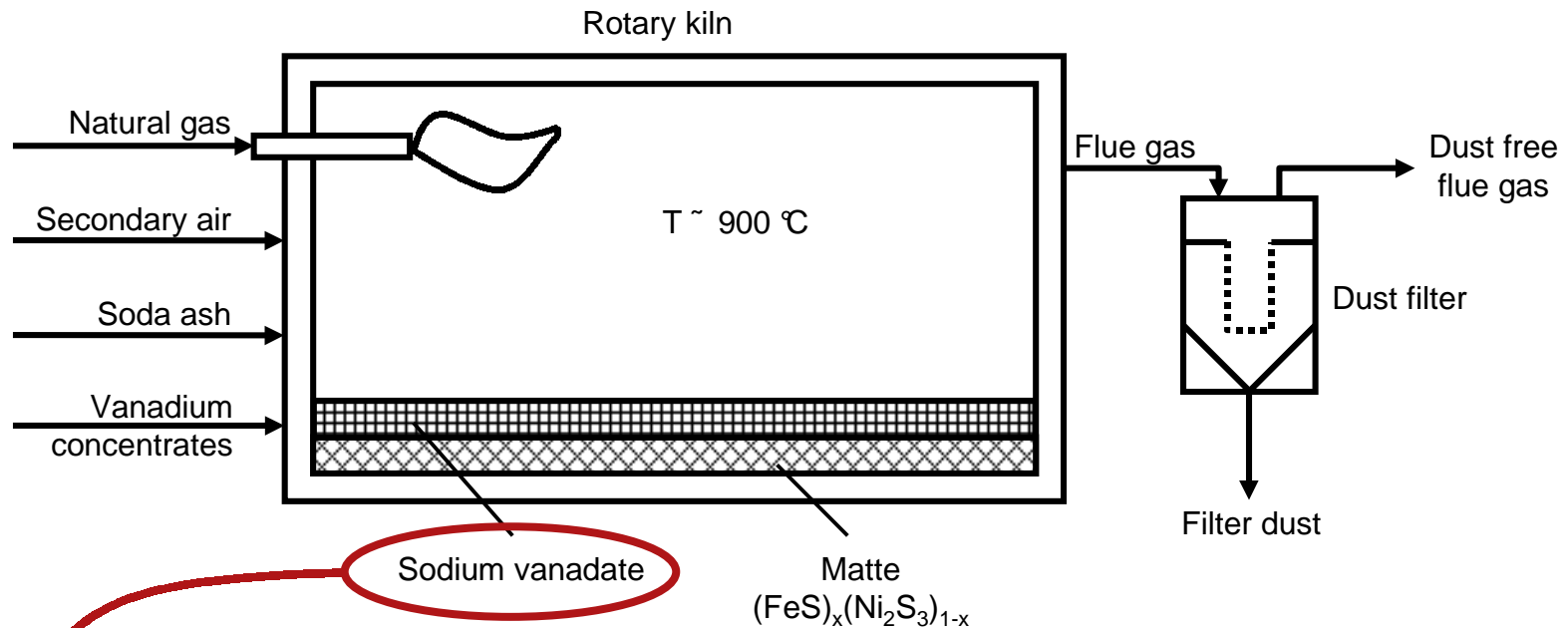


Modelling of the Vanadium Production from Petroleum Residues with FactSage

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Herzogenrath, Germany

Processing of vanadium concentrates



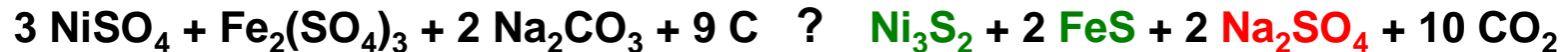
- Sodium meta-vanadate: $(\text{Na}_2\text{O})(\text{V}_2\text{O}_5) = \text{Na}_2\text{V}_2\text{O}_6 = 2 \text{NaVO}_3$
- Sodium pyro-vanadate: $(\text{Na}_2\text{O})_2(\text{V}_2\text{O}_5) = \text{Na}_4\text{V}_2\text{O}_7$
- Sodium ortho-vanadate: $(\text{Na}_2\text{O})_3(\text{V}_2\text{O}_5) = \text{Na}_6\text{V}_2\text{O}_8 = 2 \text{Na}_3\text{VO}_4$

Important chemical reactions

Formation of sodium vanadate and matte



Prevention of SO_x

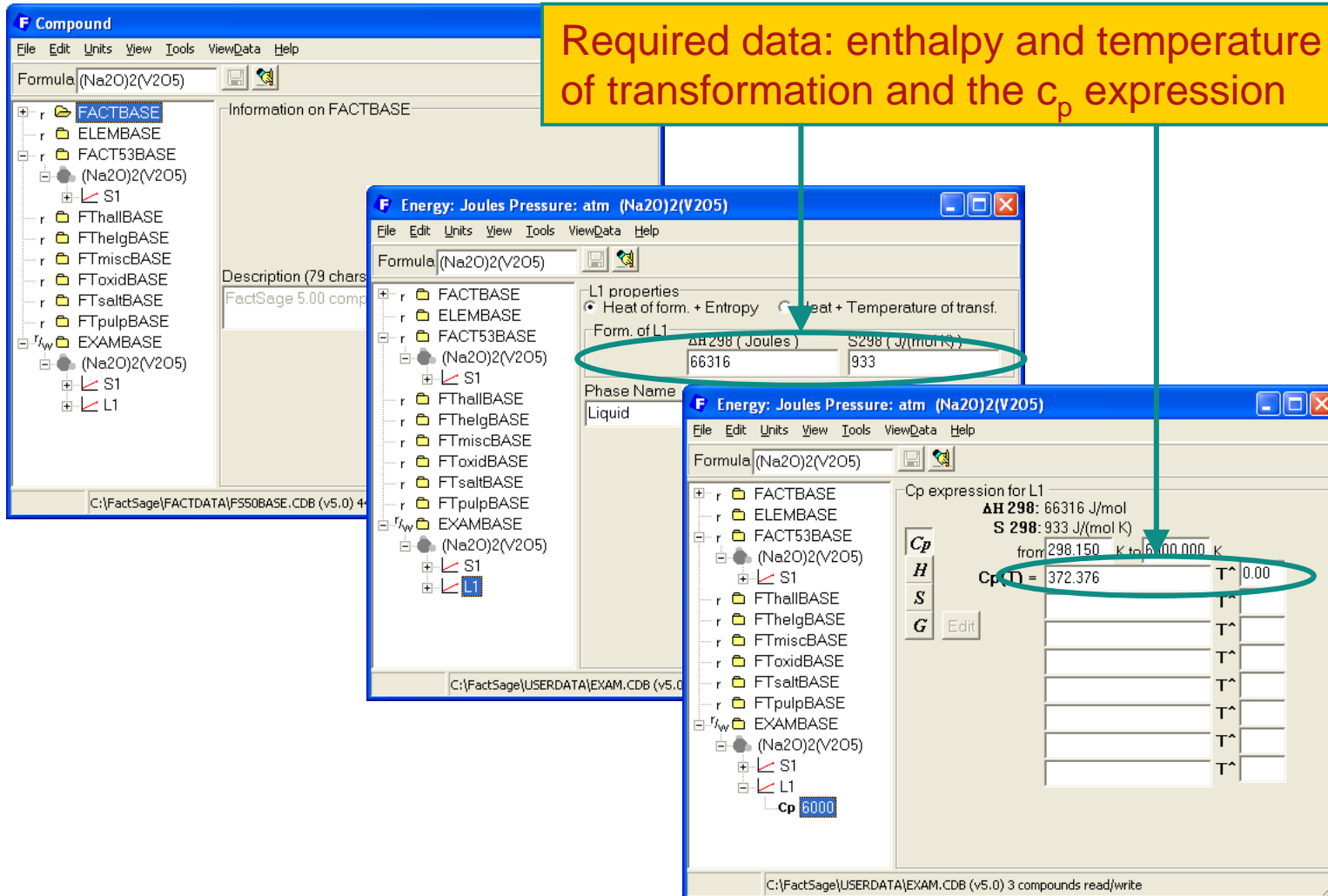


Questions to be answered:

- How much soda ash is required to form the sodium vanadate and to avoid the formation of SO_x in the flue gas?
- Under which conditions do the sodium vanadate and the matte form simultaneously?

Matching the FactSage database

Required data: enthalpy and temperature of transformation and the c_p expression



The image displays three overlapping windows from the FactSage software interface, illustrating the extraction of thermodynamic data for the compound $(\text{Na}_2\text{O})_2(\text{V}_2\text{O}_5)$.

- Top Window (Compound):** Shows the compound tree structure. The selected compound is $(\text{Na}_2\text{O})_2(\text{V}_2\text{O}_5)$ under the L1 phase.
- Middle Window (Energy: Joules Pressure: atm):** Displays L1 properties for the selected compound. The "Form. of L1" section shows the enthalpy of formation (ΔH_{298}) as 66316 Joules and the entropy (S_{298}) as 933 J/(mol K). The phase name is "Liquid".
- Bottom Window (Energy: Joules Pressure: atm):** Shows the Cp expression for the liquid phase. The expression is $C_p(T) = 372.376 T^{0.00}$, where T is temperature in Kelvin. The temperature range is from 298.150 K to 6000.000 K.

Source of thermochemical data

Compound	Formula	Melting point [K]	c_p (liq) [J/(mole·K)]
Sodium meta-vanadat	$(\text{Na}_2\text{O})(\text{V}_2\text{O}_5)$ = 2NaVO_3	903	284.512
Sodium pyro-vanadate	$(\text{Na}_2\text{O})_2(\text{V}_2\text{O}_5)$ = $\text{Na}_4\text{V}_2\text{O}_7$	933	372.376
Sodium ortho-vanadate	$(\text{Na}_2\text{O})_3(\text{V}_2\text{O}_5)$ = $2 \text{Na}_3\text{VO}_4$	1139	358.140

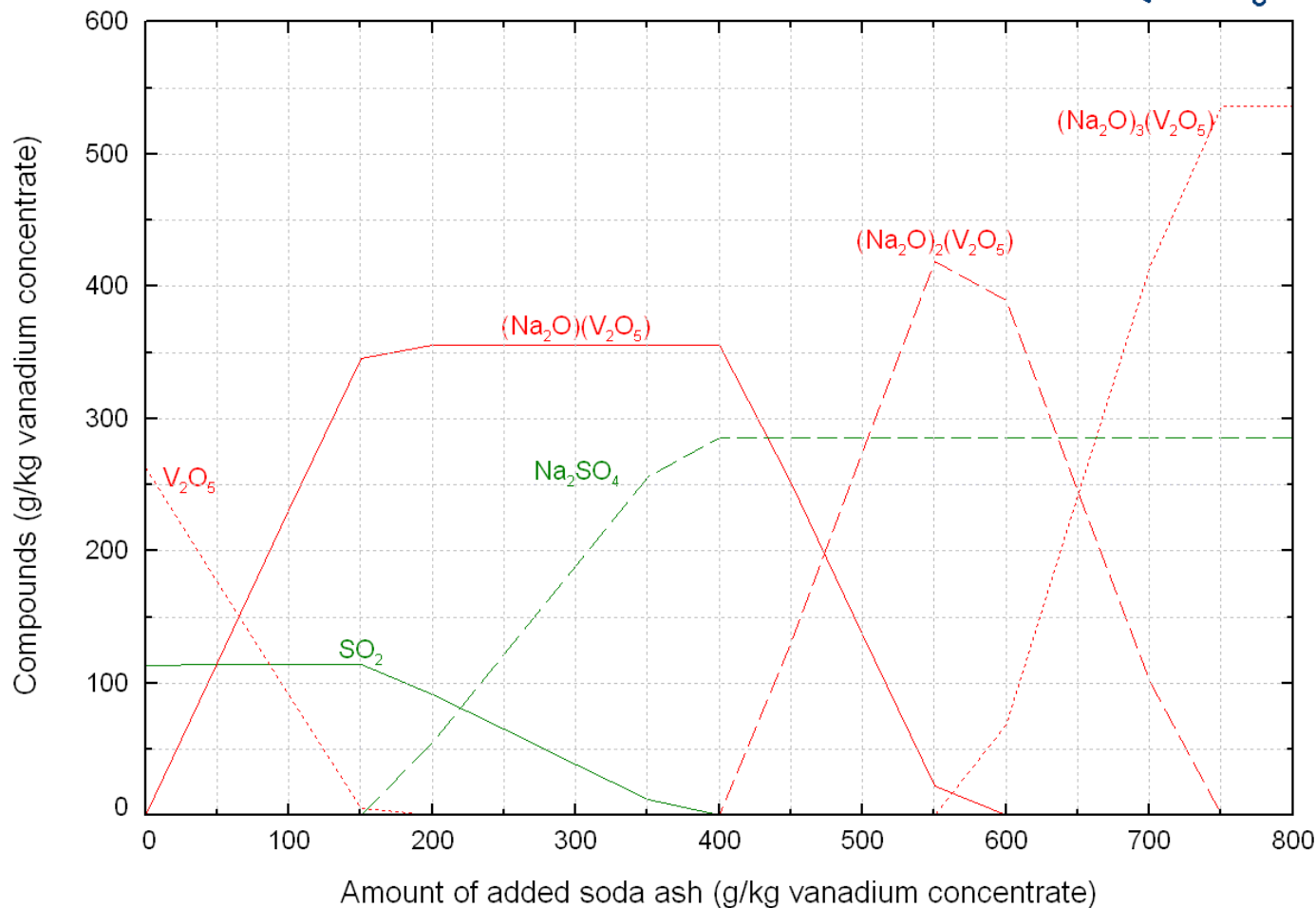
Barin I. (1995): Thermochemical Data of Pure Substances, Vol. II, 3rd edition, VHC Weinheim

estimated

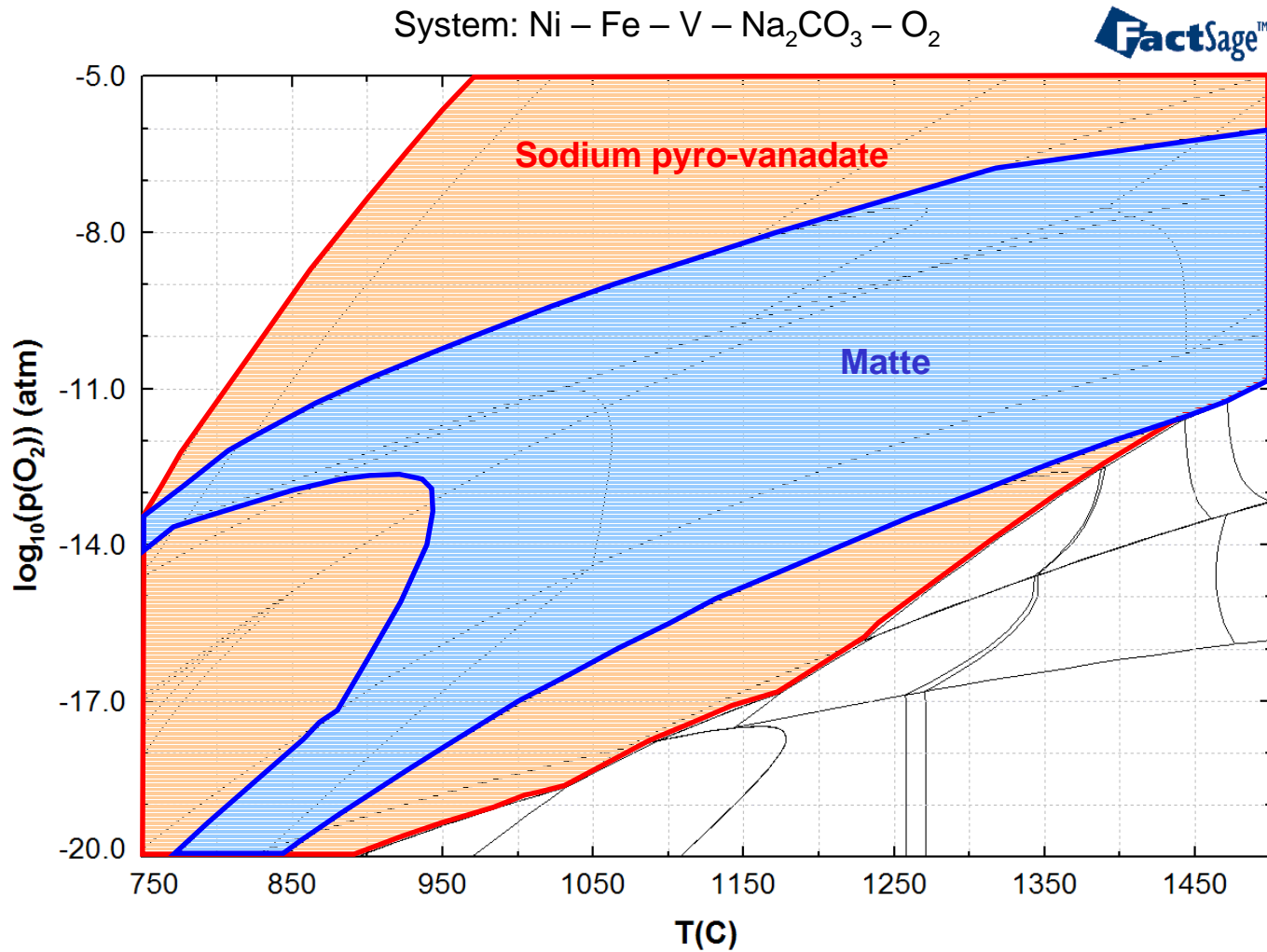
Weast R.C. et al. (1984-1985): CRC Handbook of Chemistry and Physics, 65th edition, CRC Press, Inc., Boca Raton, Florida

Formation of sodium vanadate and SO₂ at 900 °C

System: All analysed elements, T = 900 °C



Formation of sodium vanadate and matte



Summary



- Successful integration of a new data base to calculate liquid sodium vanadate
- Equilib module: Required amount of soda
- Phase Diagram module: predominance area of sodium vanadate and matte

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Thank you for your attention