, 445–446 (1960).

## TCSALT Silicon (Si): NaF-SiF<sub>4</sub>

Oxyfluoride melts could be of interest in geophysics or in the aluminium industry, which uses a cryolite-based electrolyte (NaF + AlF<sub>3</sub> with additives) as a solvent for alumina in the aluminium production process. Moreover, in Al-electrolysis cells, the corrosion of the silica-rich refractory materials of the cathode lining is mainly due to the penetration of the cryolite bath through the cathode carbon blocks. The Al-Na-Si-F-O system is the core system for such applications.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

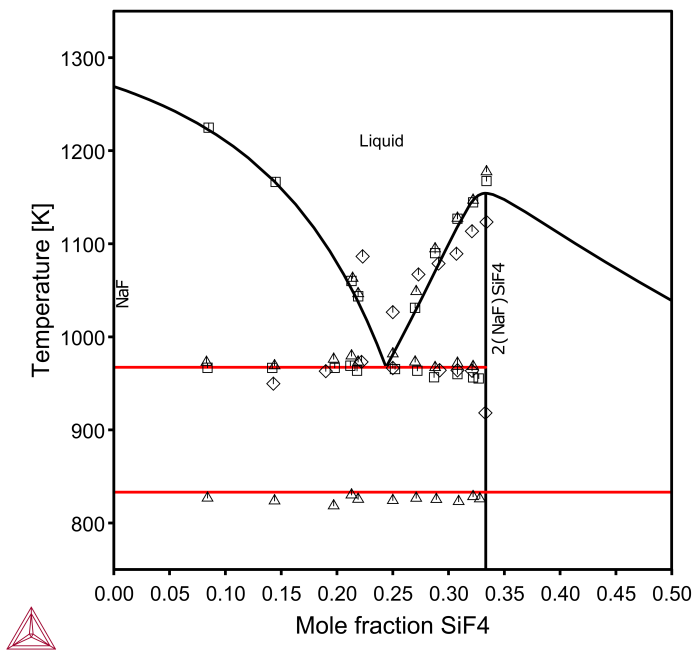


Figure 18: Calculated NaF-SiF<sub>4</sub> section with experimental data from [1971Che; 1981Chi].

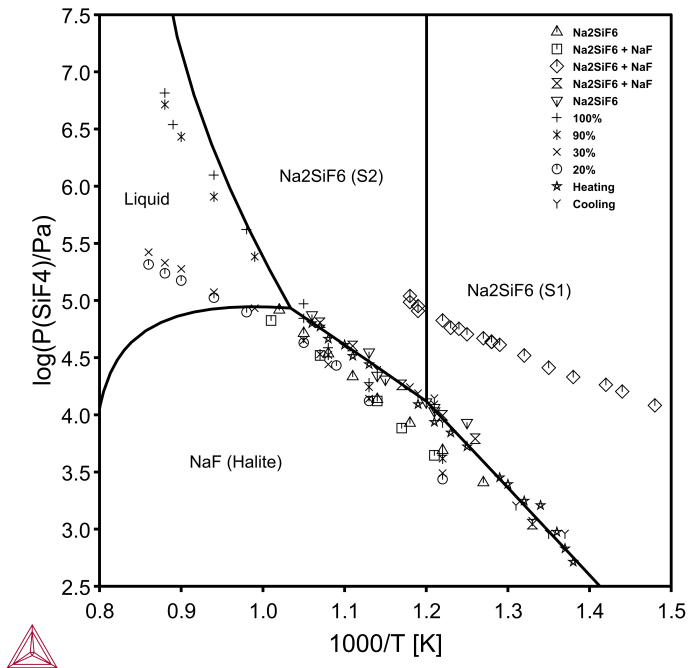



Figure 19: Calculated partial pressure of  $\text{SiF}_4$  with experimental data from [1926Han; 1945Cai; 1971Che; 1981Chi].

## References

- [1926Han] G. Hantke, Die thermische Dissoziation einiger Silicofluoride. *Angew. Chemie* 39, 1065–1071 (1926).
- [1945Cai] R. Caillat, *Ann. Chim.* 20, 367–420 (1945).
- [1971Che] R. V. Chernov, Y. K. Delimarskii, I. G. Kovzun, *Ukrainian Chem. J. (Ukr. Khim. Zh. Russ. Ed.)* 37, 984–988 (1971).
- [1981Chi] P. Chiotti, The pseudobinary system NaF-Na<sub>2</sub>SiF<sub>6</sub>. *J. Less Common Met.* 80, 105–113 (1981).

## TCSALT Validation of KCl-ZnCl<sub>2</sub> System

There is considerable interest in the application of molten salt reactions using Zn chloride. These examples using the TCS Molten Salts Database (TCSALT) show calculations for the KCl-ZnCl<sub>2</sub> system along with some validation of the results compared to experimental data.

 For additional examples, see [TCSALT Zinc \(Zn\): KCl-NaCl-ZnCl<sub>2</sub>](#)

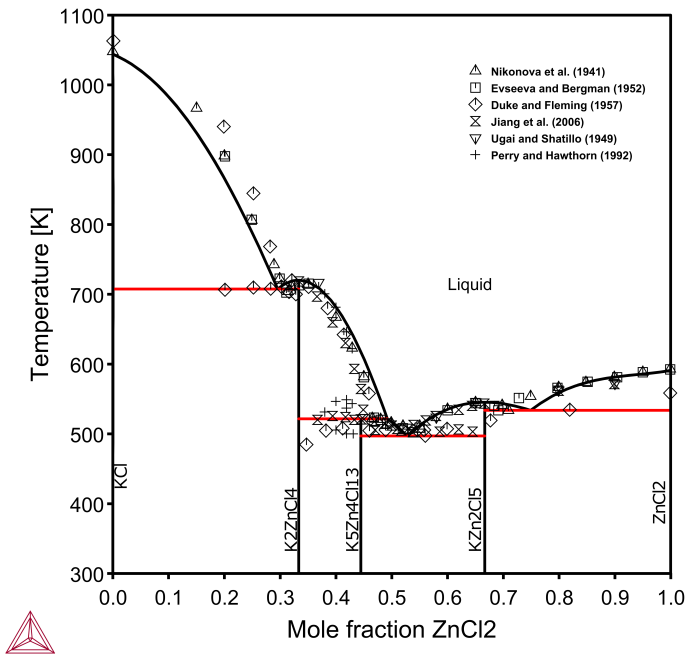


Figure 20: Calculated KCl-ZnCl<sub>2</sub> phase diagram compared to experimental data in [2014Man].

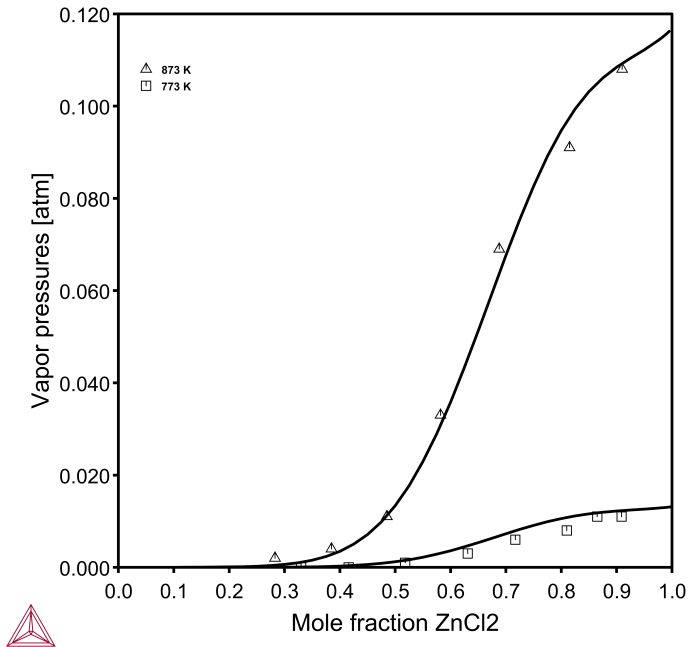


Figure 21: Vapour pressure of the KCl-ZnCl<sub>2</sub> liquid with experimental data from [1970Blo].

## References

- [1970Blo] H. Bloom, T. Spurling, J. Wong, Transpiration vapour pressures and activities in the molten salt systems ZnCl<sub>2</sub> + NaCl and ZnCl<sub>2</sub> + KCl. *Aust. J. Chem.* 23, 501–509 (1970).
- [2014Man] V. R. Manga, S. Bringuier, J. Paul, S. Jayaraman, P. Lucas, P. Deymier, K. Muralidharan, Molecular dynamics simulations and thermodynamic modeling of NaCl–KCl–ZnCl<sub>2</sub> ternary system. *Calphad* 46, 176–183 (2014).

## TCSALT Neodymium (Nd): KCl-NdCl<sub>3</sub>

Neodymium is a metal that is widely used in the field of key rare-earth functional materials, such as NdFeB magnetic materials, rare-earth alloys, and rare-earth hydrogen-storage materials. The main preparation method is molten salt electrolysis, and the electrolytic system mainly includes chloride and fluoride salt systems.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for the KCl-NdCl<sub>3</sub> system along with some validation of the results compared to experimental data.

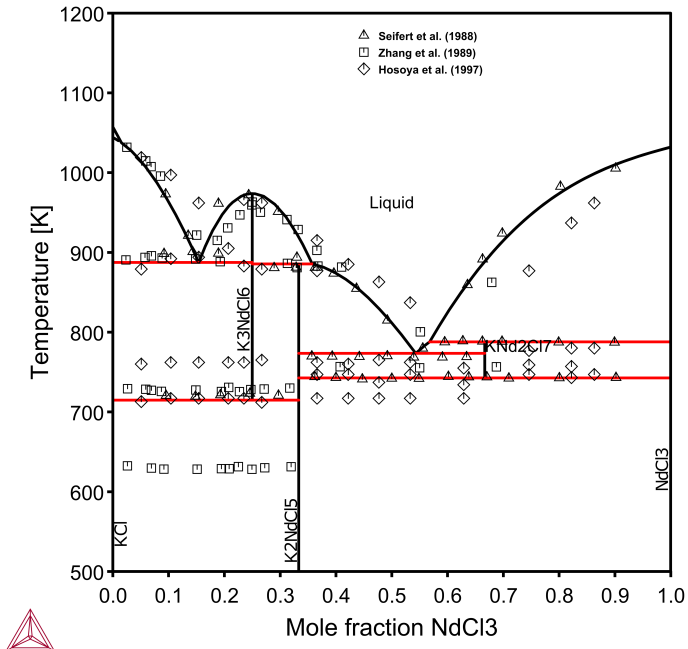


Figure 22: Calculated KCl-NdCl<sub>3</sub> section with experimental data in [2023Hao].

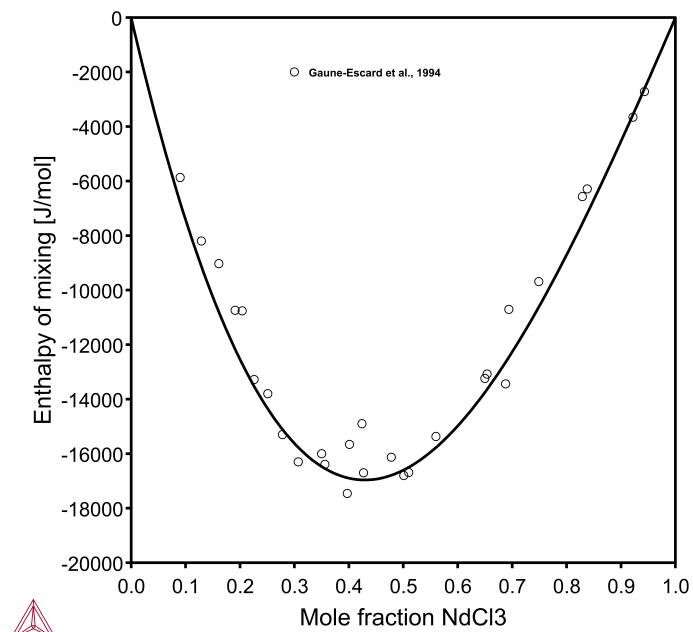


Figure 23: Calculated enthalpy of mixing at 1065 K with data in [2023Hao].

## Reference

[2023Hao] L. Hao, S. Sridar, W. Xiong, Thermodynamic description of molten salt systems: KCl-LiCl-NaCl and KCl-LiCl-NdCl<sub>3</sub>. *J. Mol. Liq.* 382, 121869 (2023).

## TCSALT Validation for Oxygen (O) Systems

Aluminum is highly reactive with oxygen, and such oxides can no longer be reduced in conventional recycling cycles. Therefore, reactions with oxygen play a special role in the field of recycling. Oxygen itself is practically insoluble as a gas in liquid aluminum. Oxidation of an aluminum melt takes place above 727 °C. Due to its high affinity for oxygen, an oxide layer forms instantly on fresh surfaces of solid and liquid aluminum in air. This layer is dense and protects the aluminum from further oxidation. The reaction takes place with atmospheric oxygen and humidity.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

### CaCl<sub>2</sub>-CaO

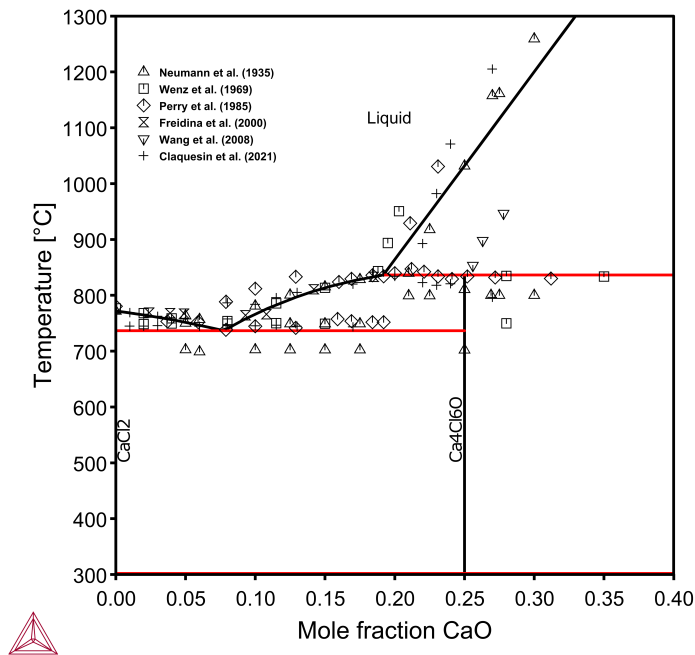


Figure 24: Calculated CaCl<sub>2</sub>-CaO phase diagram compared to experimental data in [2021Cla].

## LiCl-Li<sub>2</sub>O

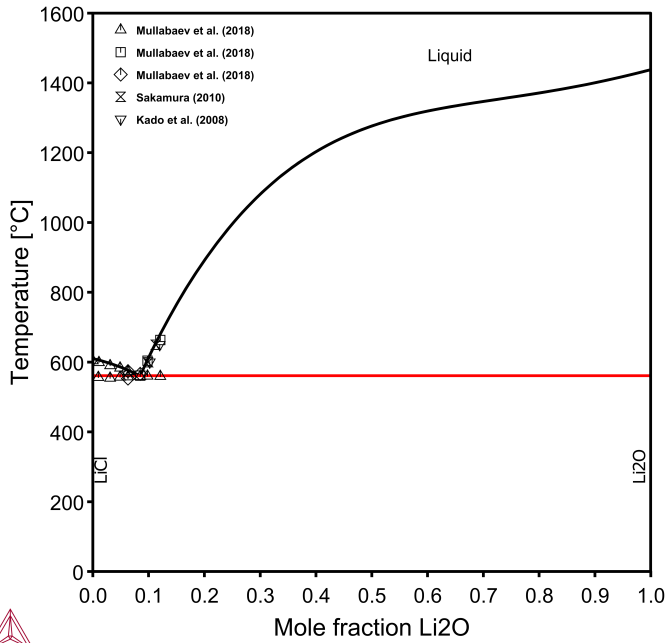


Figure 25: Calculated and experimental LiCl-Li<sub>2</sub>O section [2008Kad; 2010Sak; 2018Mul].

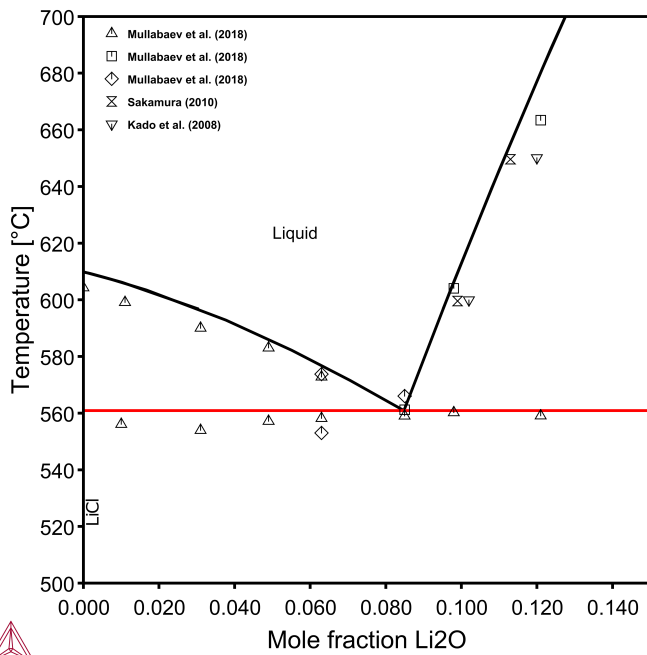


Figure 26: A zoomed in section of the previous plot of the calculated and experimental LiCl-Li<sub>2</sub>O section [2008Kad; 2010Sak; 2018Mul].

## CaCl<sub>2</sub>-CaF<sub>2</sub>-CaO

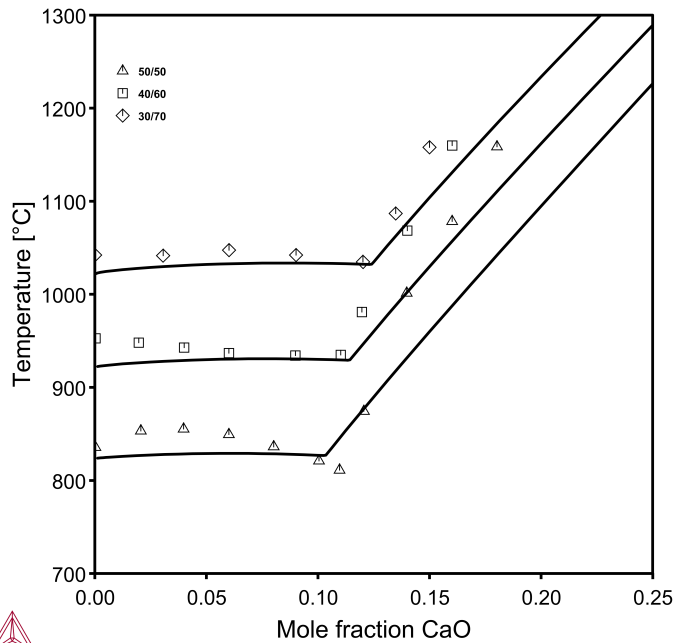


Figure 27: Liquidus at different CaCl<sub>2</sub>-CaF<sub>2</sub> ratio (50/50, 40/60, 30/70 mol-%) with experimental data [2021Cla].

## References

- [2008Kad] Y. Kado, T. Goto, R. Hagiwara, Dissolution Behavior of Lithium Oxide in Molten LiCl-KCl Systems. J. Chem. Eng. Data 53, 2816–2819 (2008).
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- [2021Cla] J. Claquesin, M. Gibilaro, L. Massot, O. Lemoine, G. Bourges, P. Chamelot, Thermodynamic Properties of CaCl<sub>2</sub>-CaF<sub>2</sub>-CaO System: Phase Diagram Investigation. Mater. Sci. Appl. 12, 139–151 (2021).

## TCSALT Validations Examples with CO<sub>3</sub>

Molten carbonate salts (containing CO<sub>3</sub><sup>2-</sup>) are high-temperature electrolytes primarily used for electrochemical capture/conversion into solid carbon, and as heat transfer fluids in concentrated solar power (CSP).

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

### Li<sub>2</sub>CO<sub>3</sub>-Na<sub>2</sub>CO<sub>3</sub>

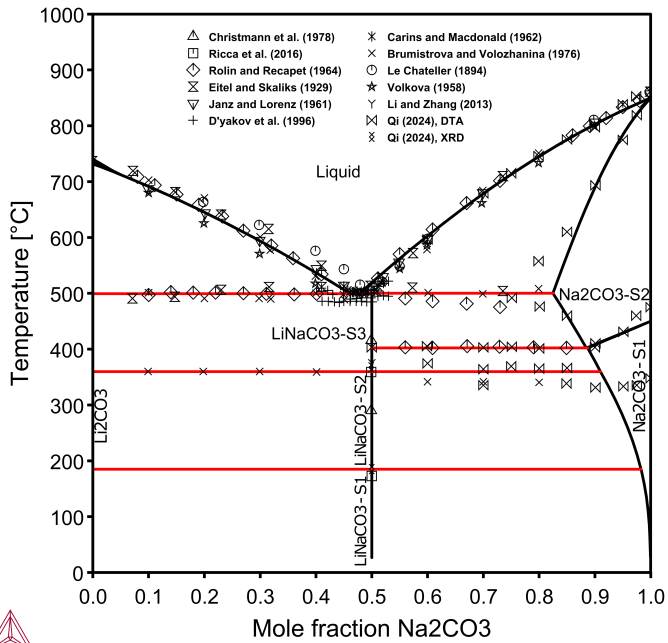


Figure 28: Calculated Li<sub>2</sub>CO<sub>3</sub>-Na<sub>2</sub>CO<sub>3</sub> section with experimental data in [2024Qi].

### K<sub>2</sub>CO<sub>3</sub>-KCl

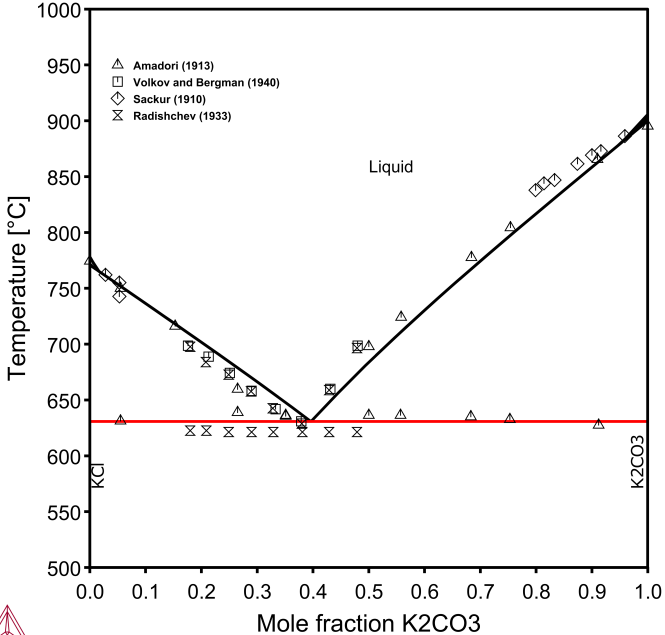


Figure 29: Calculated KCl-K<sub>2</sub>CO<sub>3</sub> section with experimental data in [2024Qi].

### K<sub>2</sub>CO<sub>3</sub>-Li<sub>2</sub>CO<sub>3</sub>-Na<sub>2</sub>CO<sub>3</sub>

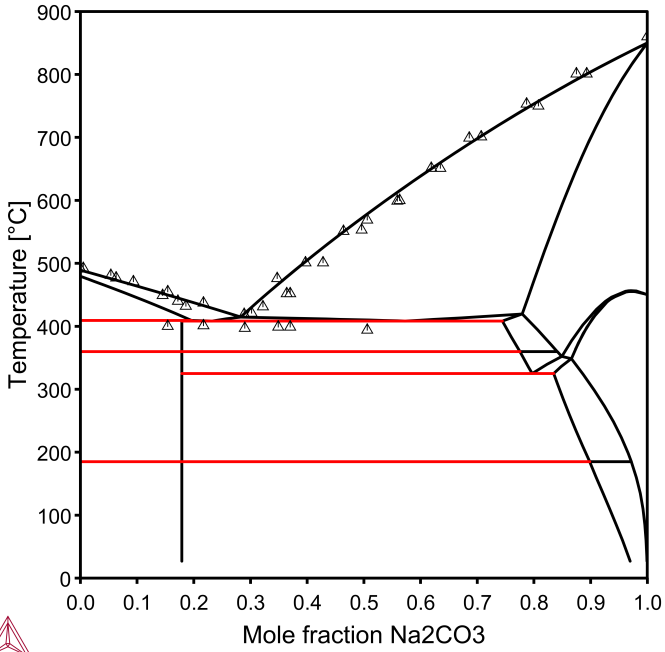


Figure 30: Calculated section Na<sub>2</sub>CO<sub>3</sub>-Li<sub>1.218</sub>K<sub>0.782</sub>CO<sub>3</sub> with experimental data from [2024Qi].

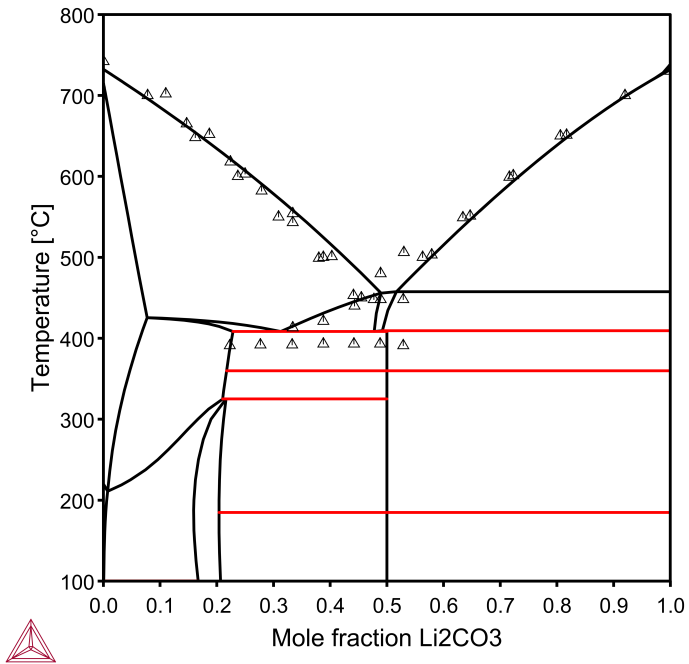


Figure 31: Calculated section  $\text{Li}_2\text{CO}_3\text{-Na}_{1.446}\text{K}_{0.554}\text{CO}_3$  with experimental data from [2024Qi].

## Reference

[2024Qi] J. Qi, Thermodynamics of salt system:  $\text{Li}^+$ ,  $\text{K}^+$ ,  $\text{Na}^+$  //  $\text{Cl}^-$ ,  $\text{CO}_3^{2-}$ , PhD thesis, RWTH Aachen (2024).

## TCSALT Validation Examples with SO<sub>4</sub>

Sulfate (SO4-2) molten salts, such as Na<sub>2</sub>SO<sub>4</sub>, K<sub>2</sub>SO<sub>4</sub> and Mg(SO<sub>4</sub>)<sub>2</sub>, are high-temperature ionic liquids commonly used in solar energy storage, catalysis (e.g., sulfuric acid production), and as reaction media for synthesizing advanced ceramic or battery materials. They are characterized by high thermal stability, high heat-storage capacity, and potential for high-temperature corrosion.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

### K<sub>2</sub>SO<sub>4</sub>-CaSO<sub>4</sub>

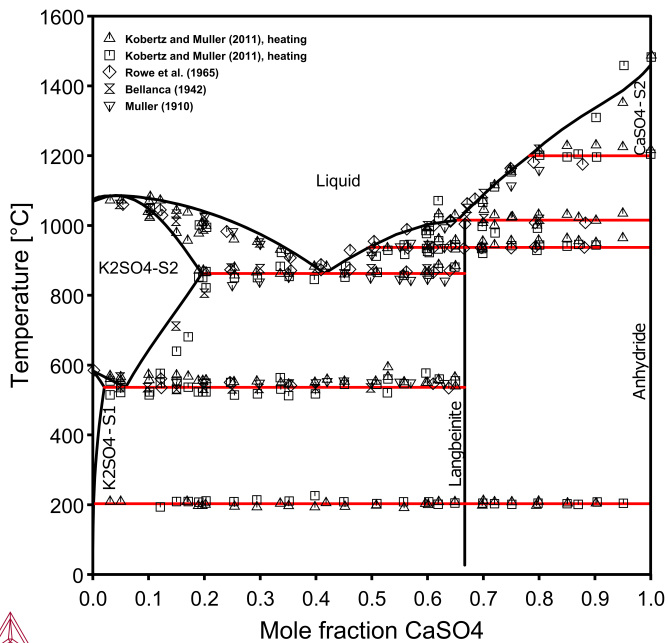


Figure 32: Calculated K<sub>2</sub>SO<sub>4</sub>-CaSO<sub>4</sub> section with experimental data in [2021Yaz].

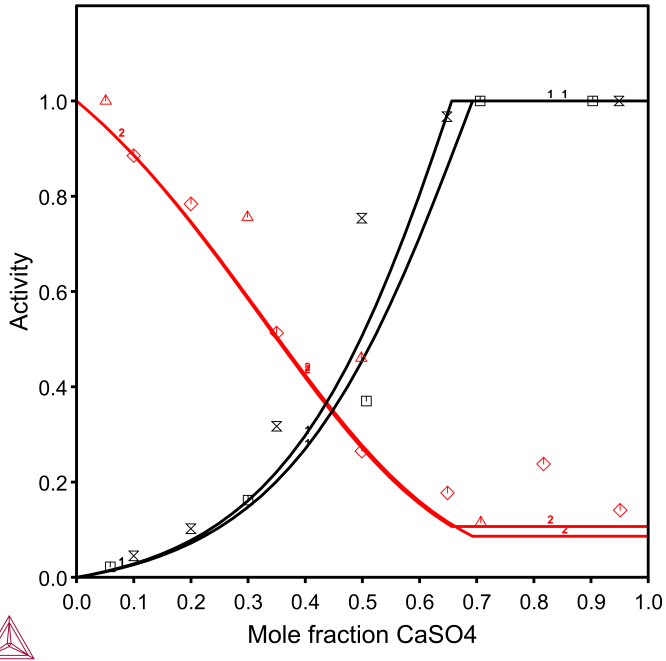


Figure 33: Calculated activities at 1020 °C and 1077 °C with experimental data in [2021Yaz].

### K<sub>2</sub>SO<sub>4</sub>-Na<sub>2</sub>SO<sub>4</sub>

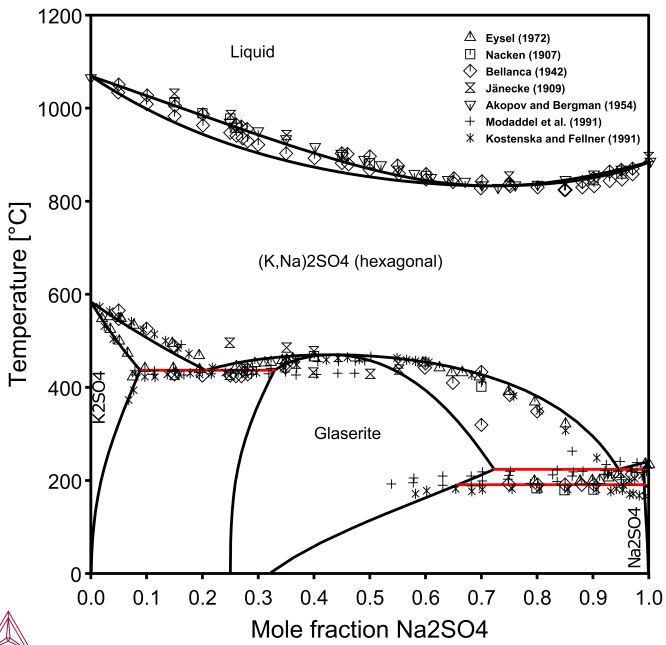


Figure 34: Calculated K<sub>2</sub>SO<sub>4</sub>-Na<sub>2</sub>SO<sub>4</sub> section with experimental data in [2021Yaz].

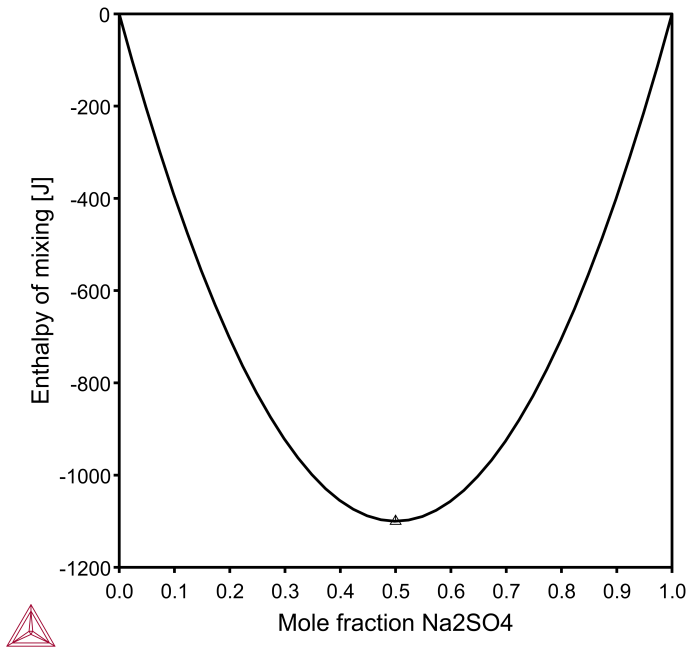


Figure 35: Calculated enthalpy of mixing of liquid phase for  $K_2SO_4$ - $Na_2SO_4$ , with experimental data in [2021Yaz].

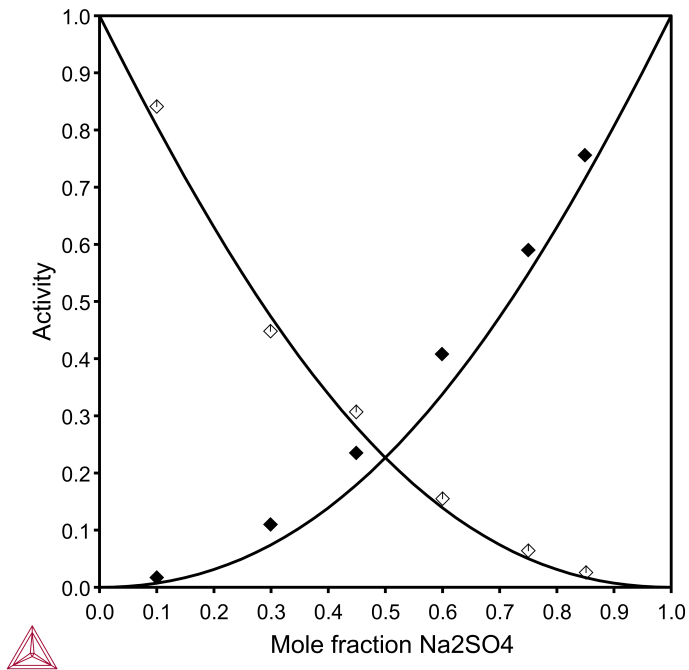


Figure 36: Calculated activity of liquid phase for  $K_2SO_4$ - $Na_2SO_4$ , with experimental data in [2021Yaz].

**K<sub>2</sub>SO<sub>4</sub>-K<sub>2</sub>CO<sub>3</sub>**

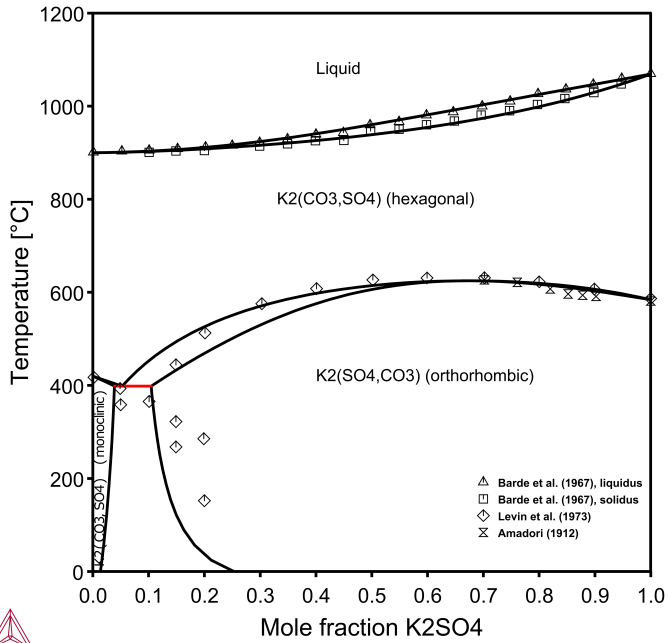


Figure 37: Calculated  $K_2CO_3$ - $K_2SO_4$  section with experimental data in [2007Lin].

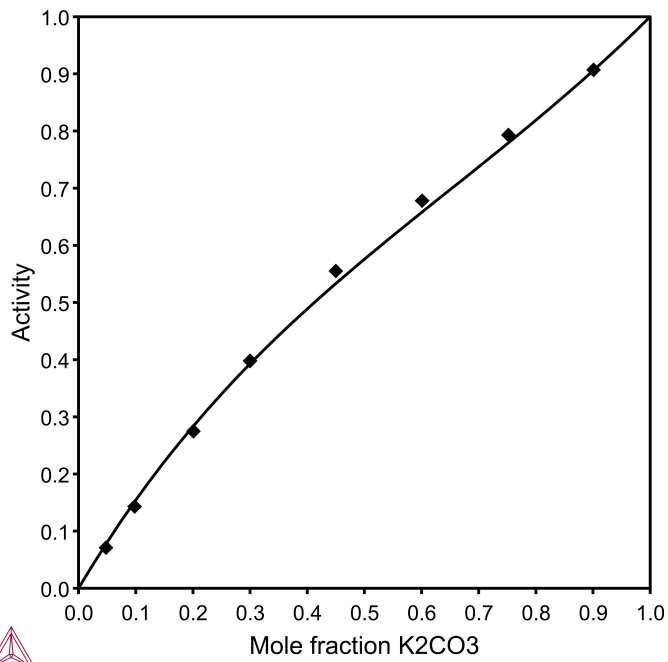


Figure 38: Calculated activity at 1073 K, with experimental data in [2007Lin].

## CaSO<sub>4</sub>-K<sub>2</sub>SO<sub>4</sub>-MgSO<sub>4</sub>

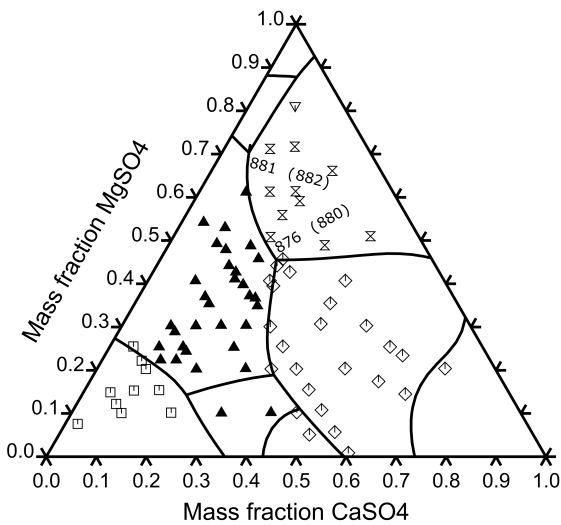


Figure 39: Calculated liquidus projection. Calculated invariant temperatures with experimental data from [1967Row].

## References

- [1967Row] J. J. Rowe, G. W. Morey, C. C. Silber, The ternary system K<sub>2</sub>SO<sub>4</sub>-MgSO<sub>4</sub>-CaSO<sub>4</sub>. J. Inorg. Nucl. Chem. 29, 925–942 (1967).
- [2007Lin] D. Lindberg, R. Backman, P. Chartrand, Thermodynamic evaluation and optimization of the (Na<sub>2</sub>CO<sub>3</sub>+ Na<sub>2</sub>SO<sub>4</sub>+ Na<sub>2</sub>S + K<sub>2</sub>CO<sub>3</sub>+ K<sub>2</sub>SO<sub>4</sub>+ K<sub>2</sub>S) system. J. Chem. Thermodyn. 39, 942–960 (2007).
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## TCSALT Calculation Examples

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## TCSALT NaCl-KCl-NaF-KF Example

The NaCl-KCl-NaF-KF molten salt mixture is a reciprocal system and a core system in the TCS Molten Salts Database (TCSALT). It is designed to combine the low cost of chloride salts with the favorable heat transfer properties of fluorides. Example applications can be in electrochemical processing, thermal energy storage, and molten salt reactors.

 For additional examples of this same system, see [TCSALT Validation of NaCl-KCl-NaF-KF System](#)

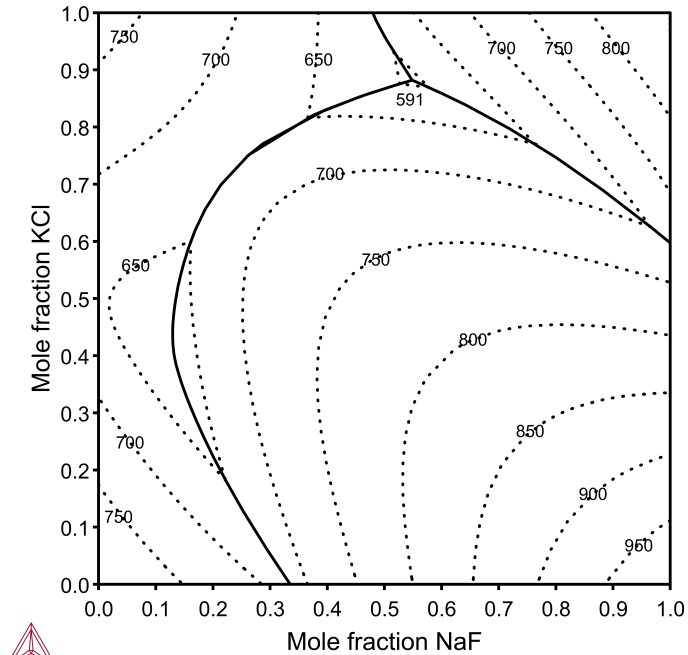


Figure 40: Calculated reciprocal KCl-KF-NaCl-NaF liquidus projection.

## TCSALT Calculations with Mg and Ca

Molten alkali-alkaline earth halide solutions are of much technological importance in, for example, the production of Mg and Na. A large amount of experimental thermodynamic and phase diagram data exists for these systems. NaCl, KCl, MgCl<sub>2</sub>, NaF, and KF are used extensively as fluxing agents for liquid aluminum treatment. For example, the electrolytes used for Mg production are based mainly on NaCl, CaCl<sub>2</sub>, and MgCl<sub>2</sub> salts, which can also be used as fluxes for Mg casting.

These examples using the TCS Molten Salts Database (TCSALT) are showing calculations of various systems, where some validation of the results are compared to experimental data.



For additional examples, see [TCSALT Validation for MgCl<sub>2</sub>-NaCl](#)

### CaCl<sub>2</sub>-CaF<sub>2</sub>-MgCl<sub>2</sub>-MgF<sub>2</sub>

The phase diagram of the CaCl<sub>2</sub>-CaF<sub>2</sub>-MgCl<sub>2</sub>-MgF<sub>2</sub> reciprocal ternary system was calculated thermodynamically from available data on the binary subsystems and from available data on the CaCl<sub>2</sub>-MgF<sub>2</sub> join. This join is very nearly quasi-binary (appr 1% MgCl<sub>2</sub> calculated in CaCl<sub>2</sub> solution) and divides the system into two quasi-ternary systems: the CaCl<sub>2</sub>-MgF<sub>2</sub>-CaF<sub>2</sub> system with a ternary eutectic calculated at 639 °C and a peritectic at 717 °C, and the CaCl<sub>2</sub>-MgF<sub>2</sub>-MgCl<sub>2</sub> system with a ternary eutectic calculated at 567 °C.

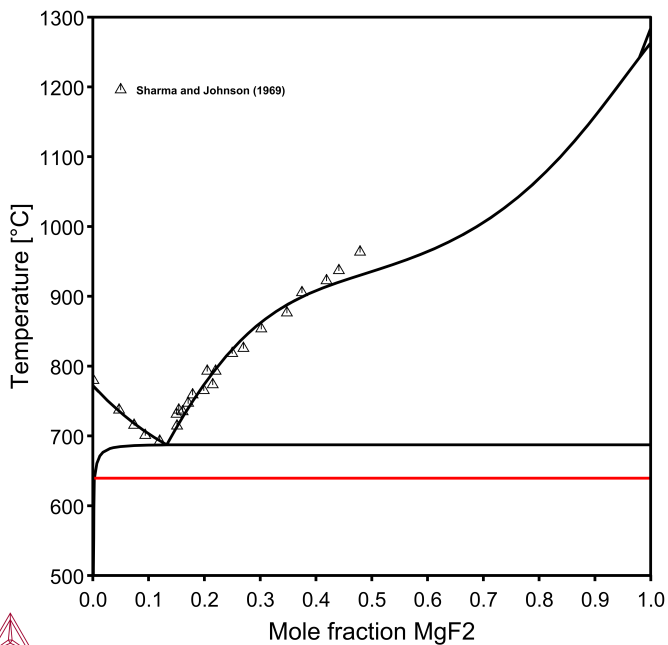


Figure 41: Calculated CaCl<sub>2</sub>-MgF<sub>2</sub> “binary” system with experimental data from [1969Sha].

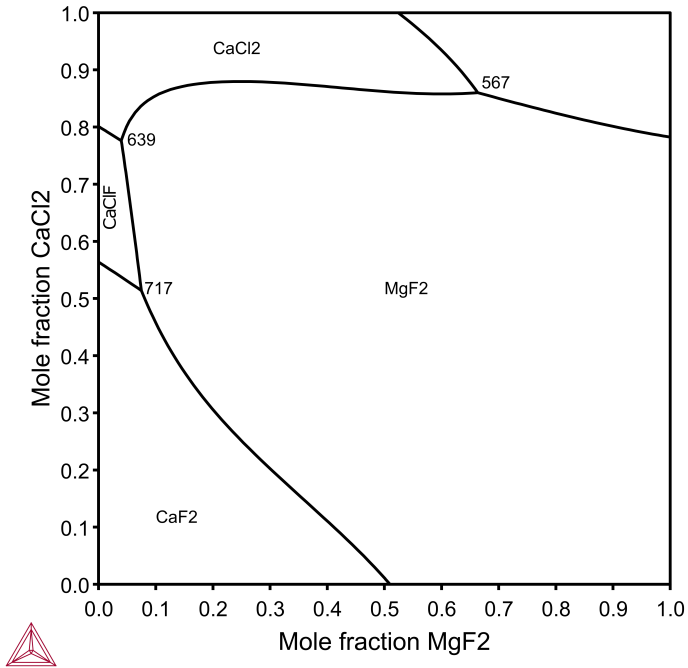


Figure 42: Calculated liquidus projection of the  $\text{CaF}_2$ - $\text{MgF}_2$ - $\text{CaCl}_2$ - $\text{MgCl}_2$  system. The temperature is in  $^\circ\text{C}$ .

### CaCl<sub>2</sub>-CaF<sub>2</sub>-KCl-KF-NaCl-NaF

Molten salts used in metallurgical applications are often based on alkali-earth chloride fluoride mixtures. For instance, such molten salts can be used as fluxes for metal treatment.

Only extrapolation from binary, ternary and reciprocal systems. The agreement is very good.

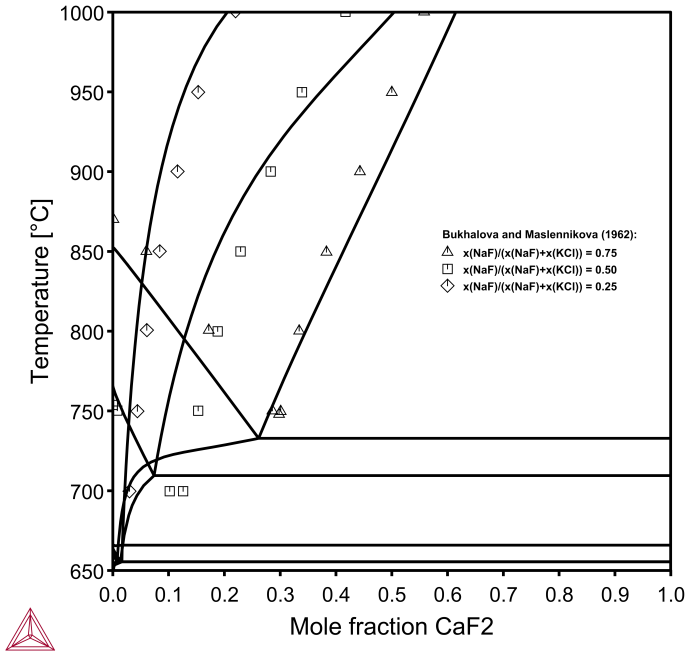


Figure 43: Calculated liquidus of the 2(NaF)-2(KCl)-CaF<sub>2</sub> isopleth for constant NaF/(NaF+KCl) molar ratios of 0.25, 0.5, and 0.75 [1962Buk].

## References

- [1962Buk] G.A. Bukhalova, G.N. Maslennikova, D.M. Rabkin, Russ. J. Inorg. Chem. 7 (1962) 847-849.
- [1969Sha] R. A. SHARMA, I. JOHNSON, Phase Diagrams for the Systems MgCl<sub>2</sub>-MgF<sub>2</sub>, CaCl<sub>2</sub>-MgF<sub>2</sub>, and NaCl-MgF<sub>2</sub>. J. Am. Ceram. Soc. 52, 612–615 (1969).

## TCSALT Examples Related to Aluminum Production

Chloroaluminate melts are of considerable industrial interest. They may be used as electrolytes to produce aluminum. NaF, CaF<sub>2</sub>, LiF, and MgF<sub>2</sub> are important components in the Hall-Heroult electrolysis cells for Al production.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various aluminum systems.

 For additional examples, see [TCSALT Validations for Aluminum \(Al\) Systems](#)

### AlCl<sub>3</sub>-KCl-NaCl

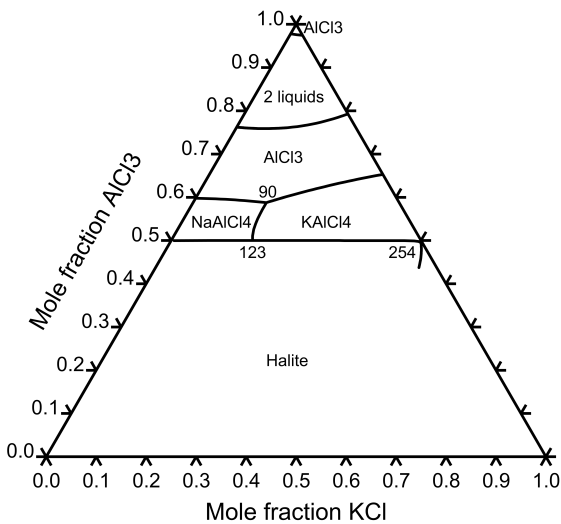


Figure 44: Calculated liquidus projection of the AlCl<sub>3</sub>-NaCl-KCl system.

### AlF<sub>3</sub>-KF-NaF

The development of low-temperature aluminium electrolysis makes it possible to reduce energy consumption and greenhouse gas emissions. The KF-NaAlF<sub>3</sub>-based electrolyte is a promising low-temperature electrolyte for aluminium reduction.

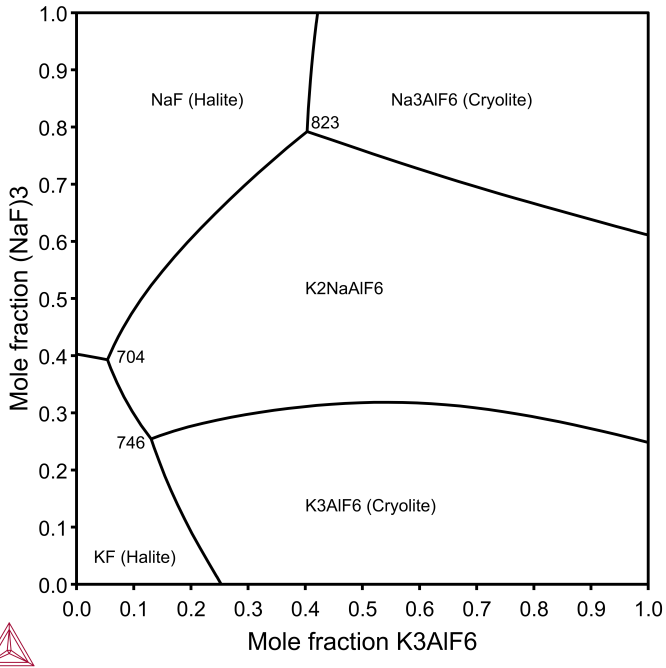


Figure 45: Calculated  $K_3F_3$ - $K_3AlF_6$ - $Na_3F_3$ - $Na_3AlF_6$  liquidus projection.

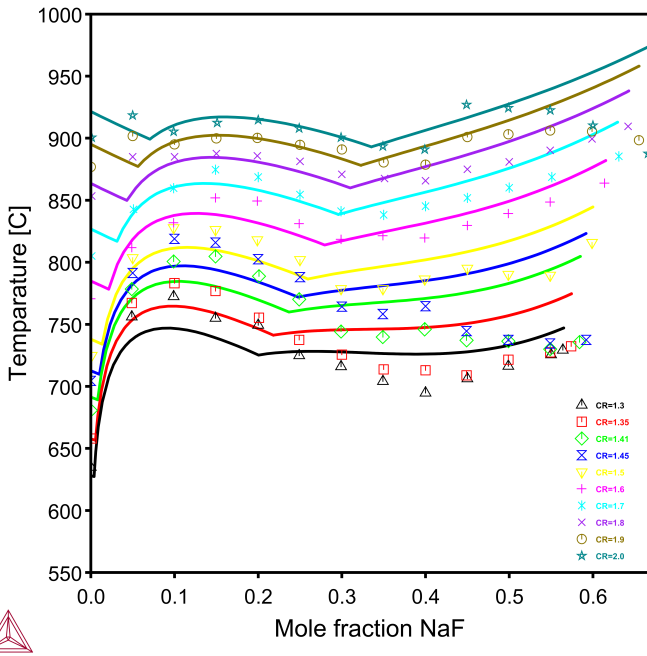


Figure 46: Calculated liquidus at CR=1.3-2. Experimental points are liquidus temperatures. CR is the Cryolite ratio:  $([NaF]+[KF])/[AlF_3]$ . Experimental data from [2020Yan].

## Reference

[2020Yan] H. Yan, Z. Liu, W. Ma, L. Huang, C. Wang, Y. Liu, KF-NaF-AlF<sub>3</sub> System: Liquidus Temperature and Phase Transition. JOM 72, 247–252 (2020).

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## TCSALT Examples of Lithium (Li) Systems

Li can be substituted for Na/K.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for various systems along with some validation of the results compared to experimental data.

 For additional examples, see [TCSALT Validation of Lithium \(Li\) Systems](#)

### KCl-LiCl-MgCl<sub>2</sub>

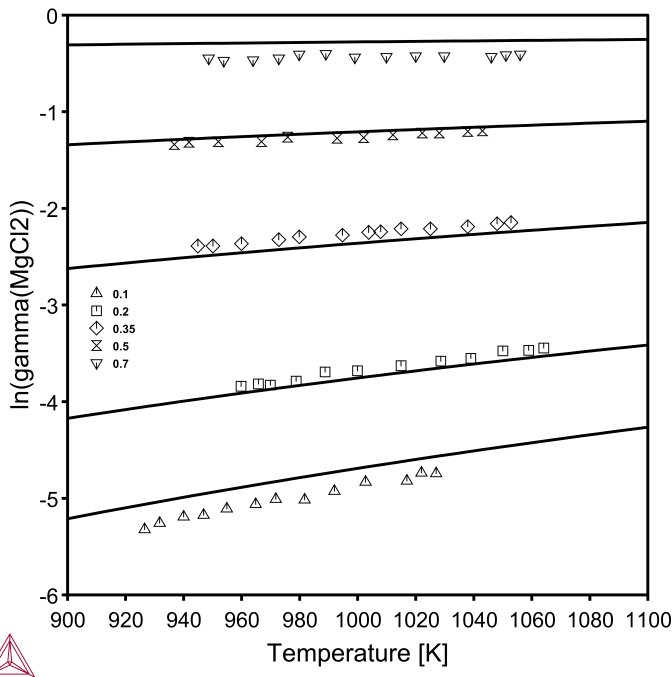


Figure 47: Calculated activity coefficient of MgCl<sub>2</sub> in the liquid for a LiCl/(LiCl+KCl) molar ratio of 2/3. Experimental data from [1995Dav].

### CaCl<sub>2</sub>-KCl-LiCl-CaF<sub>2</sub>-KF-LiF

Various quaternary reciprocal sections of the LiF-KF-CaF<sub>2</sub>-LiCl-KCl-CaCl<sub>2</sub> system have been measured by the visual-polythermal method. Points extracted from reported liquidus projections on these sections are shown on the calculated liquidus below.

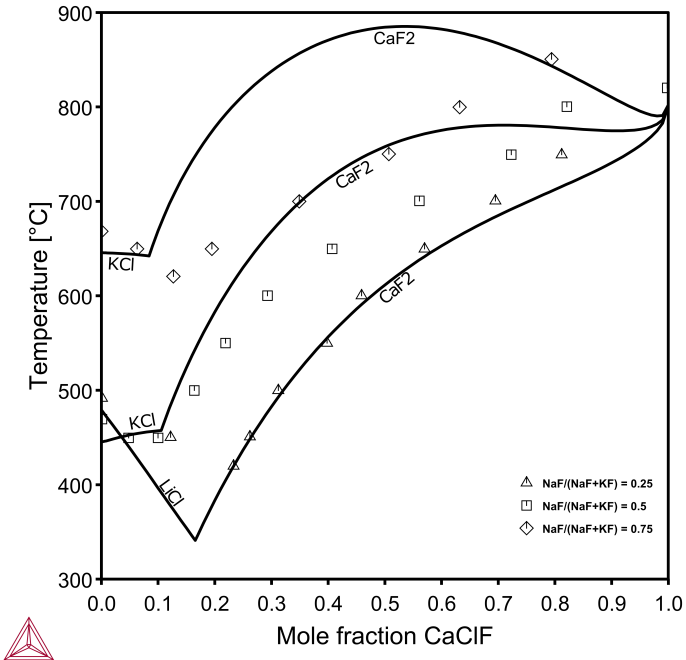


Figure 48: LiF-KF-CaF<sub>2</sub>-LiCl-KCl-CaCl<sub>2</sub> system: calculated liquidus lines of the LiCl-KCl-CaCl<sub>2</sub> isopleth for constant LiCl/(LiCl + KCl) molar ratios of 0.25, 0.50, and 0.75 (labels on lines indicate the primary solid phases). Experimental data from [1964Zak].

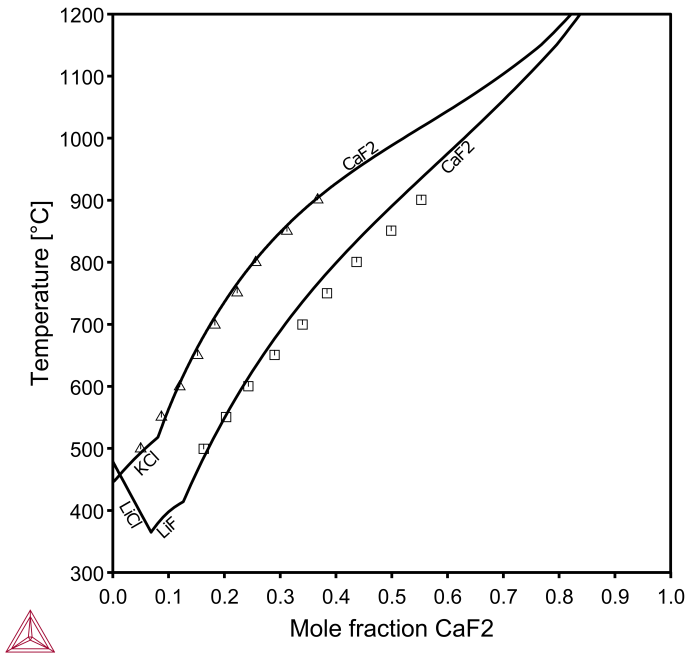


Figure 49: LiF-KF-CaF<sub>2</sub>-LiCl-KCl-CaCl<sub>2</sub> system: calculated liquidus lines of the LiCl-KCl-CaF<sub>2</sub> isopleth for constant LiCl/(LiCl + KCl) molar ratios of 0.50, and 0.75 (labels on lines indicate the primary solid phases). Experimental data from [1964Zak].

## References

- [1964Zak] M. A. Zakharchenko, N. V. Belogorskaya, S. M. Aslanov, Russ. J. Inorg. Chem. 9, 93–95 (1964).
- [1995Dav] B. R. Davis, W. T. Thompson, Thermodynamic Properties of Magnesium Chloride-Alkali Chloride (MgCl<sub>2</sub>-LiCl-KCl) Electrolytes. Can. Metall. Q. 34, 347–352 (1995).

## TCSALT Strontium (Sr): LiCl-SrCl<sub>2</sub>-LiF-SrF<sub>2</sub>

Using the TCS Molten Salts Database (TCSALT) the calculated liquidus projection of the (LiF-LiCl-SrF<sub>2</sub>-SrCl<sub>2</sub>) system is shown together with the calculated and experimental temperatures of the ternary invariant points of the liquidus projection. Ten sections of the ternary reciprocal system were measured by the visual-polythermal method. Some sections are calculated with good agreement to the experimental data.

 For additional examples, see [TCSALT Validation of KF-LiF-SrF<sub>2</sub> System](#)

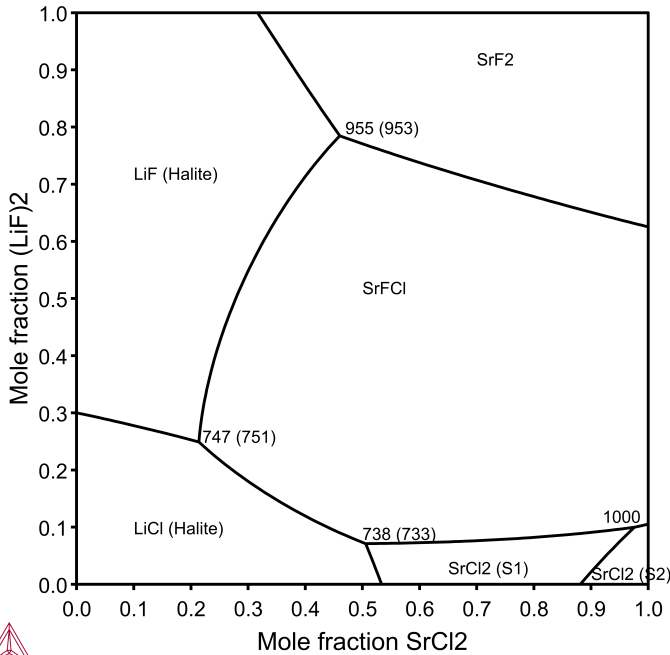


Figure 50: Calculated reciprocal LiF-LiCl-SrF<sub>2</sub>-SrCl<sub>2</sub> liquidus projection. Calculated and experimental[1954Ban] temperatures of the invariant points in Kelvin.

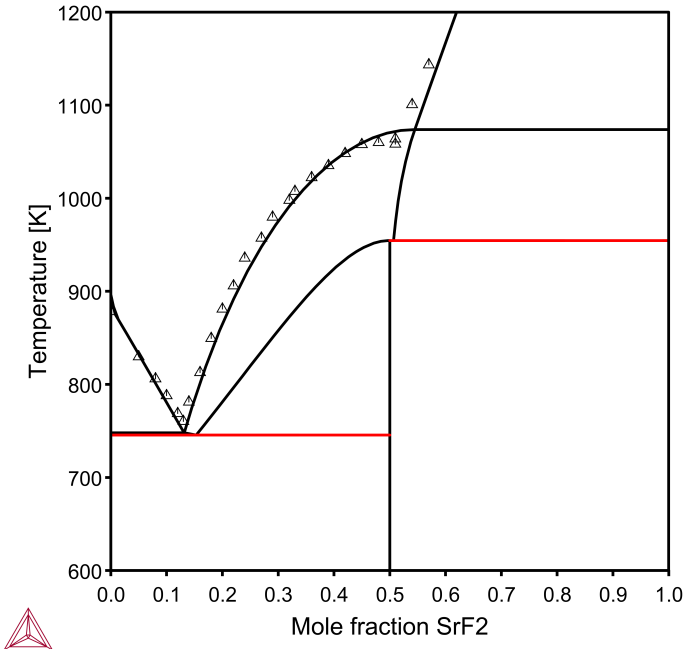


Figure 51: Calculated LiCl-SrF<sub>2</sub> section with experimental data from [1954Ban].

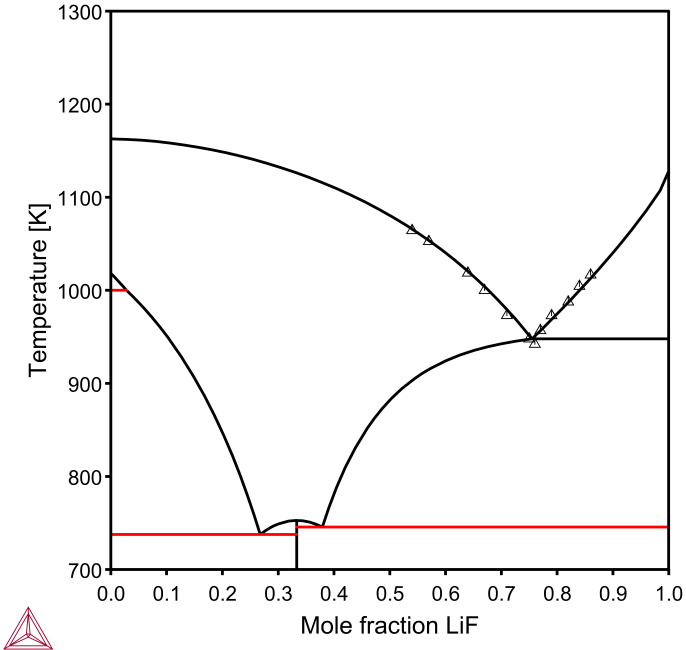


Figure 52: Calculated (75% SrCl<sub>2</sub> + 25% SrF<sub>2</sub>) - LiF section with experimental data from [1954Ban].

## **| Reference**

[1954Ban] E.I. Banashek, A.G. Bergman, *Izvest. Sektora Fiz.-Khim. Anal., Inst. Obshchei i Neorg. Khim., Akad. Nauk S.S.S.R.* 25 (1954) 245–254.

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## TCSALT Zinc (Zn): KCl-NaCl-ZnCl<sub>2</sub>

There is considerable interest in the application of molten salt reactions using Zn chloride.

These examples using the TCS Molten Salts Database (TCSALT) show calculations for the KCl-ZnCl<sub>2</sub> system along with some validation of the results compared to experimental data.

 For additional examples, see [TCSALT Validation of KCl-ZnCl<sub>2</sub> System](#)

One of these applications is the electrodeposition of refractory metals such as tungsten and molybdenum using molten ZnCl<sub>2</sub>-NaCl-KCl system as electrolyte. Interest in these systems is also related to the recycling of heavy-metal halide waste generated in industrial processes, which must consider phase equilibria for the prevention of environmental pollution and the recovery of resources.

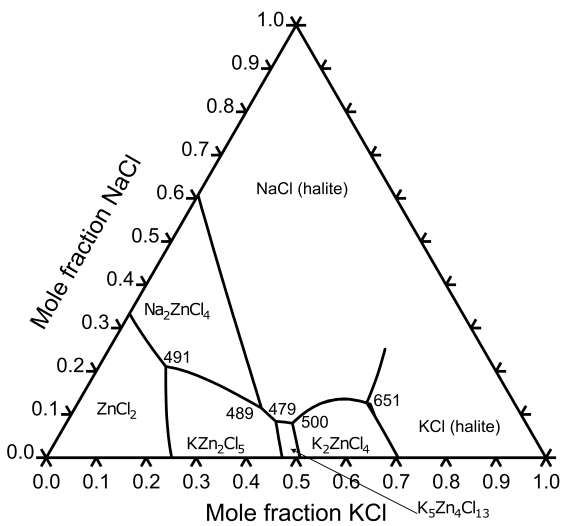


Figure 53: Calculated liquidus projection of the NaCl-KCl-ZnCl<sub>2</sub> ternary. Temperatures in Kelvin.

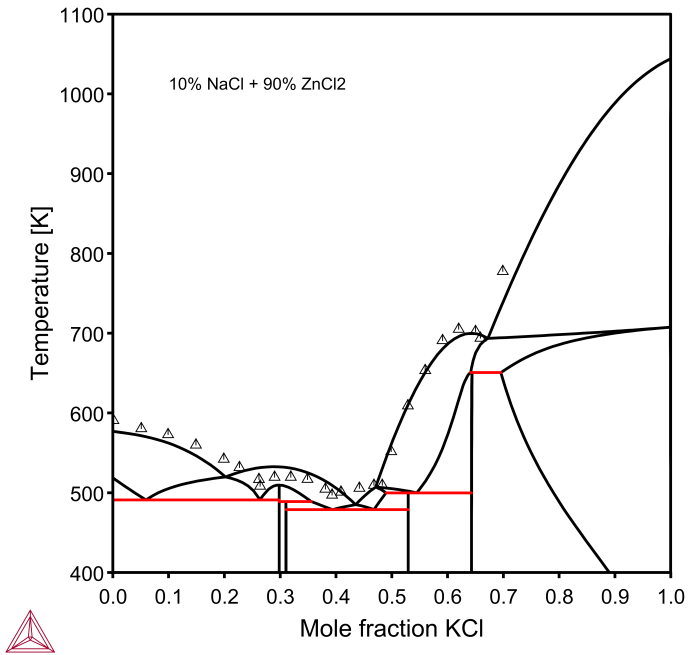


Figure 54: Calculated liquidus temperatures for (10% NaCl + 90% ZnCl<sub>2</sub>) - KCl section with experimental data from [1941Nik].

## Reference

[1941Nik] I. N. Nikonova, S. P. Pavlenko, A. G. Bergman, *Izv. Akad. Nauk SSSR Ser. Khim.* 3, 391–400 (1941).

## TCSALT Examples with NO<sub>2</sub> and NO<sub>3</sub>

Molten nitrate (NO<sub>3</sub>-1) and nitrite (NO<sub>2</sub>-1) salts are commonly used as high-temperature heat transfer fluids and thermal energy storage media.

### KNO<sub>2</sub>-KNO<sub>3</sub>

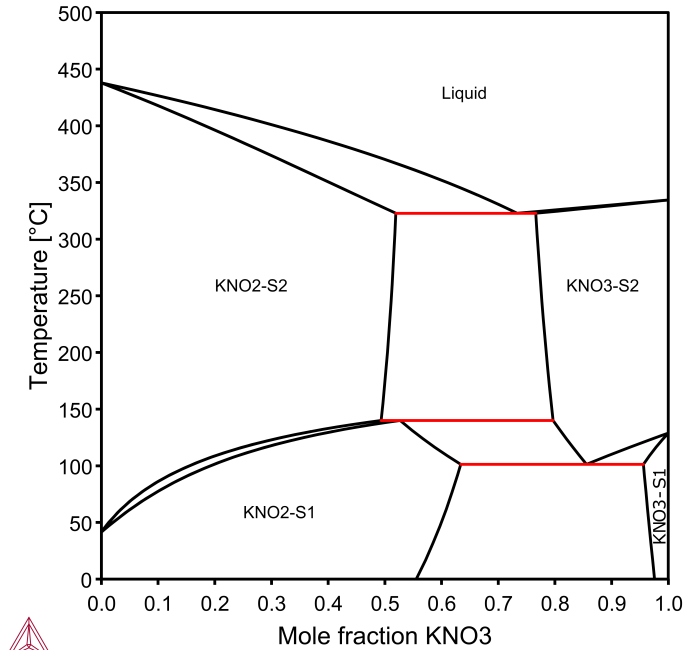


Figure 55: Calculated KNO<sub>2</sub>-KNO<sub>3</sub> section.

### KNO<sub>3</sub>-LiNO<sub>3</sub>-NaNO<sub>3</sub>

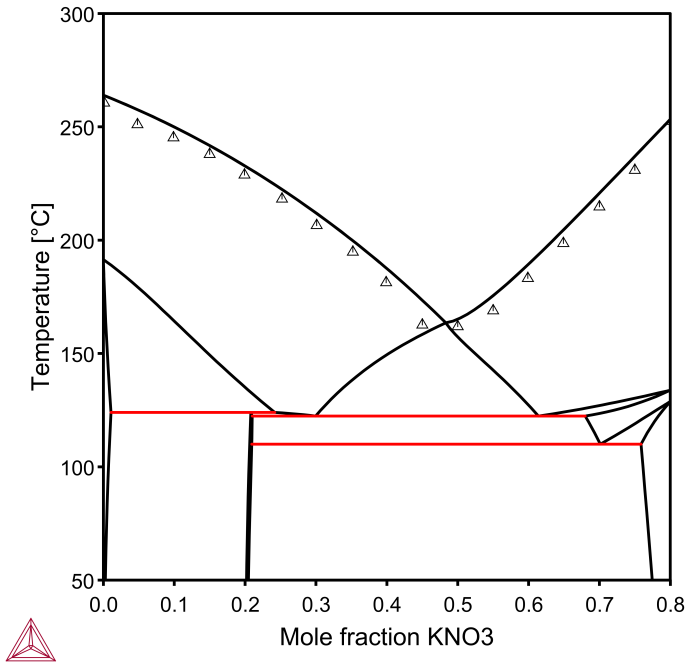


Figure 56: Calculated section for LiNO<sub>3</sub>-KNO<sub>3</sub>-NaNO<sub>3</sub> ternary system with 0.2 mole fraction LiNO<sub>3</sub> with experimental data from [2013Cos].

### LiNO<sub>3</sub>-Mg(NO<sub>3</sub>)<sub>2</sub>-NaNO<sub>3</sub>

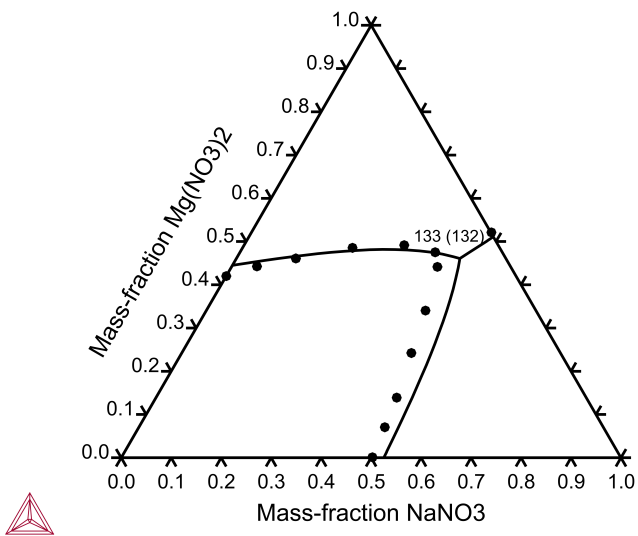


Figure 57: Calculated liquidus projection. Experimental temperature in °C with experimental data from [2020Zho].

## References

- [2013Cos] K. Coscia, T. Elliott, S. Mohapatra, A. Oztekin, S. Neti, Binary and Ternary Nitrate Solar Heat Transfer Fluids. *J. Sol. Energy Eng.* 135 (2013).
- [2020Zho] Y. Zhong, J. Yuan, M. Wang, J. Li, Phase Diagrams of Binary Systems  $\text{Mg}(\text{NO}_3)_2$ - $\text{KNO}_3$ ,  $\text{Mg}(\text{NO}_3)_2$ - $\text{LiNO}_3$  and ternary system  $\text{Mg}(\text{NO}_3)_2$ - $\text{LiNO}_3$ - $\text{NaNO}_3$ . *J. Chem. Eng. Data* 65, 3420–3427 (2020).
-

## TCSALT Examples of Density

The TCS Molten Salts Database (TCSALT) can be used to calculate density. These examples show calculations of various systems, where some validation of the results are compared to experimental data.

### $\text{Li}_2\text{CO}_3\text{-Na}_2\text{CO}_3\text{-K}_2\text{CO}_3$

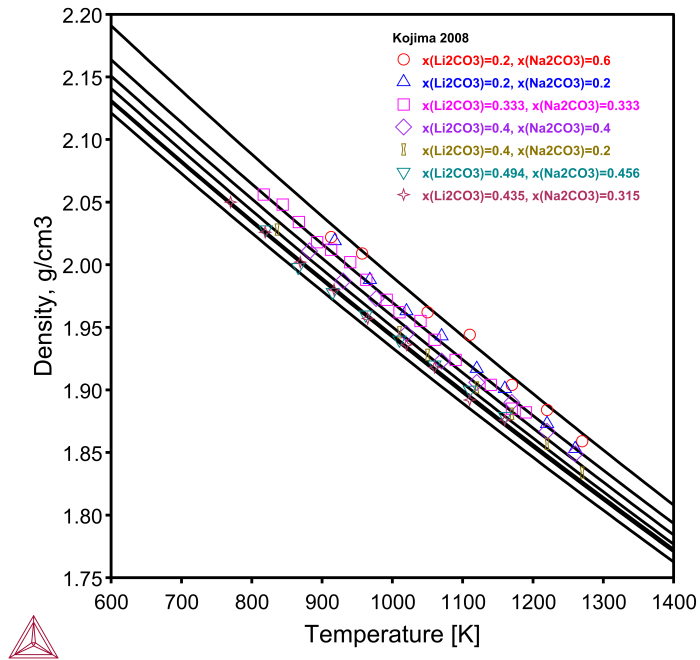


Figure 58: Calculated density of  $\text{Li}_2\text{CO}_3\text{-Na}_2\text{CO}_3\text{-K}_2\text{CO}_3$  system compared with literature data in [2008Koj]. Solid lines denote the calculations in the present work.

## LiF-NaF-KF

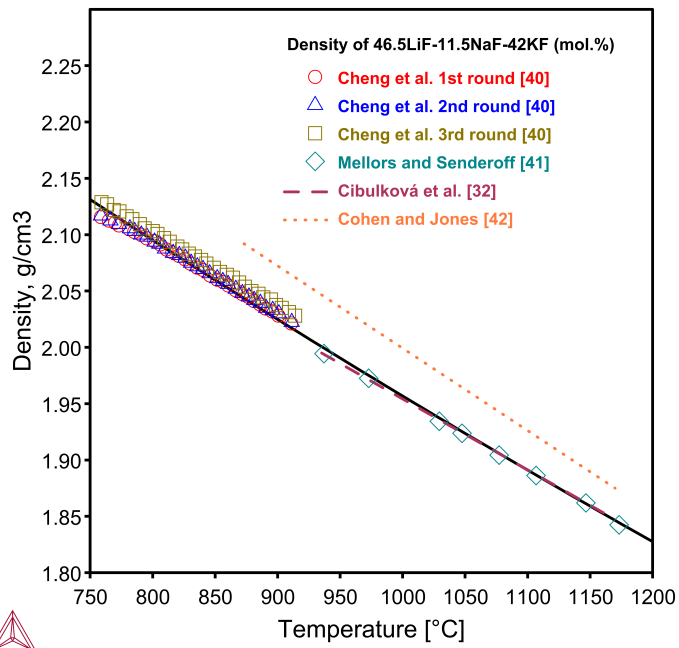


Figure 59: Calculated density of FLiNaK (46.5LiF-11.5NaF-42KF mol.%) system compared with literature data from [2026Zha]. Solid lines denote the calculations in the present work.

## CaCl<sub>2</sub>-LiCl

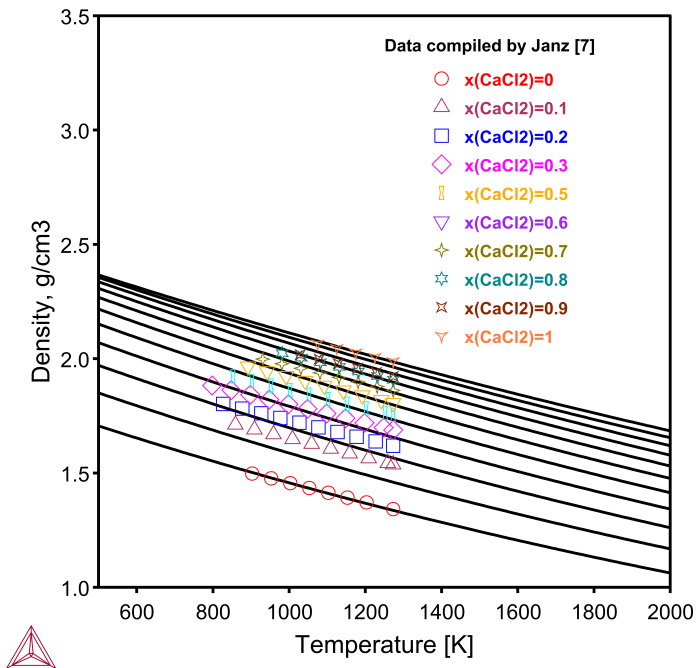


Figure 60: Calculated density of CaCl<sub>2</sub>-LiCl system compared with literature data in [2026Zha]. Solid lines denote the calculations in the present work.

## References

[2008Koj] T. Kojima, Y. Miyazaki, K. Nomura, K. Tanimoto, Density, Surface Tension, and Electrical Conductivity of Ternary Molten Carbonate System Li<sub>2</sub>CO<sub>3</sub> – Na<sub>2</sub>CO<sub>3</sub> – K<sub>2</sub>CO<sub>3</sub> and Methods for Their Estimation. J. Electrochem. Soc. 155, F150 (2008).

[2026Zha] R. Zhang, L. Kjellqvist, H. Mao, A. Markström, R. Naraghi, Q. Chen, Thermophysical Properties of Molten Salts: Insights from the TCSALT Database. Int. J. Thermophys. 47, 23 (2026).

## TCSALT Examples of Surface Tension

The TCS Molten Salts Database (TCSALT) can be used to calculate surface tension. These examples show calculations of various systems, where some validation of the results are compared to experimental data.

### $\text{Li}_2\text{CO}_3\text{-Na}_2\text{CO}_3\text{-K}_2\text{CO}_3$

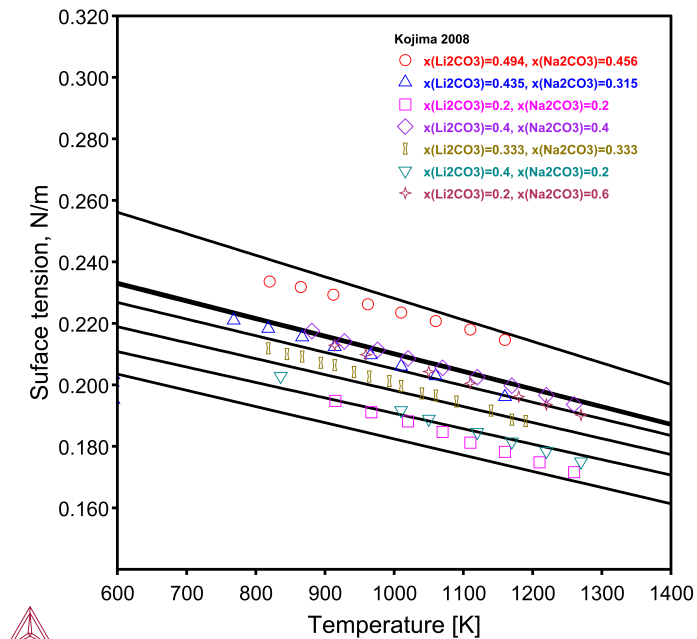


Figure 61: Calculated surface tension of  $\text{Li}_2\text{CO}_3\text{-Na}_2\text{CO}_3\text{-K}_2\text{CO}_3$  system compared with literature data from [2008Koj]. Solid lines denote the calculations in the present work.

### $K_3AlF_6$ - $Na_3AlF_6$

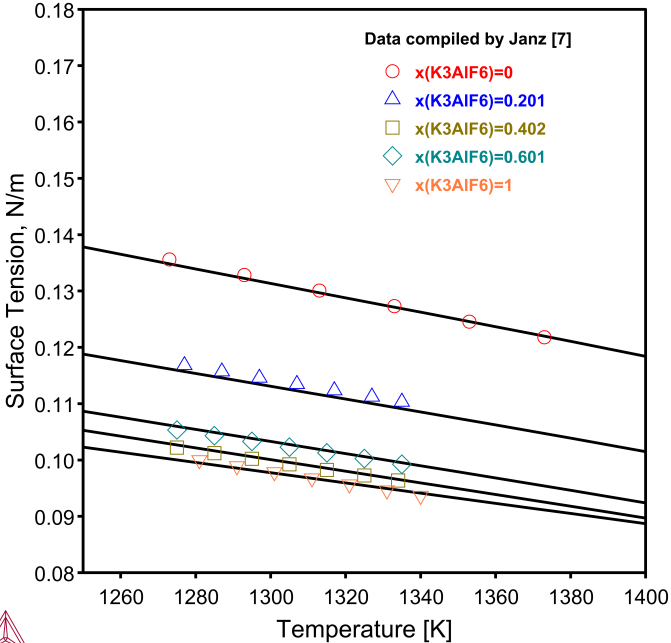


Figure 62: Calculated surface tension of  $K_3AlF_6$ - $Na_3AlF_6$  system compared with literature data [2026Zha]. Solid lines denote the calculations in the present work.

## LiCl-LiF

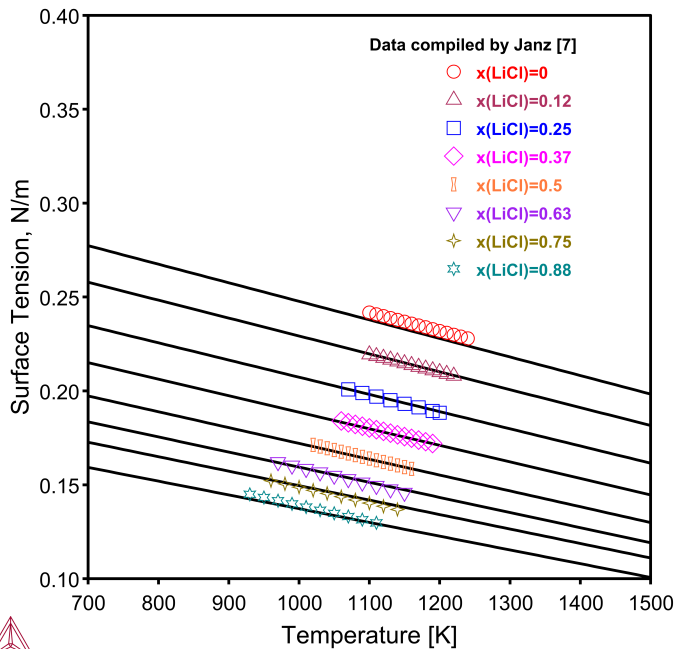


Figure 63: Calculated surface tension of LiCl-LiF system compared with literature data [2026Zha]. Solid lines denote the calculations in the present work.

## References

- [2008Koj] T. Kojima, Y. Miyazaki, K. Nomura, K. Tanimoto, Density, Surface Tension, and Electrical Conductivity of Ternary Molten Carbonate System  $\text{Li}_2\text{CO}_3 - \text{Na}_2\text{CO}_3 - \text{K}_2\text{CO}_3$  and Methods for Their Estimation. *J. Electrochem. Soc.* 155, F150 (2008).
- [2026Zha] R. Zhang, L. Kjellqvist, H. Mao, A. Markström, R. Naraghi, Q. Chen, Thermophysical Properties of Molten Salts: Insights from the TCSALT Database. *Int. J. Thermophys.* 47, 23 (2026).

## TCSALT Examples of Viscosity

The TCS Molten Salts Database (TCSALT) can be used to calculate viscosity. These examples show calculations of various systems, where some validation of the results are compared to experimental data.

### $\text{Na}_3\text{AlF}_6\text{-AlF}_3\text{-CaF}_2\text{-Al}_2\text{O}_3$

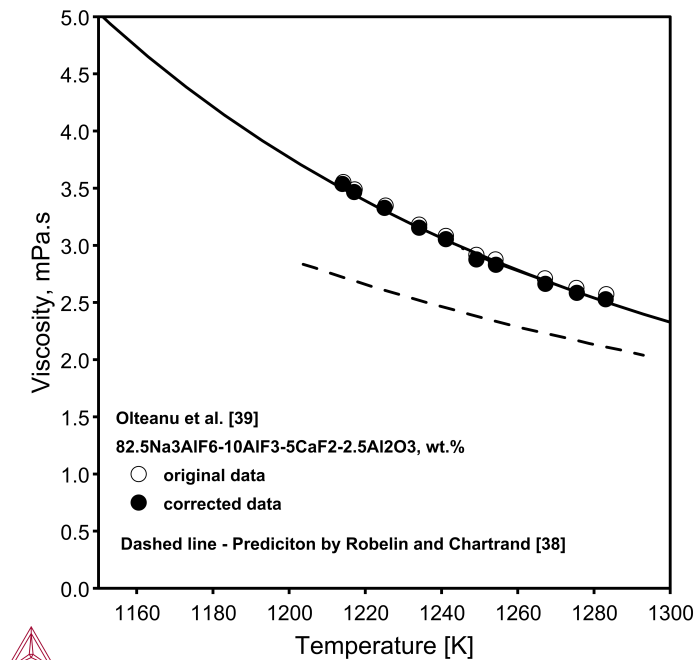


Figure 64: Calculated viscosity of the  $82.5\text{Na}_3\text{AlF}_6\text{-}10\text{AlF}_3\text{-}5\text{CaF}_2\text{-}2.5\text{Al}_2\text{O}_3$  (wt.%) system compared with literature data found in [2026Zha]. Solid and dotted lines denote the calculations in the present work.

## Ca(NO<sub>3</sub>)<sub>2</sub>-24NaNO<sub>3</sub>-44KNO<sub>3</sub>

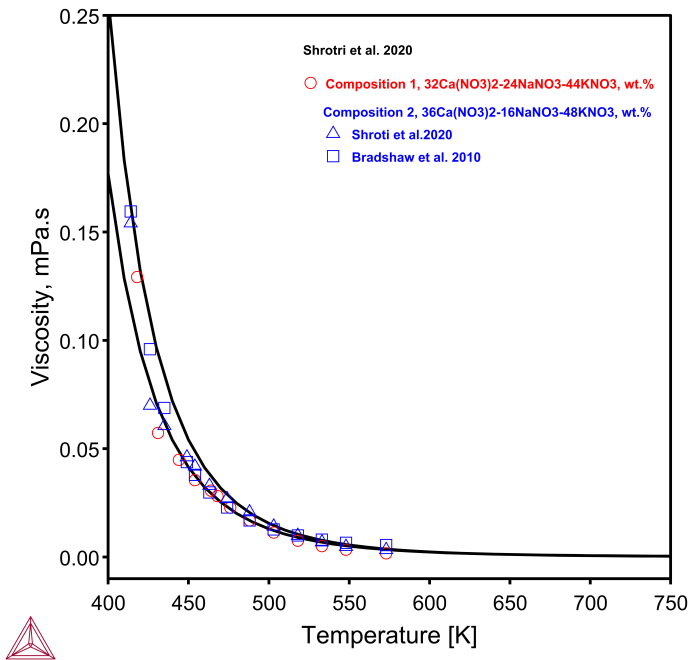


Figure 65: Calculated viscosity of the  $32\text{Ca}(\text{NO}_3)_2\text{-}24\text{NaNO}_3\text{-}44\text{KNO}_3$  (wt.%) and  $36\text{Ca}(\text{NO}_3)_2\text{-}16\text{NaNO}_3\text{-}48\text{KNO}_3$  (wt.%) systems compared with literature data reported by [2020Shr]. Solid and dotted lines denote the calculations in the present work.

## LiF-NaF-KF

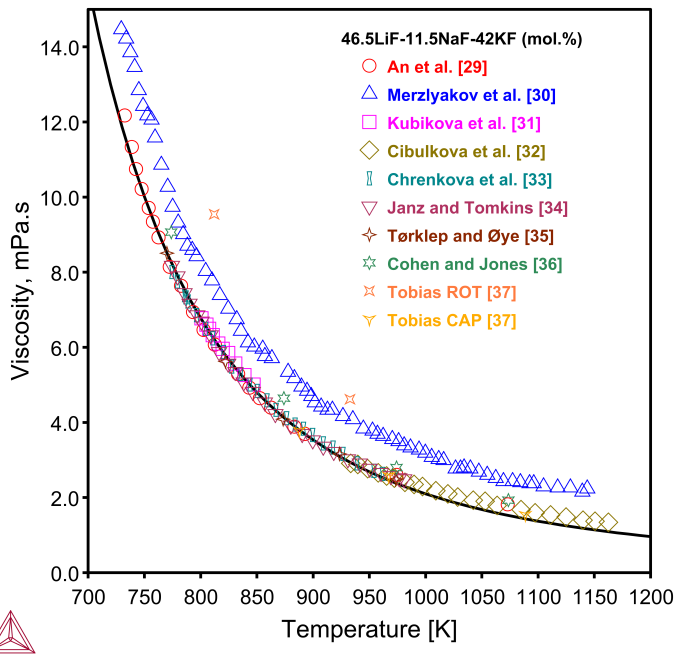


Figure 66: Calculated viscosity of FLiNaK (46.5LiF-11.5NaF-42KF mol.%) system compared with experimental data from the literature discussed in [2026Zha]. Solid line denotes the calculation in the present work.

## References

- [2020Shr] V. Shrotri, L. Muhmood, Experimental and Modeling Studies on Density of  $\text{Ca}(\text{NO}_3)_2\text{-NaNO}_3\text{-KNO}_3$  Ternary Salts with Focus on Calcium Nitrate Density Prediction. *Int. J. Thermophys.* 41, 85 (2020).
- [2026Zha] R. Zhang, L. Kjellqvist, H. Mao, A. Markström, R. Naraghi, Q. Chen, Thermophysical Properties of Molten Salts: Insights from the TCSALT Database. *Int. J. Thermophys.* 47, 23 (2026).