Thermodynamic Assessments of Na-Cr-O System

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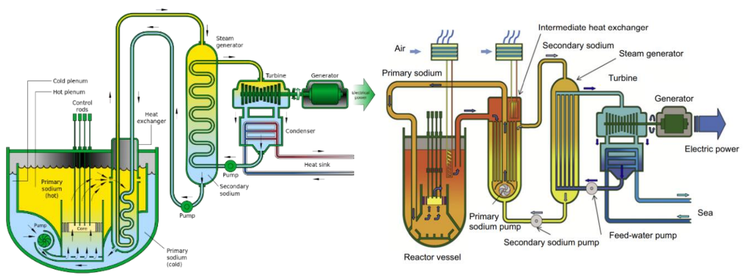
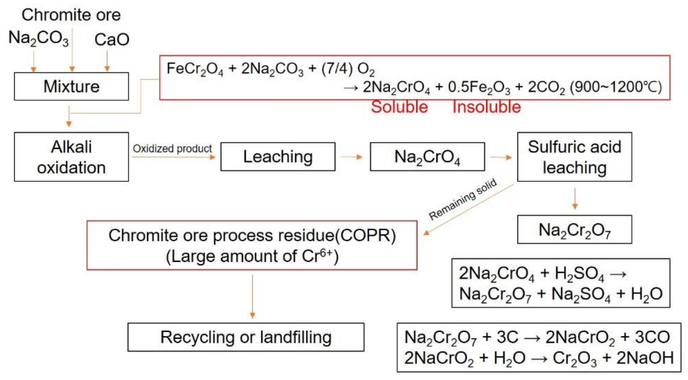
Introduction

SFR: Sodium-cooled Fast Reactor



[Pool type] [Loop type]

General chromium oxide extraction



Chromium oxide extraction in reduction condition

L. Escudero-Castejon et al. (2017)

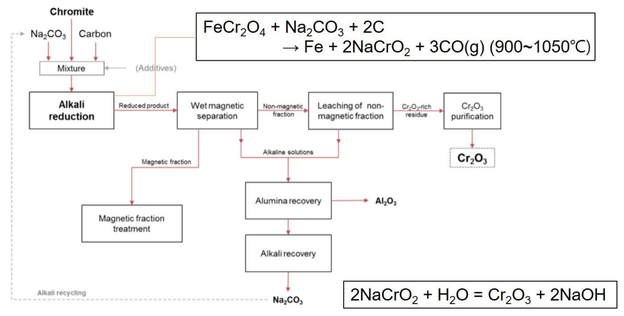
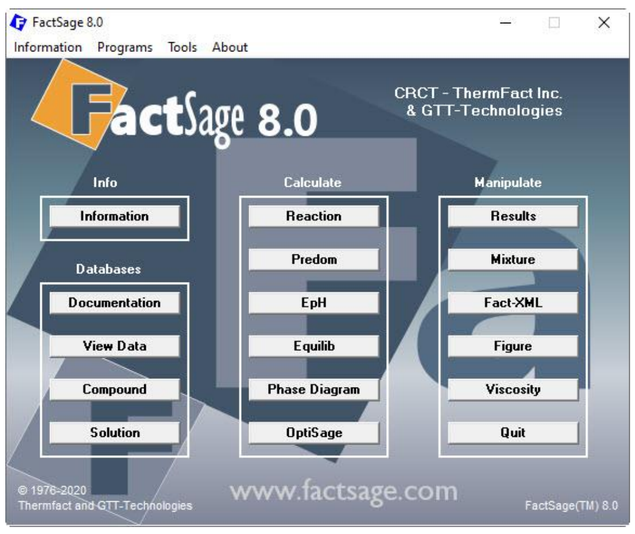


Figure 6- Process flowsheet including the main stages of the alkali reduction process

CALPHAD : Methodology

FactSage: Thermochemical software



Stoichiometric compounds

$$G_T^o = H_T^o - TS_T^o$$

$$H_T^o = \Delta H_{298K}^o + \int_{298K}^{T} C_p dT$$

$$S_T^o = \Delta S_{298K}^o + \int_{298K}^{T} \frac{C_p}{T} dT$$

Liquid solution : Modified Quasichemical Model (MQM)

$$(A-\mathrm{A}) + (B-B) = 2(A-B); \Delta g_{AB}$$

$$G^m = (n_A g_A^o + n_B g_B^o) - \mathrm{T}\Delta S^{config} + (\frac{n_{AB}}{2})\Delta g_{AB}$$

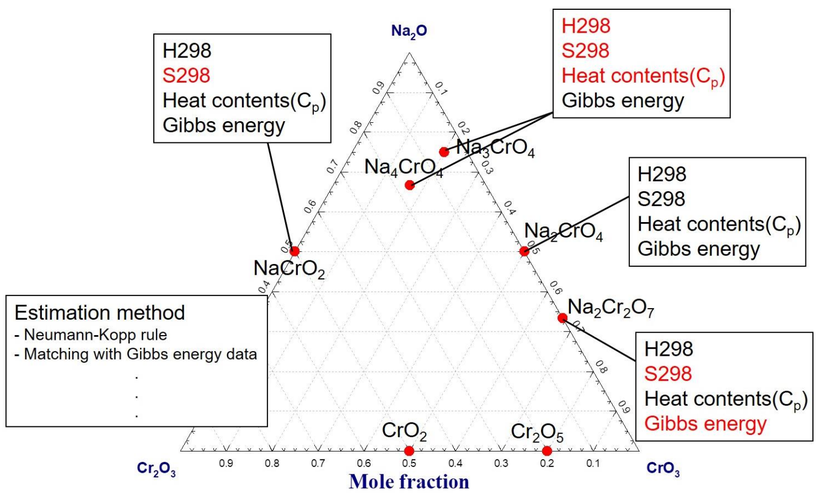
$$\Delta S^{config} = -R(n_A lnX_A + n_B lnX_B) - R[n_{AA} \ln\left(\frac{X_{AA}}{Y_A^{\,2}}\right) + n_{AA} \ln\left(\frac{X_{BB}}{Y_A^{\,2}}\right) + n_{AB} \ln\left(\frac{X_{AB}}{2Y_A Y_B}\right)]$$

$$\Delta g_{AB} = \Delta g_{AB}^o + \sum_{i\geq 1} g_{AB}^{i0} X_{AA}^i + \sum_{\mathrm{j}\geq 1} g_{AB}^{0j} X_{BB}^j$$

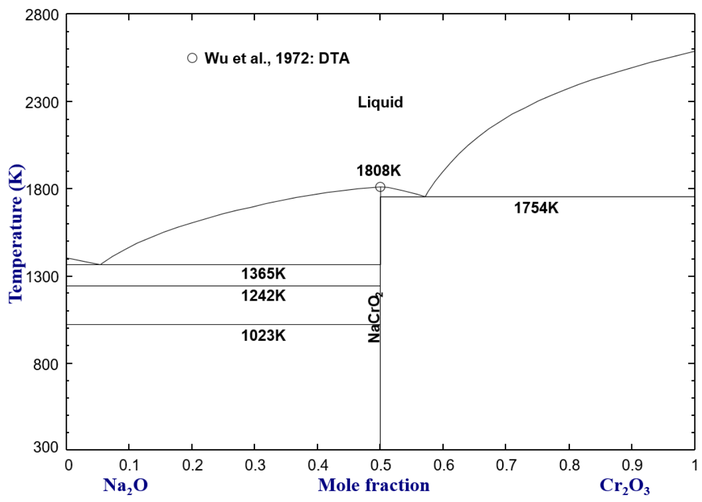
Results & Discussion

- Stoichiometric compounds in Na_2O-Cr_2O_3-CrO_3 system

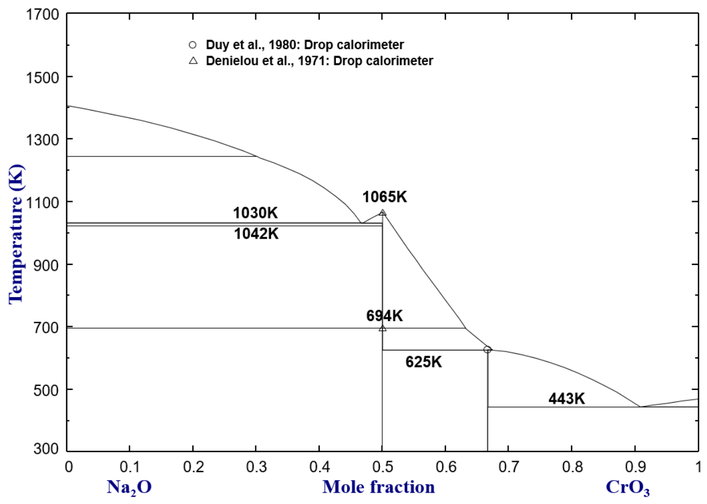
Black : experimental data
Red : estimated data



- Phase diagram of Na_2O-Cr_2O_3 system

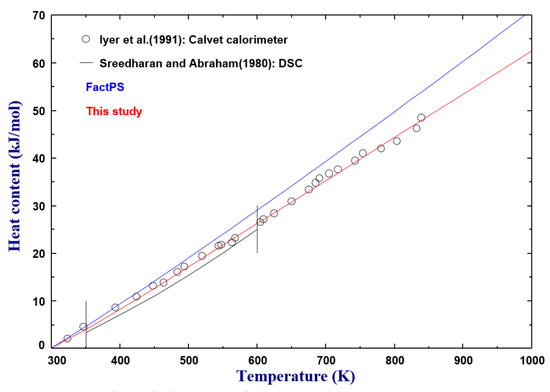


- Phase diagram of Na_2O-CrO_3 system

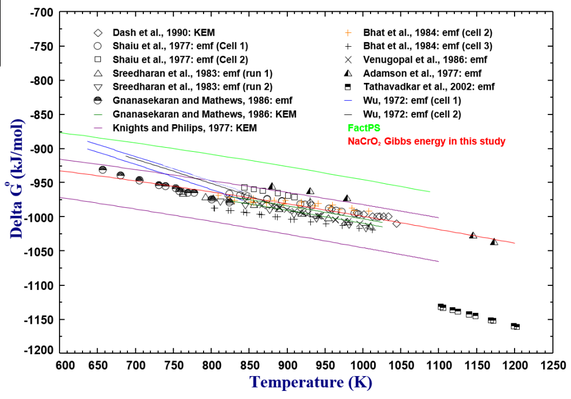


- Thermodynamic properties of $NaCrO_2$

- Heat content of $NaCrO_2$

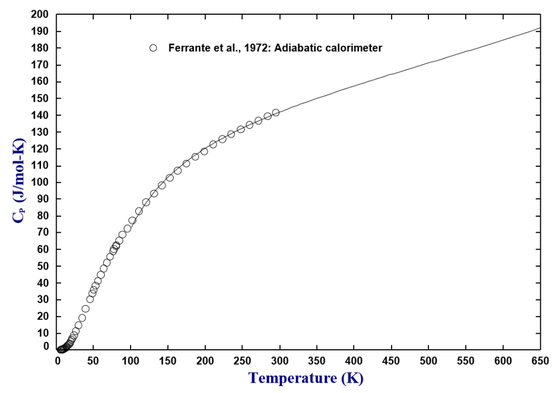


- Standard formation Gibbs energy of $NaCrO_2$

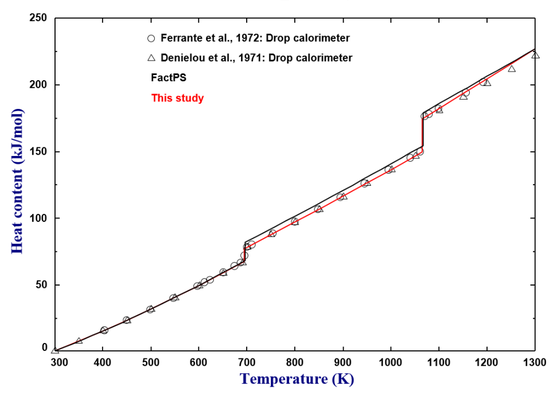


- Thermodynamic properties of Na_2CrO_4

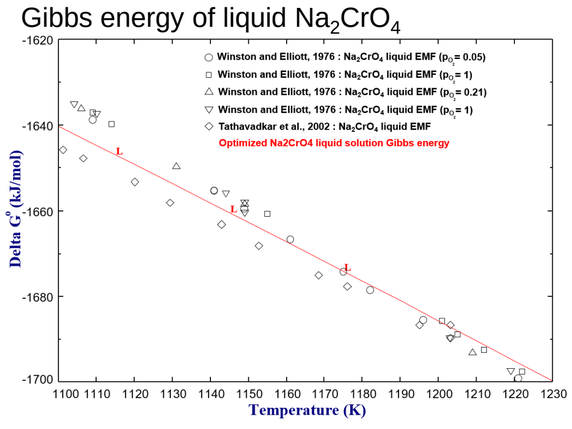
- Heat capacity of Na_2CrO_4



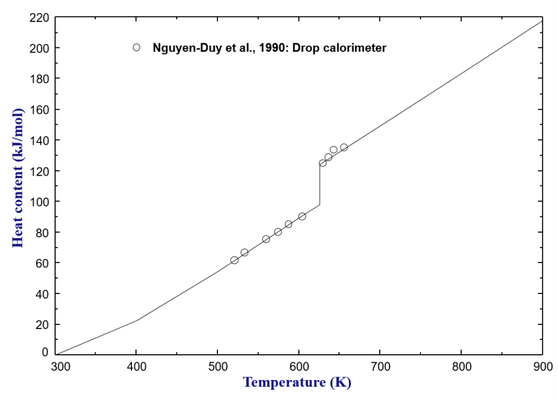
- Heat content of Na_2CrO_4



- Standard formation Gibbs energy of liquid Na_2CrO_4

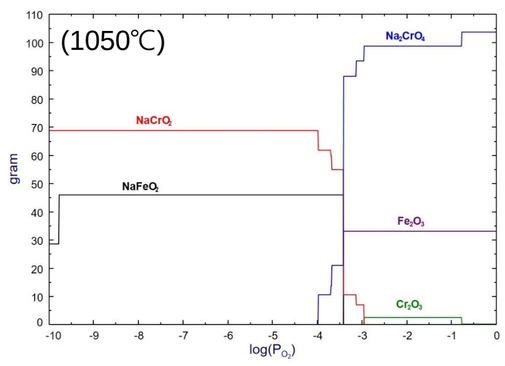


- Heat content of $Na_2Cr_2O_7$

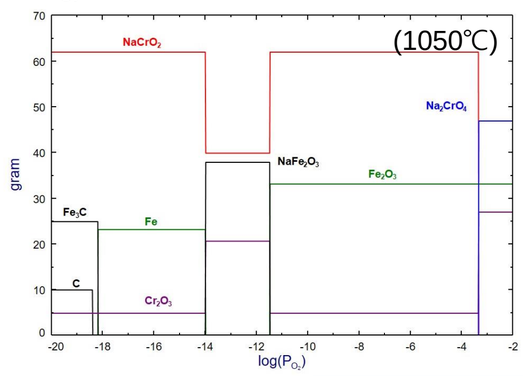


- Application

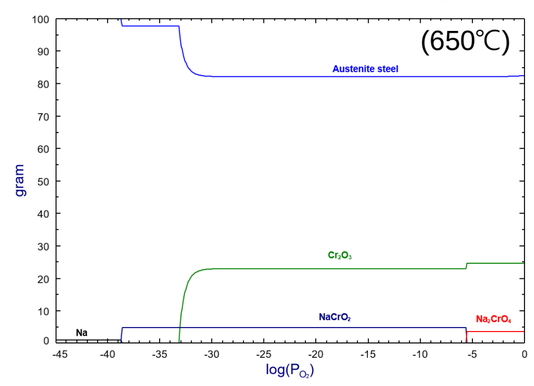
- Alkali reaction of chromite ore (based on 100g) in oxidation condition



- Alkali reaction of chromite ore (based on 100g) in carbothermic reduction condition



- Calculation of condition to prevent formation of Na-Cr oxide in SFR (based on100g of 316LN)



Conclusion

- Na_2O-Cr_2O_3, Na_2O-CrO_3 system is optimized, but it needs to be developed because of not enough experimental data.
- Alkali reaction in chromium oxide extraction process in oxidation condition and reduction condition is calculated based on optimized data respectively.
- Condition to prevent Na-Cr oxide in SFR is calculated.

Future work

- This system should be checked under various O2 partial pressure condition later.
- Na-Cr-O system will be connected with CaO-MgO-Al_2O_3-SiO_2 system.