

Recent advances in modelling of coal ash behaviour in the VerSi Project

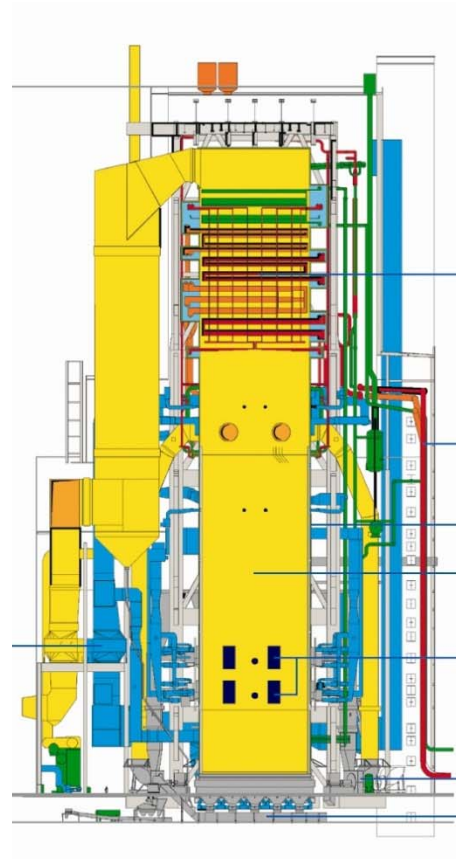
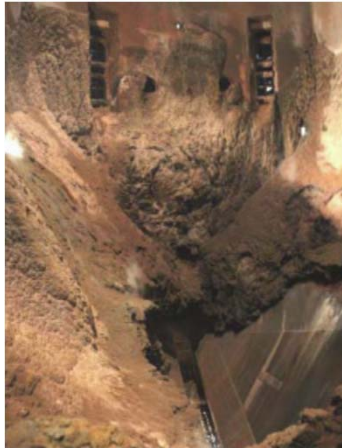
GTT User Meeting, 29th June to 1st July 2016

K. Hack¹, T.Jantzen¹, M. Dohrn², M. Müller²

¹GTT-Technologies ²FZJ IEK-2



Motivation



Forms of slagging and fouling

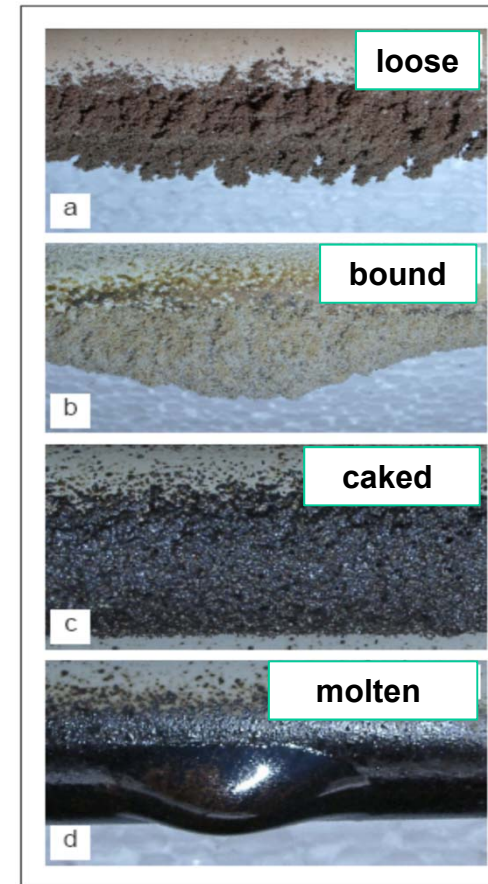
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Fouling

Sintering

Slagging

$f(T)$
 $f(\text{ash elements})$



Slagging and Sintering must be technically manageable or preventable !



The Project VerSi

GTT-Technologies

- Project Leader: University of Stuttgart, IFK Institut für Feuerungs- und Kraftwerkstechnik
- Partners: Research Center FZJ-IEK2 (Jülich)
SMEs: RECOM Services (Stuttgart),
GTT-Technologies (Herzogenrath)
- Industrial Supporters:
EON, Clyde-Bergemann, Vattenfall, ALSTOM



Goals

- Collection of plant data concerning ash/slag formation and deposits
- Generation of a suitable thermodynamic database
- Generation of a model based on interlinked local equilibria
- Generation of a model based on CFD
- Comparison of plant data with models
- Adjustment of models and practical applications



Work Plan VerSi project

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- Data and Model for Hard Coal fired Power Plant
- Data and Model for Lignite fired Power Plant
- Model adaptation for use in plant environment



Ash compositions for Hard Coals

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| Component | Unit | Columbia South Afr. Russia USA | | | |
|--------------------------------|------|--------------------------------|------|------|------|
| | | SKC | SKK | SKR | SKU |
| Al ₂ O ₃ | % | 14.6 | 25.9 | 22.1 | 20.6 |
| CaO | % | 2.1 | 7.1 | 4.9 | 3.7 |
| Fe ₂ O ₃ | % | 15.5 | 15.4 | 6.8 | 14.6 |
| K ₂ O | % | 1.4 | 0.7 | 2.9 | 2.4 |
| MgO | % | 1.1 | 0.1 | 0.2 | 0.9 |
| Na ₂ O | % | 1.8 | 0.2 | 1.3 | 0.7 |
| P ₂ O ₅ | % | 0.1 | 1.5 | 0.5 | 0.2 |
| SiO ₂ | % | 60.7 | 45.4 | 57.1 | 52.6 |
| SO ₃ | % | 1.9 | 2.5 | 3.2 | 3.0 |
| TiO ₂ | % | 0.8 | 1.4 | 0.9 | 1.1 |

Conclusion: The Al₂O₃-SiO₂-X subsystems are of major importance !
The most important third component is Fe₂O₃ → FeO_x

Note: Inclusion of TiO₂ is in progress.

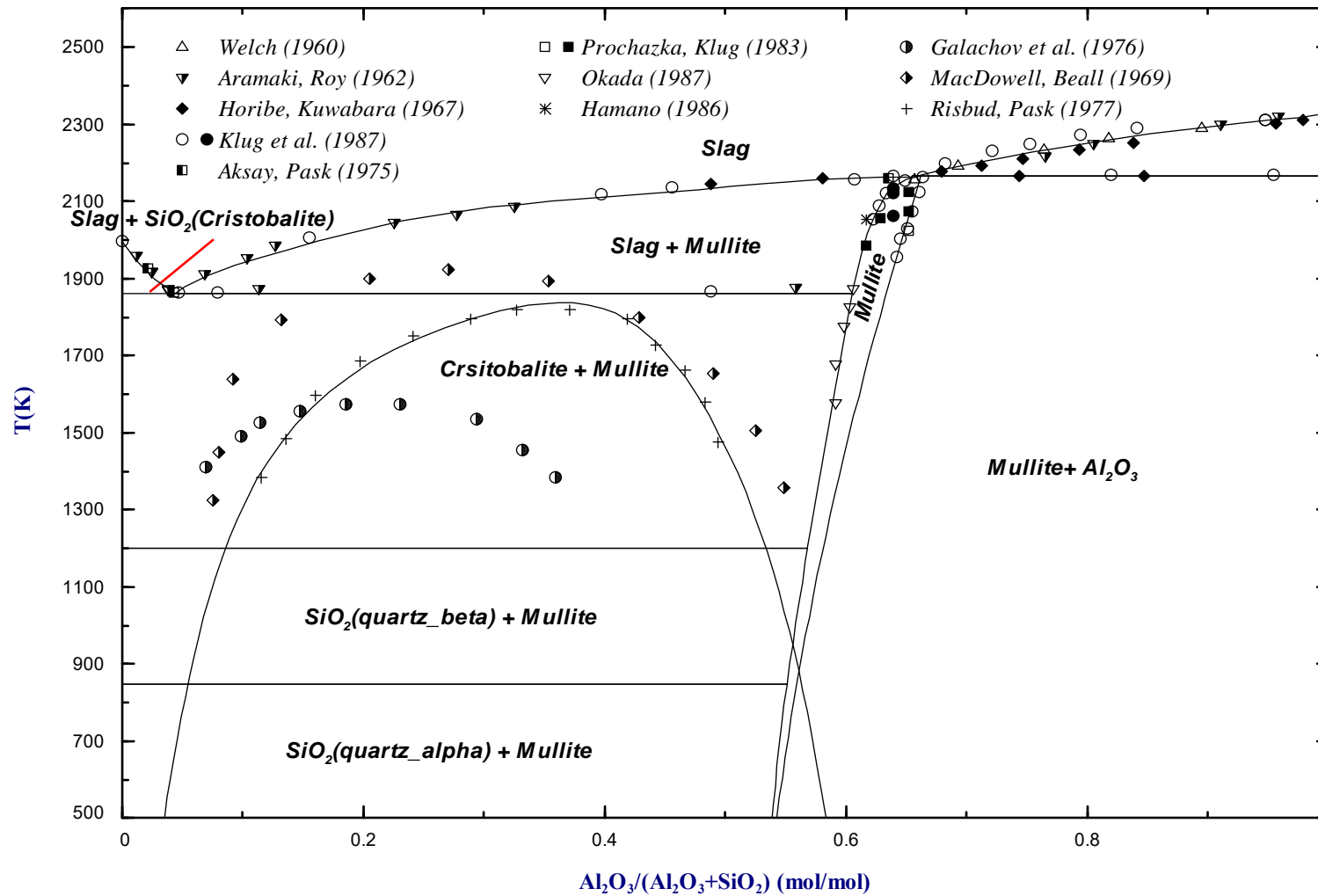


Phase diagrams pertaining to hard coal ashes

GTT-Technologies

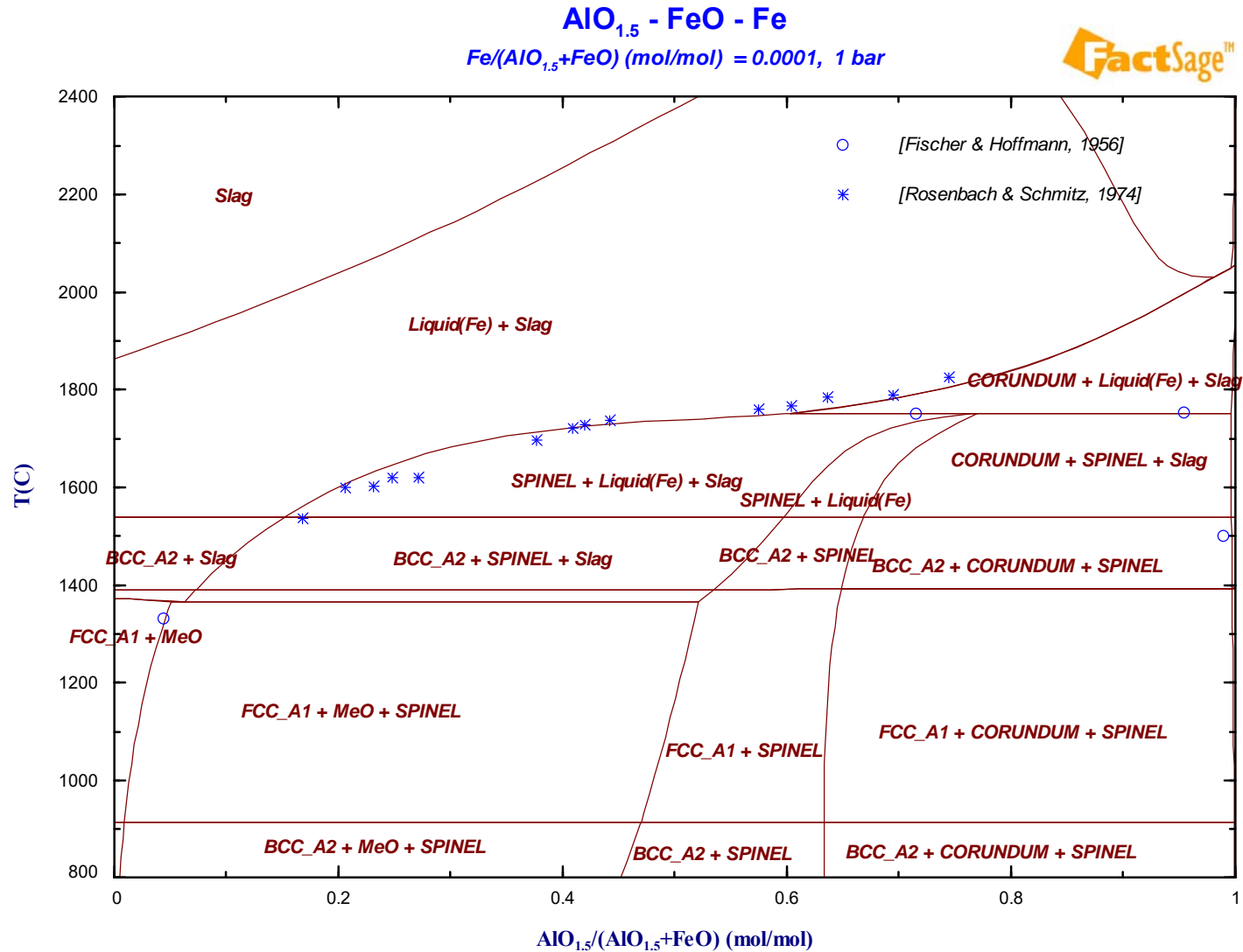
$\text{Al}_2\text{O}_3 - \text{SiO}_2$
1 atm

FactSage™



Phase diagrams pertaining to hard coal ashes

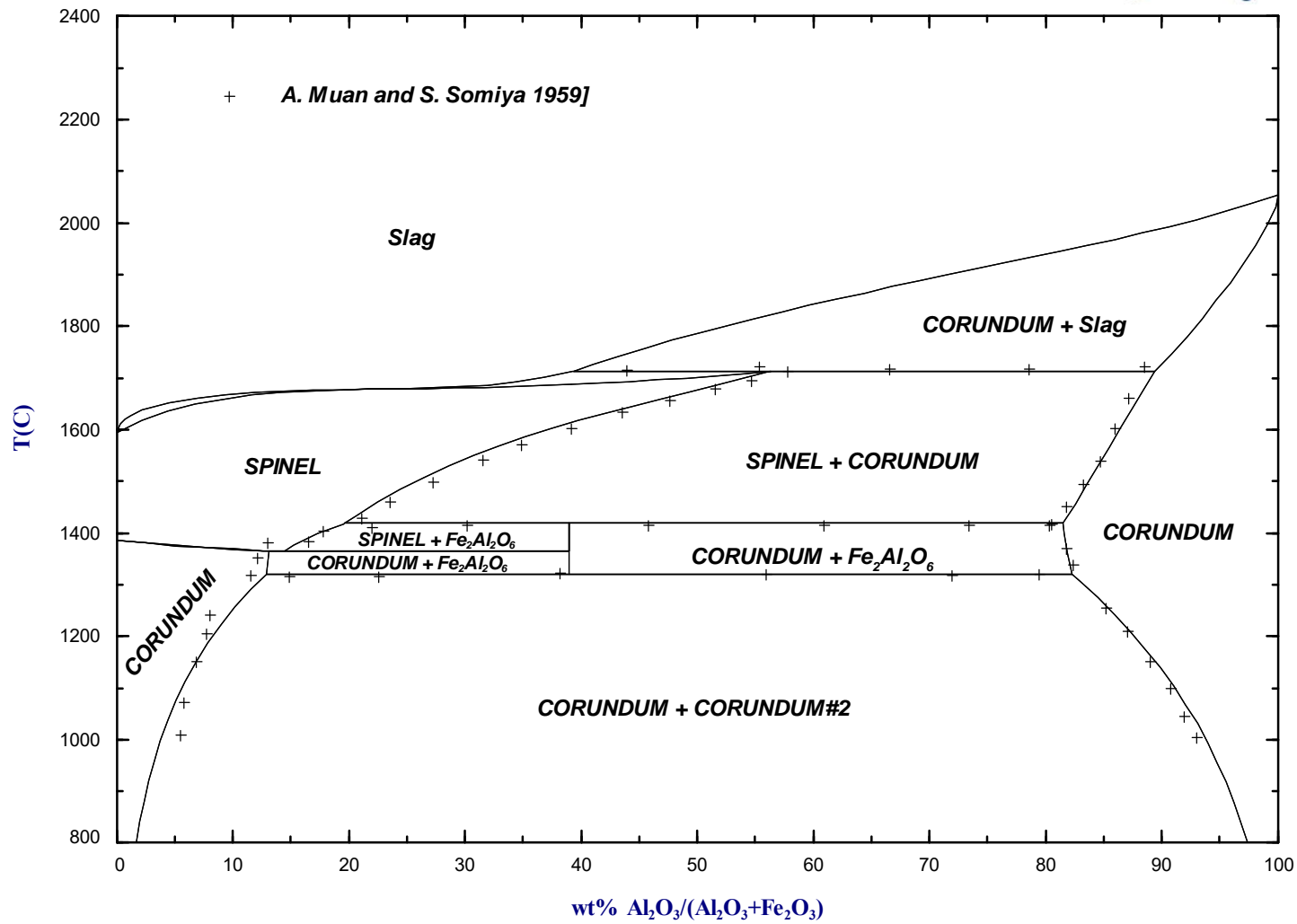
GTT-Technologies



Phase diagrams pertaining to hard coal ashes

GTT-Technologies

$\text{Al}_2\text{O}_3 - \text{Fe}_2\text{O}_3 - \text{O}_2$
 $p(\text{O}_2) = 0.21 \text{ atm}$

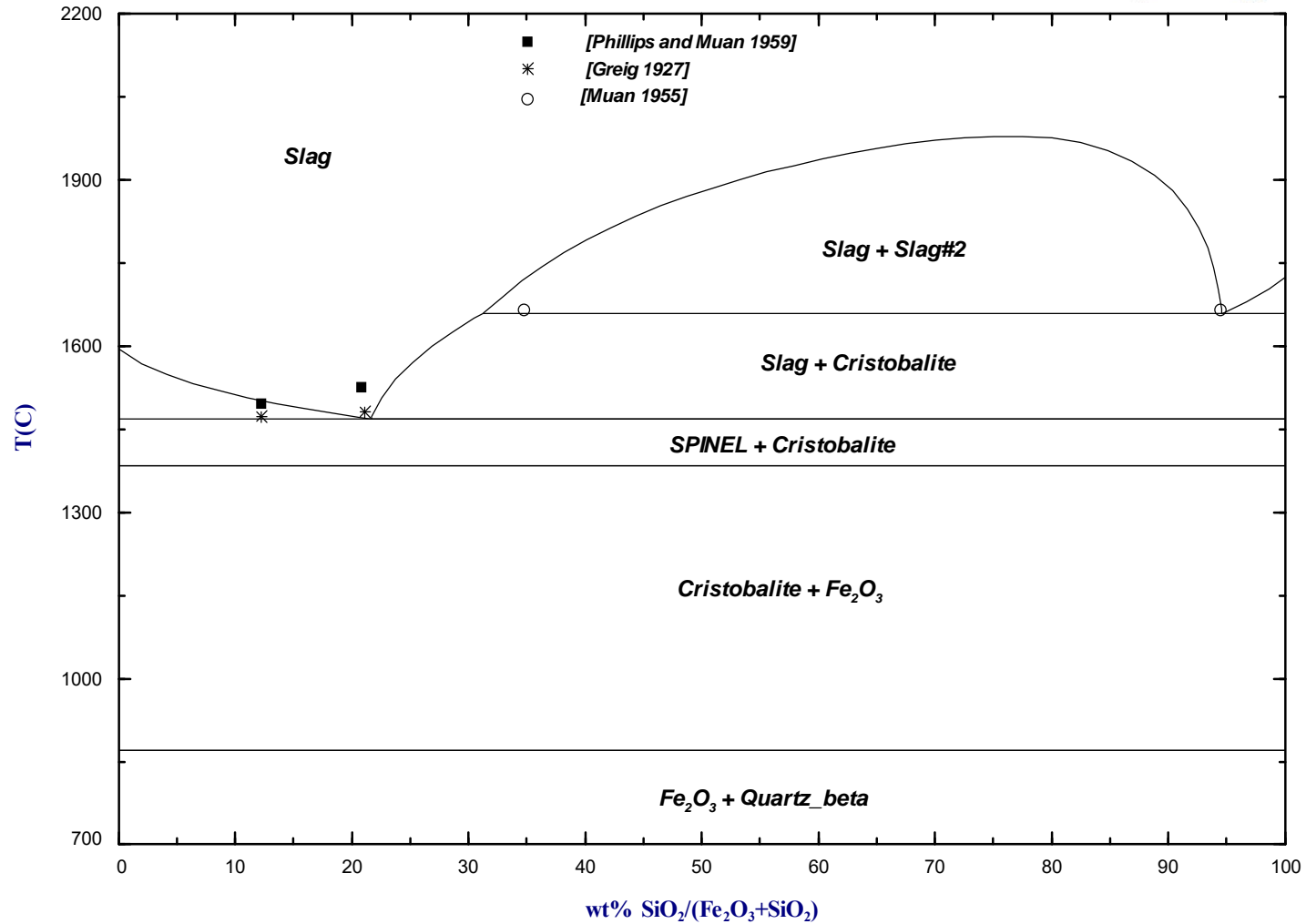


Phase diagrams pertaining to hard coal ashes

GTT-Technologies

$\text{Fe}_2\text{O}_3 - \text{SiO}_2 - \text{O}_2$
 $p(\text{O}_2) = 0.21 \text{ atm}$

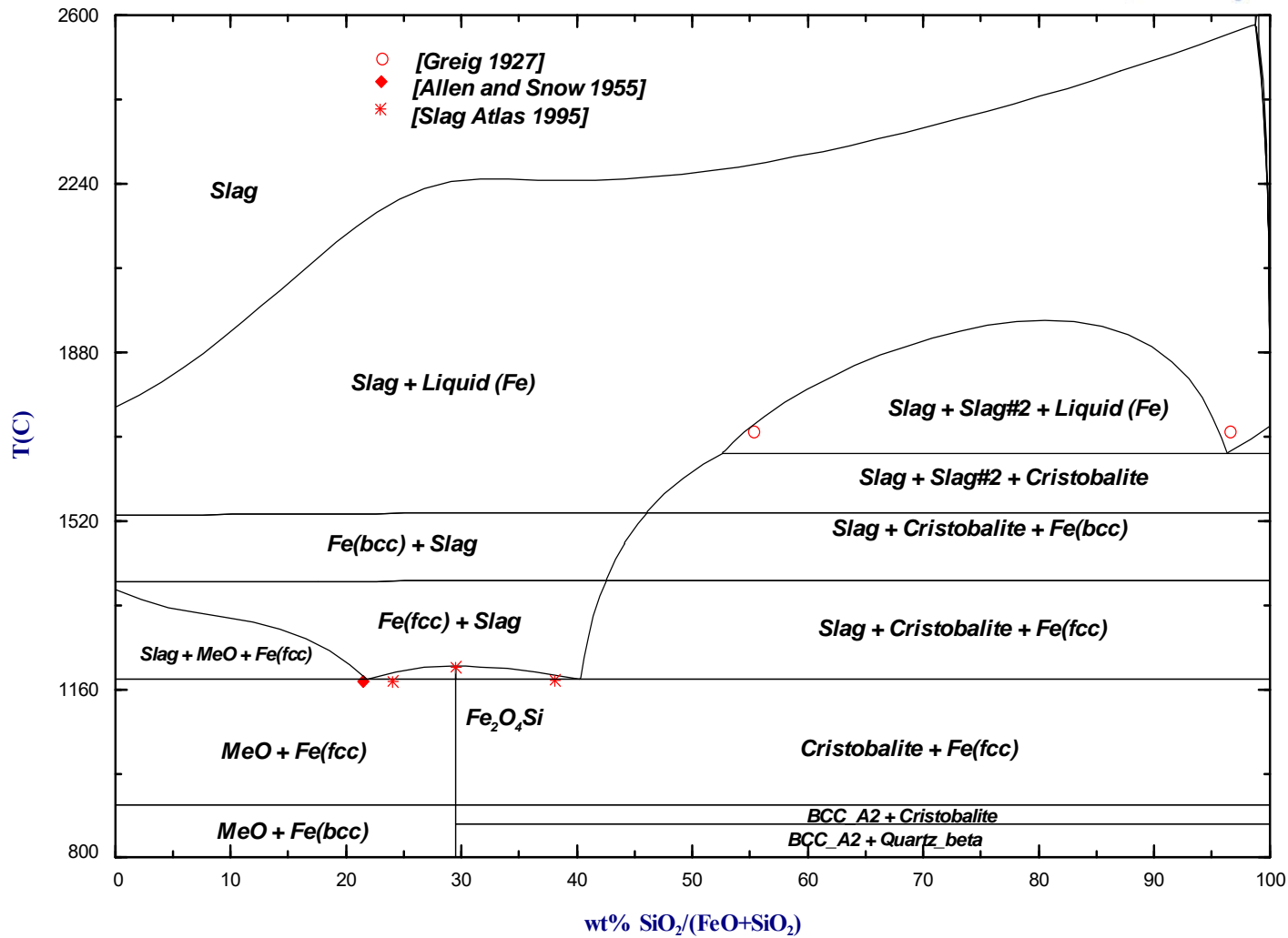
FactSage™



Phase diagrams pertaining to hard coal ashes

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FeO - SiO₂ - Fe
wt% Fe/(FeO+SiO₂) = 0.001



Phase diagrams pertaining to hard coal ashes

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$\text{Al}_2\text{O}_3 - \text{Fe}_2\text{O}_3 - \text{SiO}_2 - \text{O}_2$
 Projection (Slag), $p(\text{O}_2) = 0.21 \text{ atm}$, 1 atm

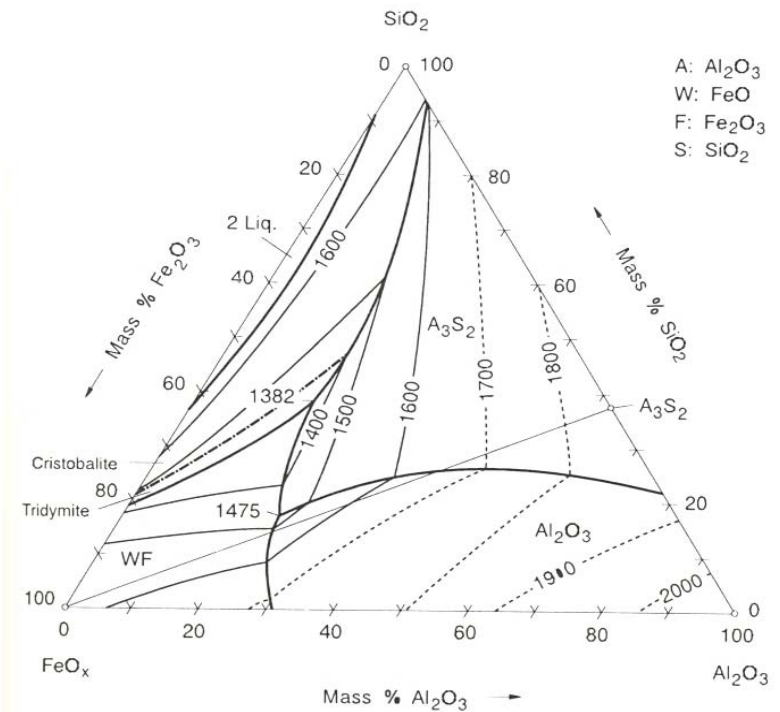
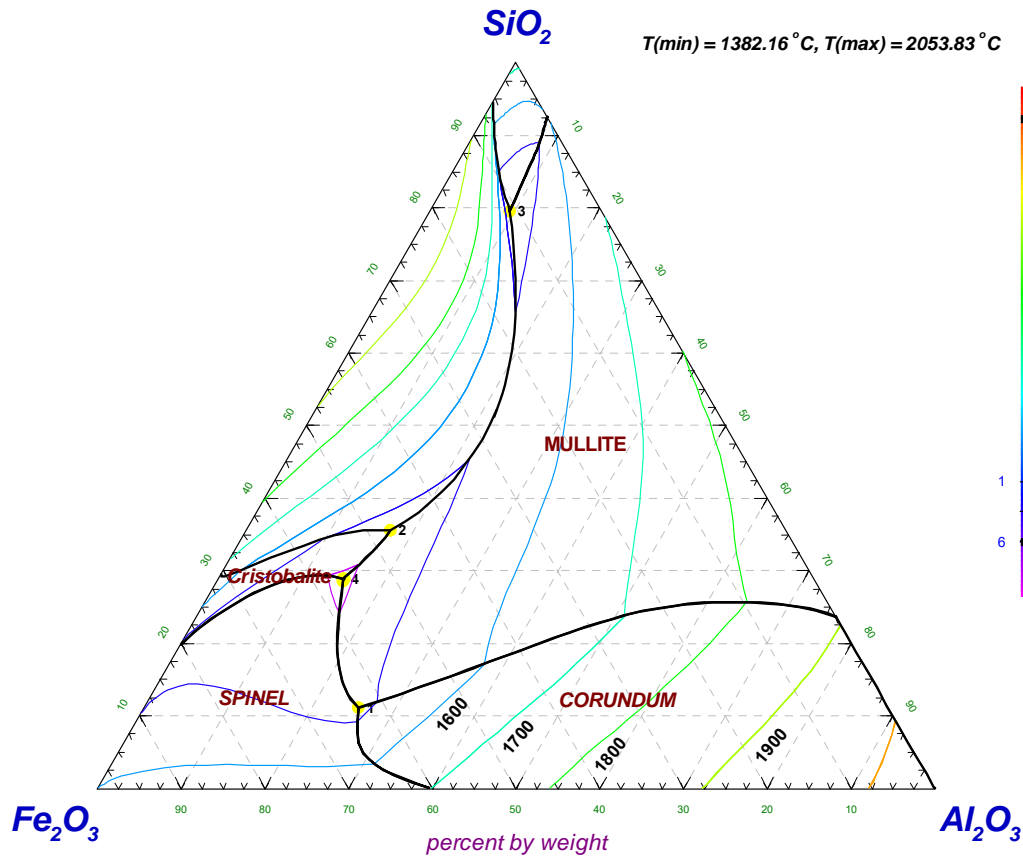


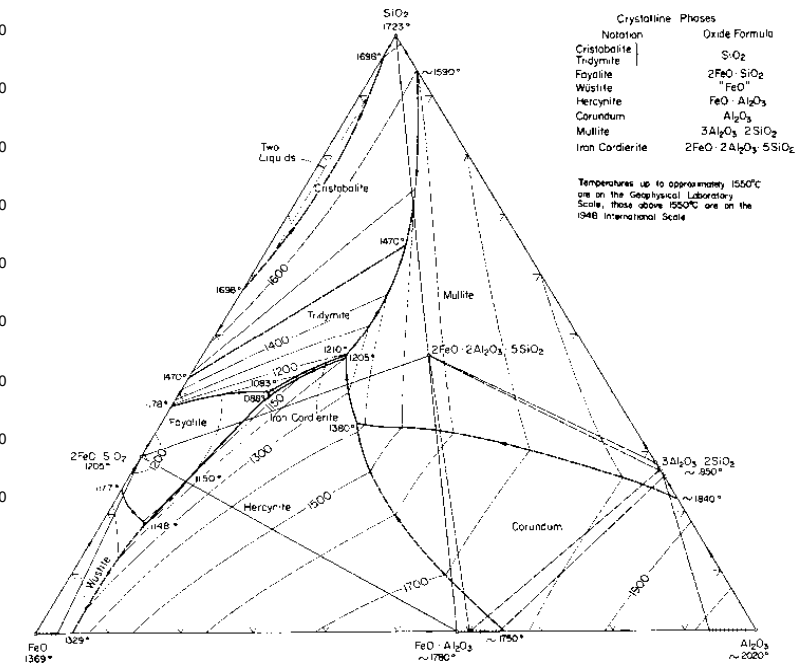
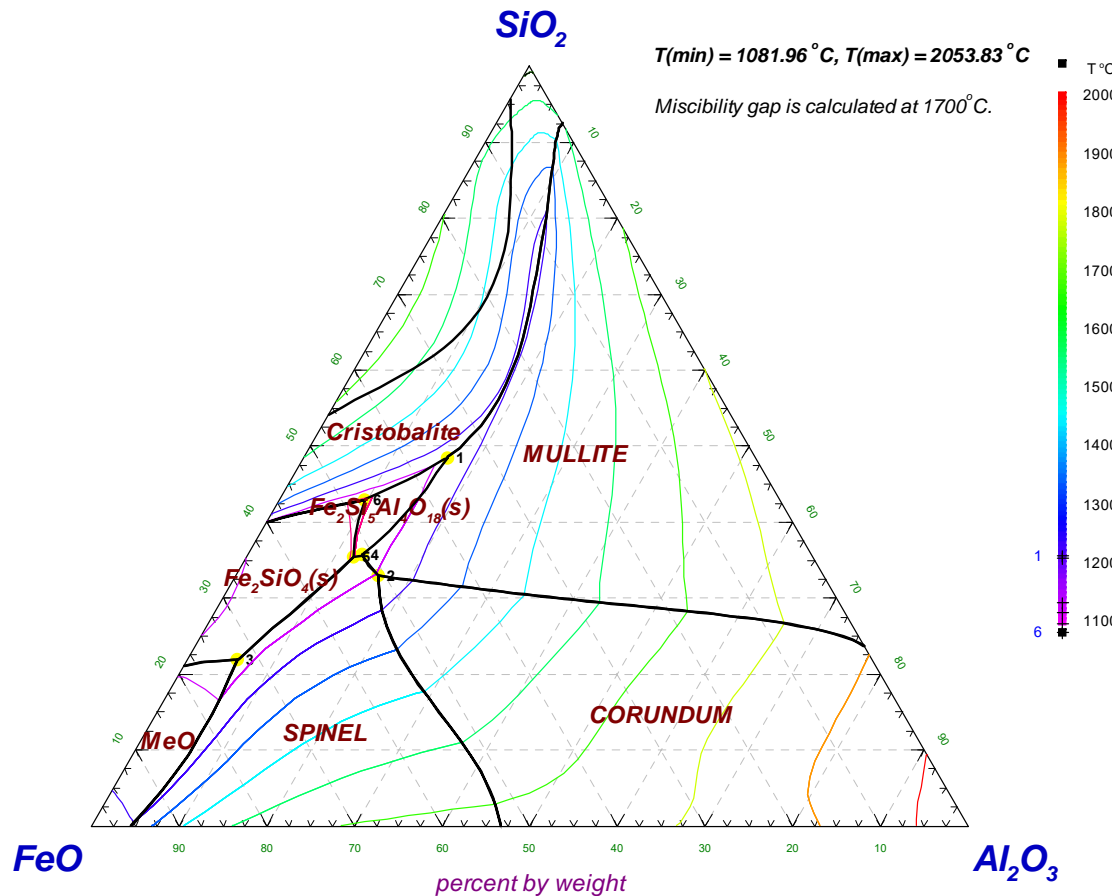
Fig. 3.184. Liquidus surface in the system $\text{Al}_2\text{O}_3\text{-FeO}_x\text{-SiO}_2$ in air after Muan [4], as revised by Idink, Woermann [5].



Phase diagrams pertaining to hard coal ashes

GTT-Technologies

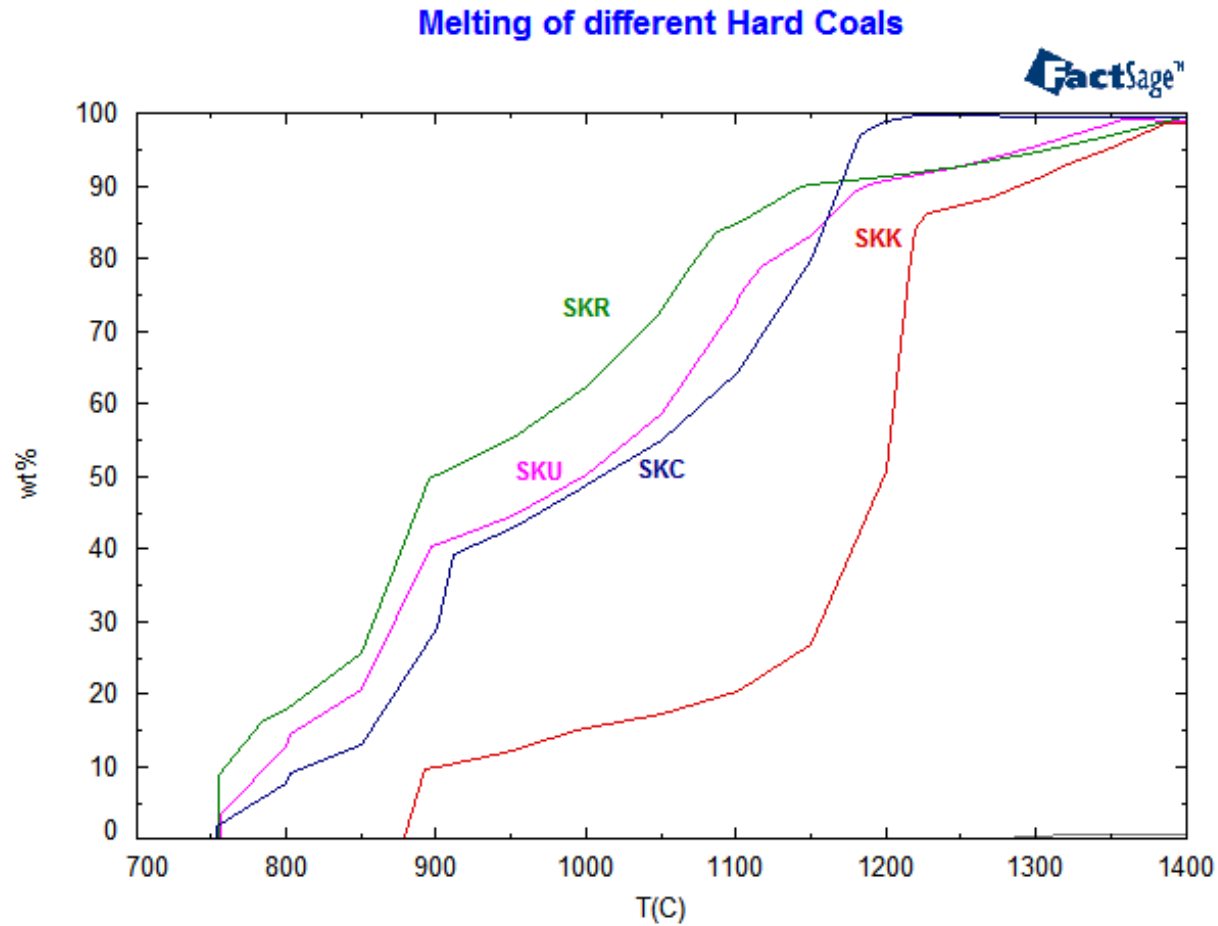
$\text{Al}_2\text{O}_3 - \text{FeO} - \text{SiO}_2$
Projection (Slag), 1 atm



E.F. Osborn, A. Muan: „Phase Equilibrium Diagrams of Oxide Systems“, Plate 9, publ. By American Ceramic Society and the Edward Orton, Jr., Ceramic Foundation, 1960.

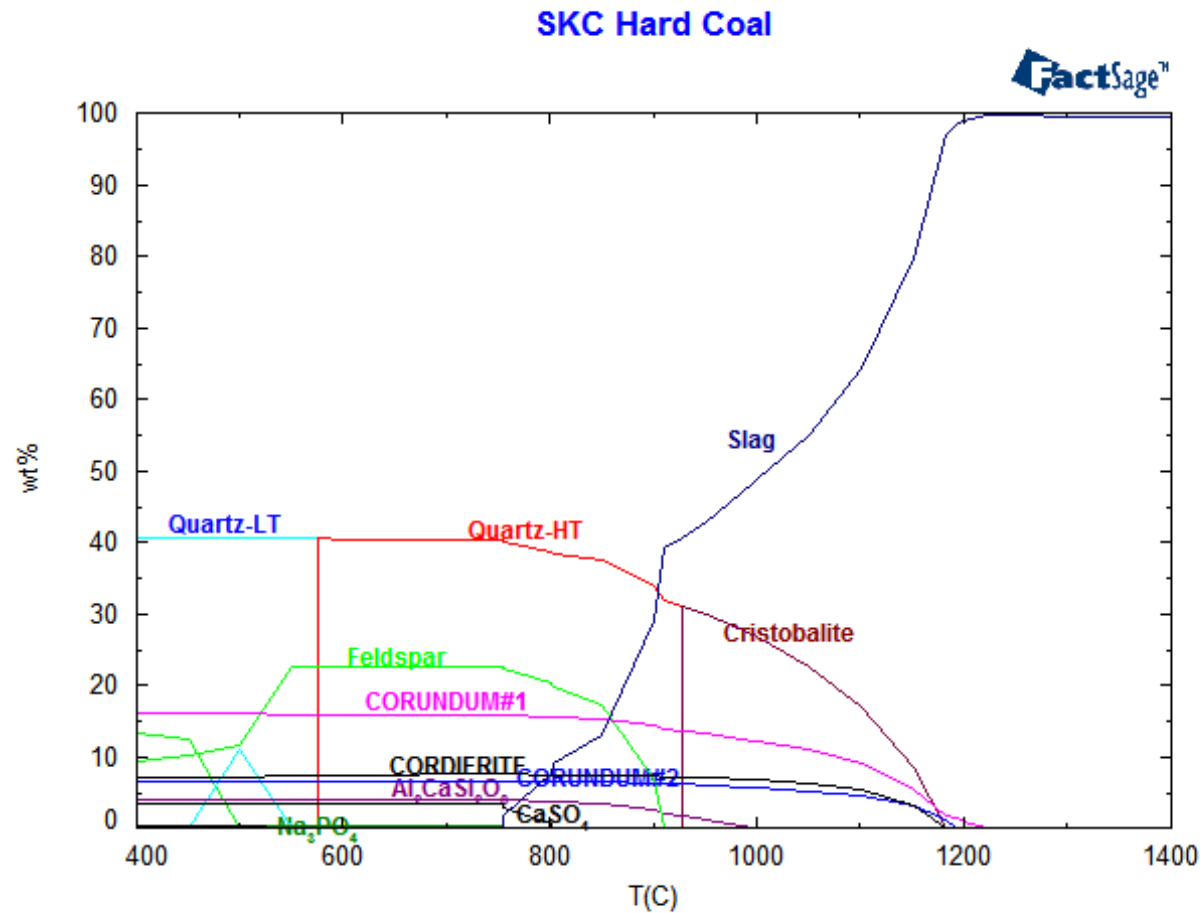


Wt% Melt as f(T)



All phase amounts during melting of SKC

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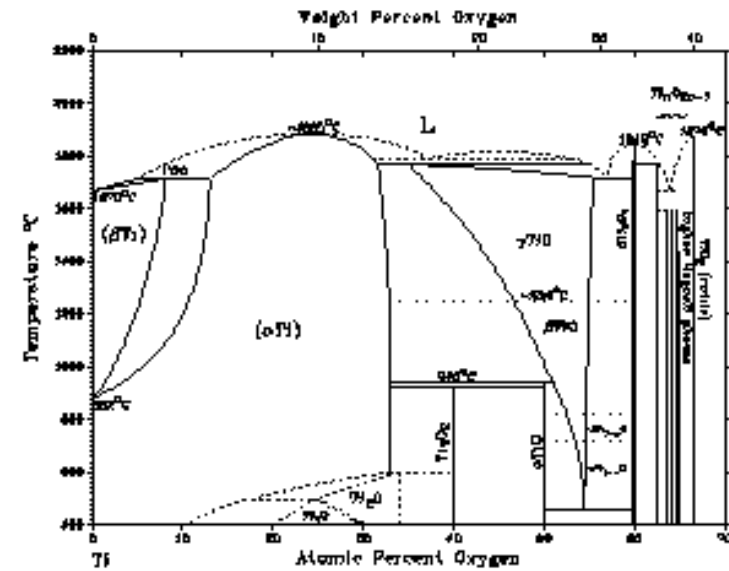
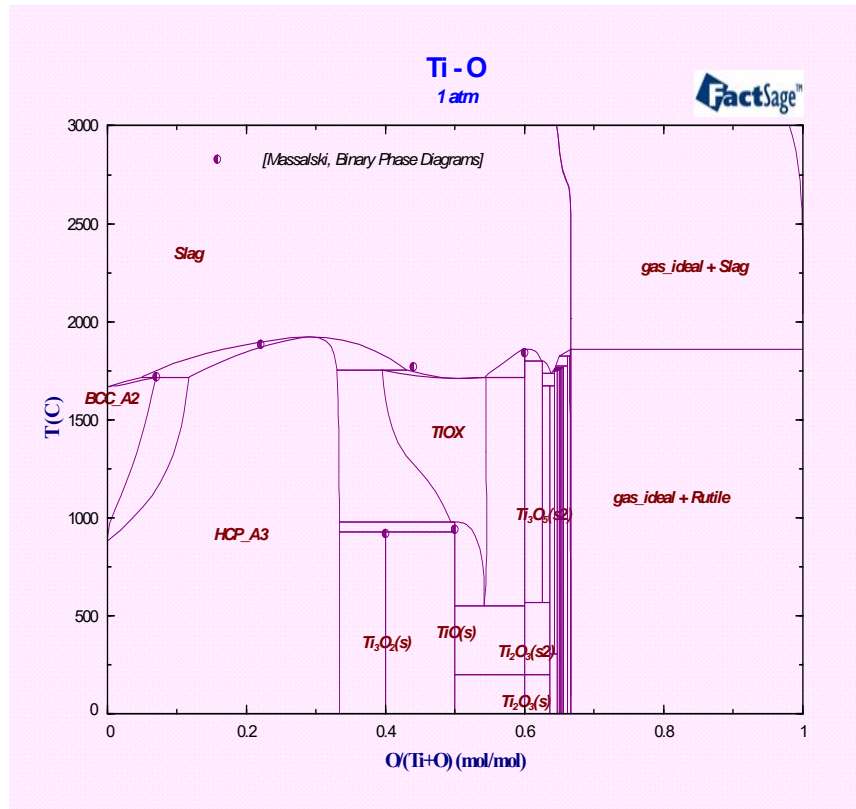
Inclusion of TiO_2

- **Binary systems**
 - *Al-O*
 - *Ti-O*
 - *Al-Ti*
 - *Al_2O_3 - TiO_2*
 - *MgO - TiO_2*
- **Ternary system**
 - *Al-O-Ti*
 - *Al_2O_3 - MgO - TiO_2*



Ti-O phase diagram

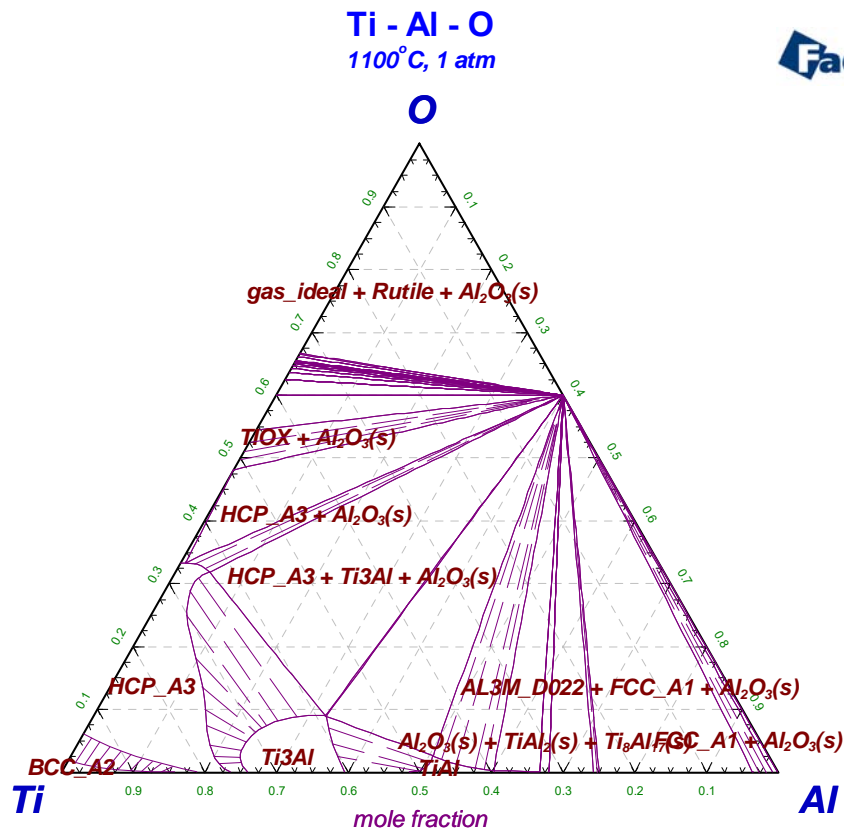
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T.B. Massalski (ed), Binary Alloy Phase Diagrams, Second Edition, ASM International, Metals Park, OH 1990.



Isothermal section at 1100°C in Al-Ti-O



FactSage™

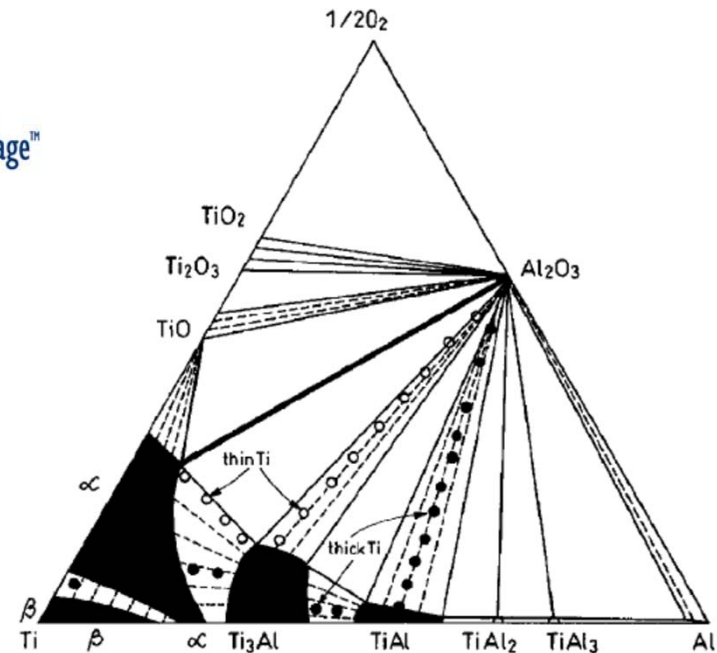


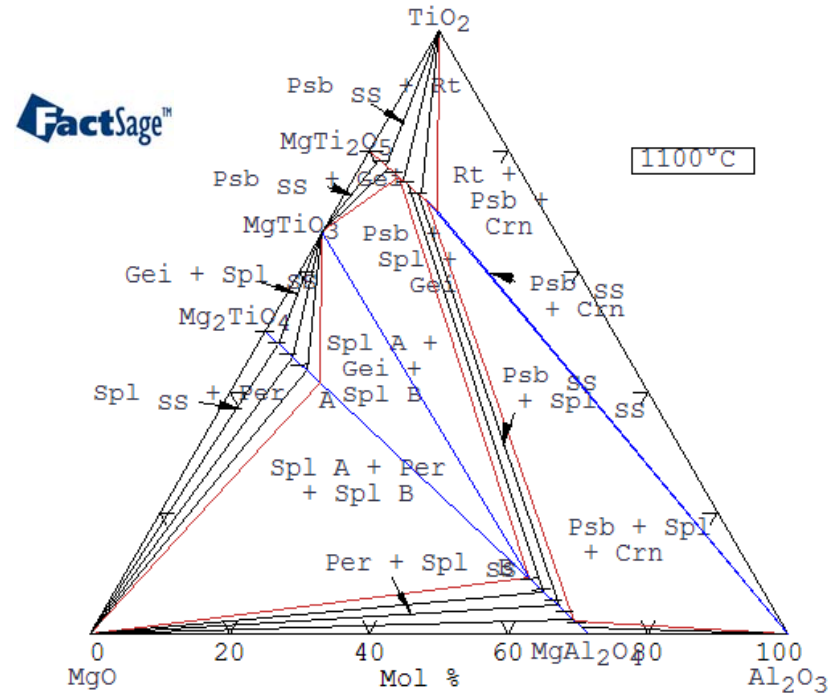
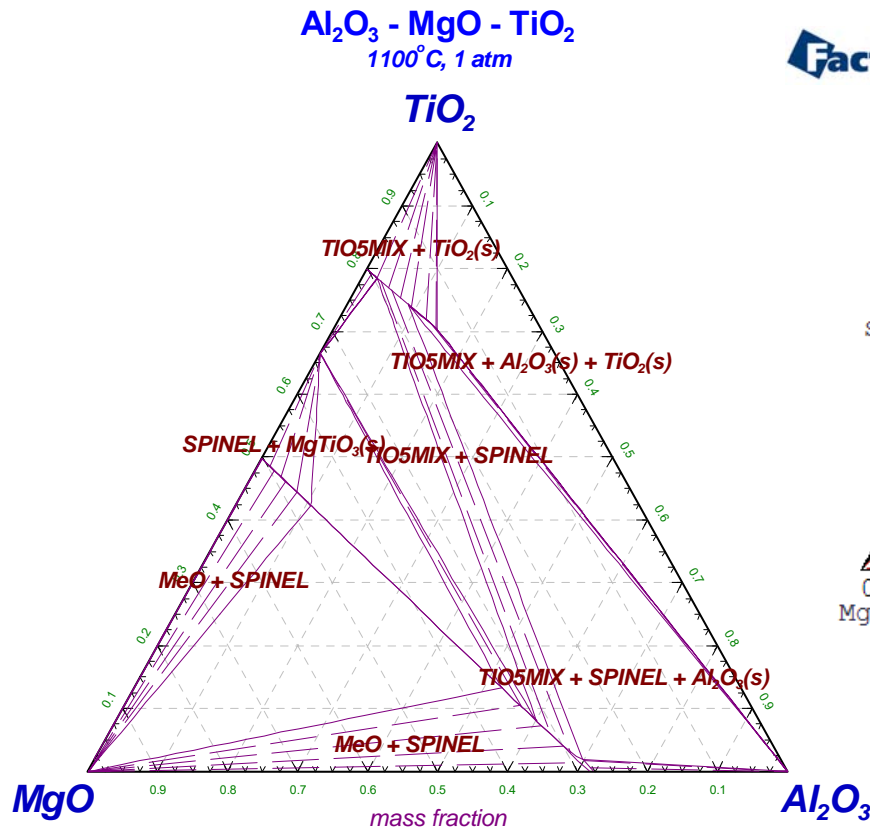
Fig. 7 Experimentally determined isothermal section of the Ti-Al-O system at 1100 °C with diffusion paths indicated [1992Li]

K. Das, P. Choudhury, S. Das. J. Phase Equilib., 23 [6], (2002), pp. 525-536.



Isothermal section at 1100°C in Al_2O_3 - MgO - TiO_2

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P. Boden, F.P. Glasser, Trans. J. Br. Ceram. Soc., 72[5], (1973), pp. 215-220.



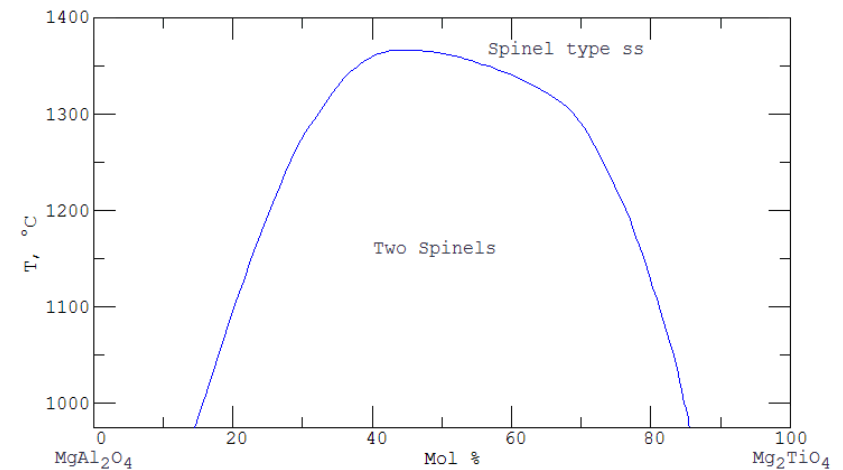
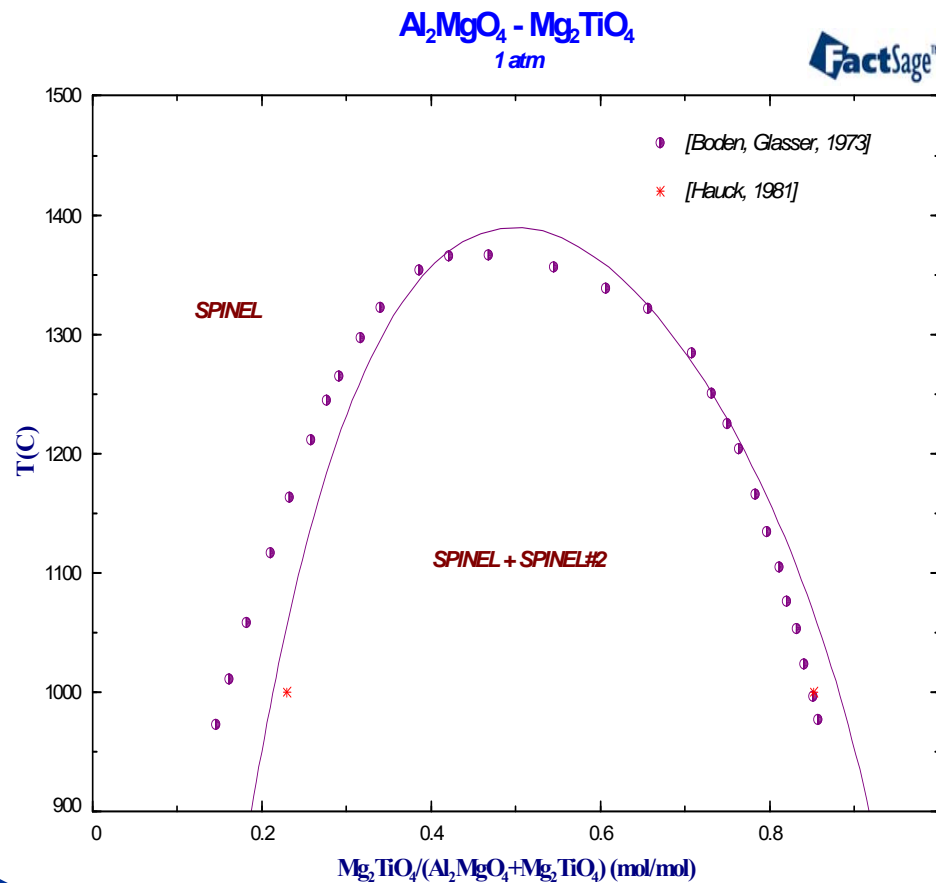
Isopleth $\text{Al}_2\text{MgO}_4\text{-Mg}_2\text{TiO}_4$ in $\text{Al}_2\text{O}_3\text{-MgO-TiO}_2$

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Spinel – solid solution phase with end-members

Al_2MgO_4 and Mg_2TiO_4

$(\text{Al}^{+3}, \text{Mg}^{+2}, \text{Ti}^{+4})_1(\text{Al}^{+3}, \text{Mg}^{+2}, \text{Va})_2(\text{Mg}^{+2}, \text{Va})_2(\text{O}^{-2})_4$

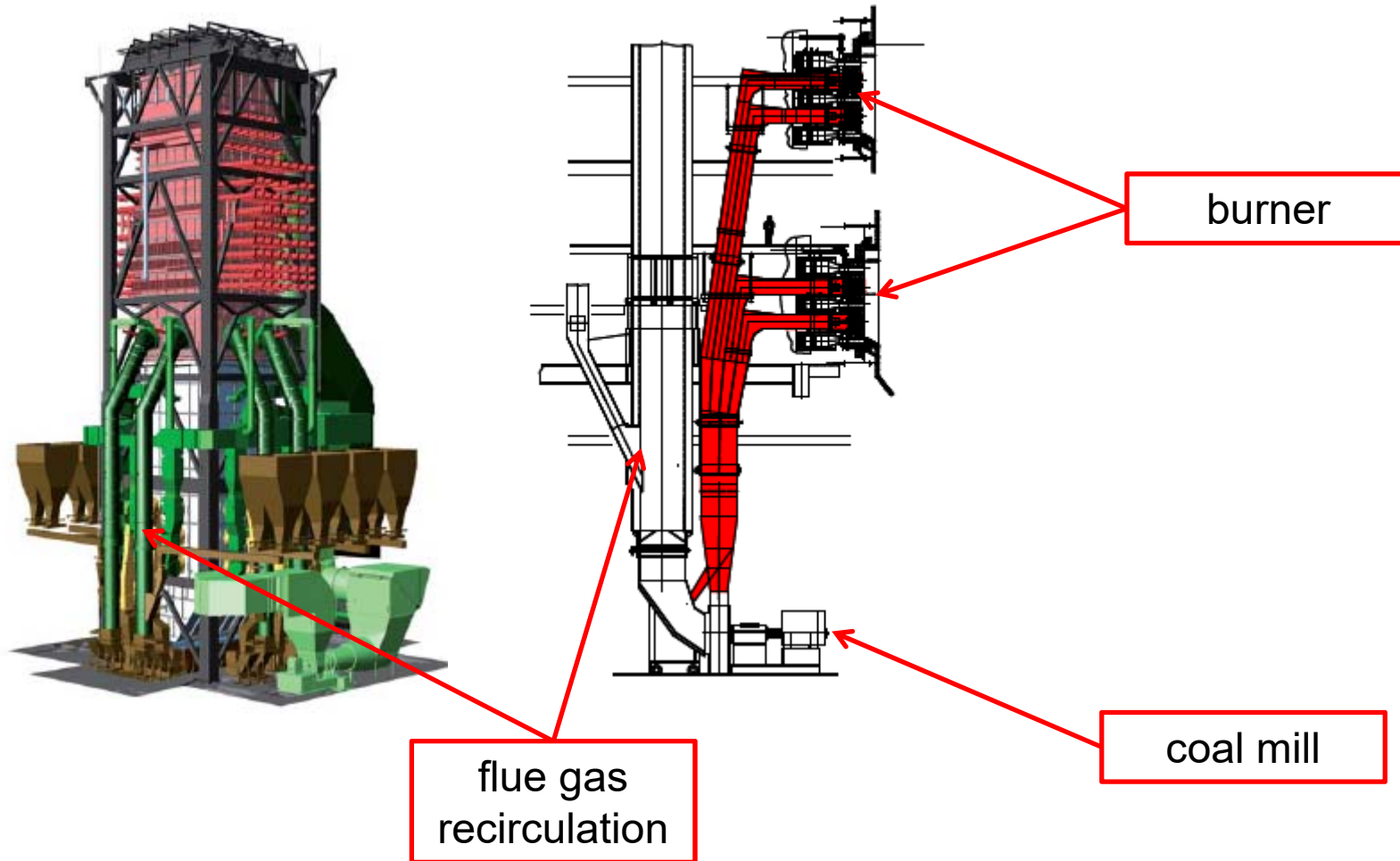


P. Boden, F.P. Glasser, Trans. J. Br. Ceram. Soc., 72[5], (1973), pp. 215-220.



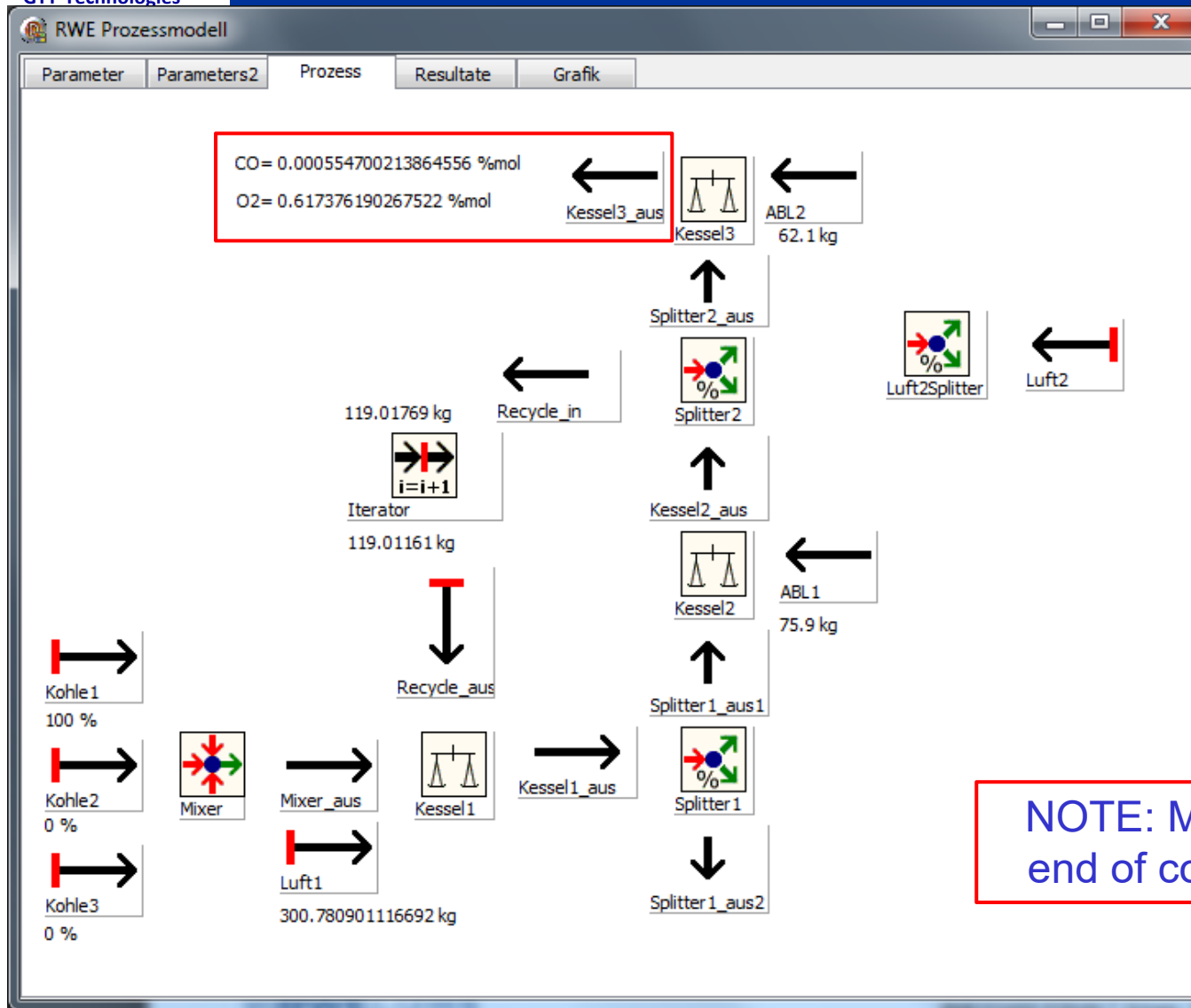
Model relevant Details of Boiler for Dust Combustion

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Furnace chamber: SimuSage model

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Kohle = Coal

Kessel = Boiler

Luft = Air

NOTE: Model ends at upper end of combustion chamber



Furnace chamber model: User interface I

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**Air supply:
On average or partitioned in four areas**

The screenshot shows the 'RWE Prozessmodell' software interface with several parameter sections:

- Kohlen:** Summe Kohle = 100 kg/s. Includes buttons for 'Kohle1 Definieren', 'Kohle2 Definieren', and 'Kohle3 Definieren' with corresponding percentage inputs (100%, 0%, 0%).
- Kessel:** Kessel 1 Temp = 1400 °C, Kessel 2 Temp = 1300 °C, Kessel 3 Temp = 1200 °C.
- Splitter:** Faktor Nassasche - Flüssig = 0.8, Faktor Nassasche - Fest = 0.5, Faktor Rauchgasrückführung = 0.8.
- Luft1:** Radio button for 'Lambda' (selected) with value 0.8, and 'Amount' section with four input fields for Luft1.1 to Luft1.4, all set to 0 kg/s.
- Luft2:** Luft2 = 200 kg/s.
- Faktor ABL1/ABL2:** 0.7.
- Iterator:** Iterationsgenauigkeit = 0.01.
- START** button at the bottom right.

The screenshot shows the 'Coal1 Edit' software interface with a table of chemical constituents and their percentages:

| Konstituente | % | Ort |
|--------------|--------------------|-------------------|
| H2O | 52.3972201013215 | NIA |
| Na2O | 0.129809156307231 | Anlage |
| K2O | 0.0254664044185653 | Bekohlung |
| CaO | 0.774186527607638 | Teilanlage |
| MgO | 0.333806403643055 | Kohleprobennehmer |
| Al2O3 | 0.252289580199826 | Material |
| SiO2 | 0.865585891604302 | Kohle |
| Fe2O3 | 0.260313030969009 | Datum |
| TiO2 | 0.0177159249585819 | 11.09.2001 |
| SO3 | 0.606917607351214 | Zeit |
| C | 31.3574097131461 | 06:00:00 |
| O2 | 10.3834237267784 | |
| H2 | 2.5958559316946 | |

Below the table, there is a 'SUM= 100%' label, an 'Import from Database' section with a 'Data Source' field containing the path 'C:\LocalData\GTT_ANWENDUNGEN\Model 2.3\KASIS-05V01.mdb', and buttons for 'Browse', 'ProbenNr : 01-010-0001', 'Import', 'Reset', 'Clear', 'Cancel', and 'Create'.

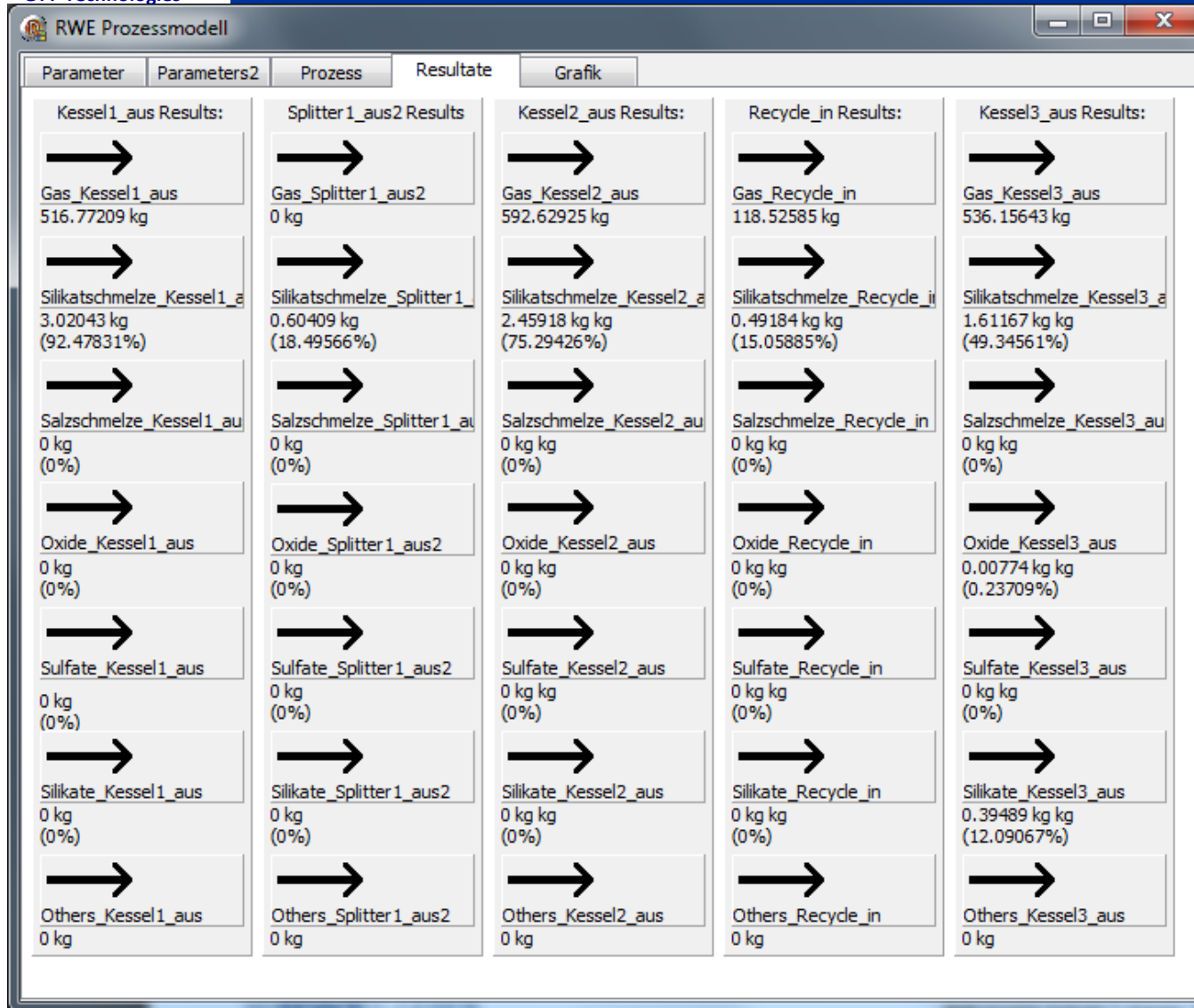
**Proportion of fluid / solid wet ash
Proportion of flue gas recirculation**

**Temperatur in combustion chamber
partitioned in three areas**



Furnace chamber model: Results I

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Phases are compiled in characteristic groups:

- Silicate melt
- Salt melt
- Solid oxides
- Solid sulphates
- others



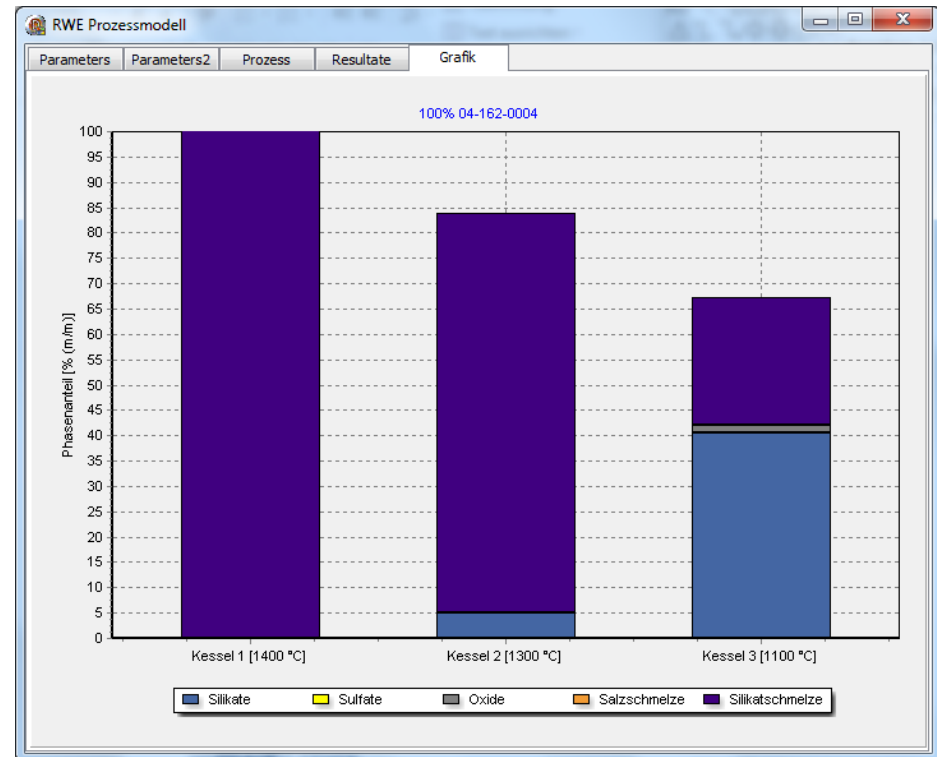
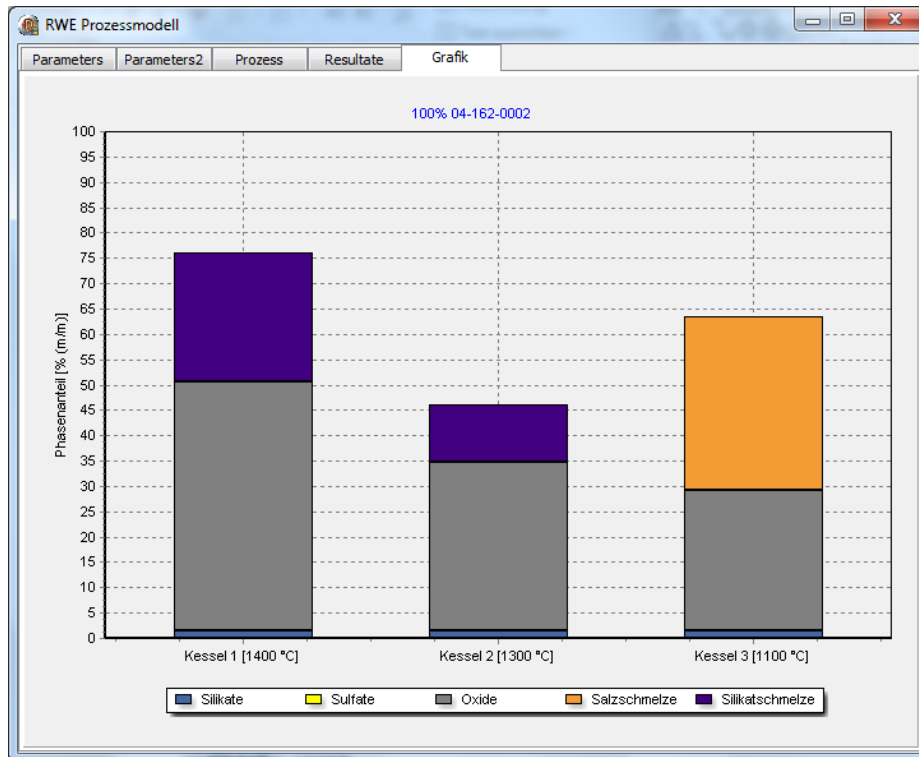
Furnace chamber model: Results IIa

Influence of coal blends on phase formation

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100% HKN

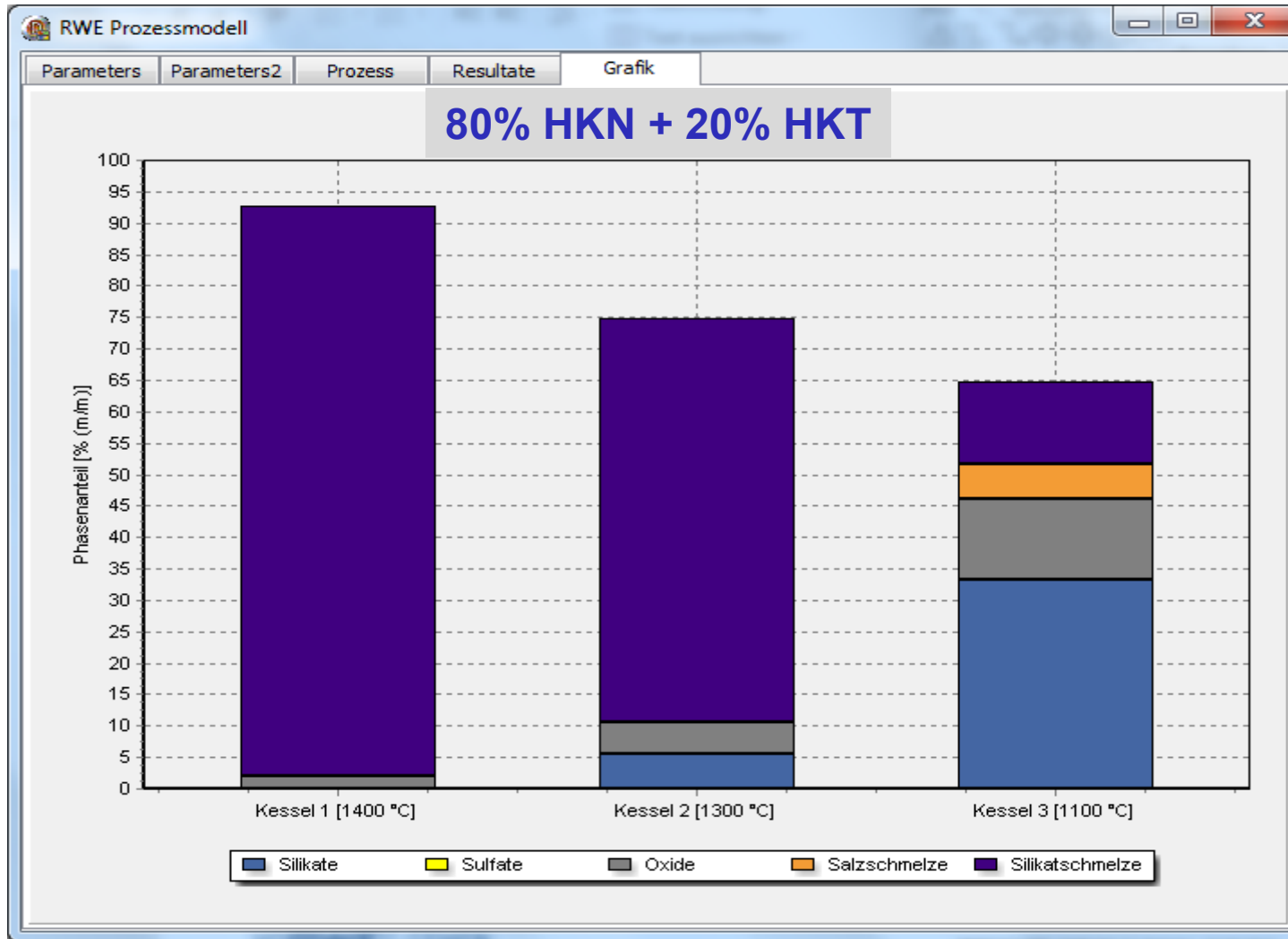
100% HKT



Furnace chamber model: Results IIb

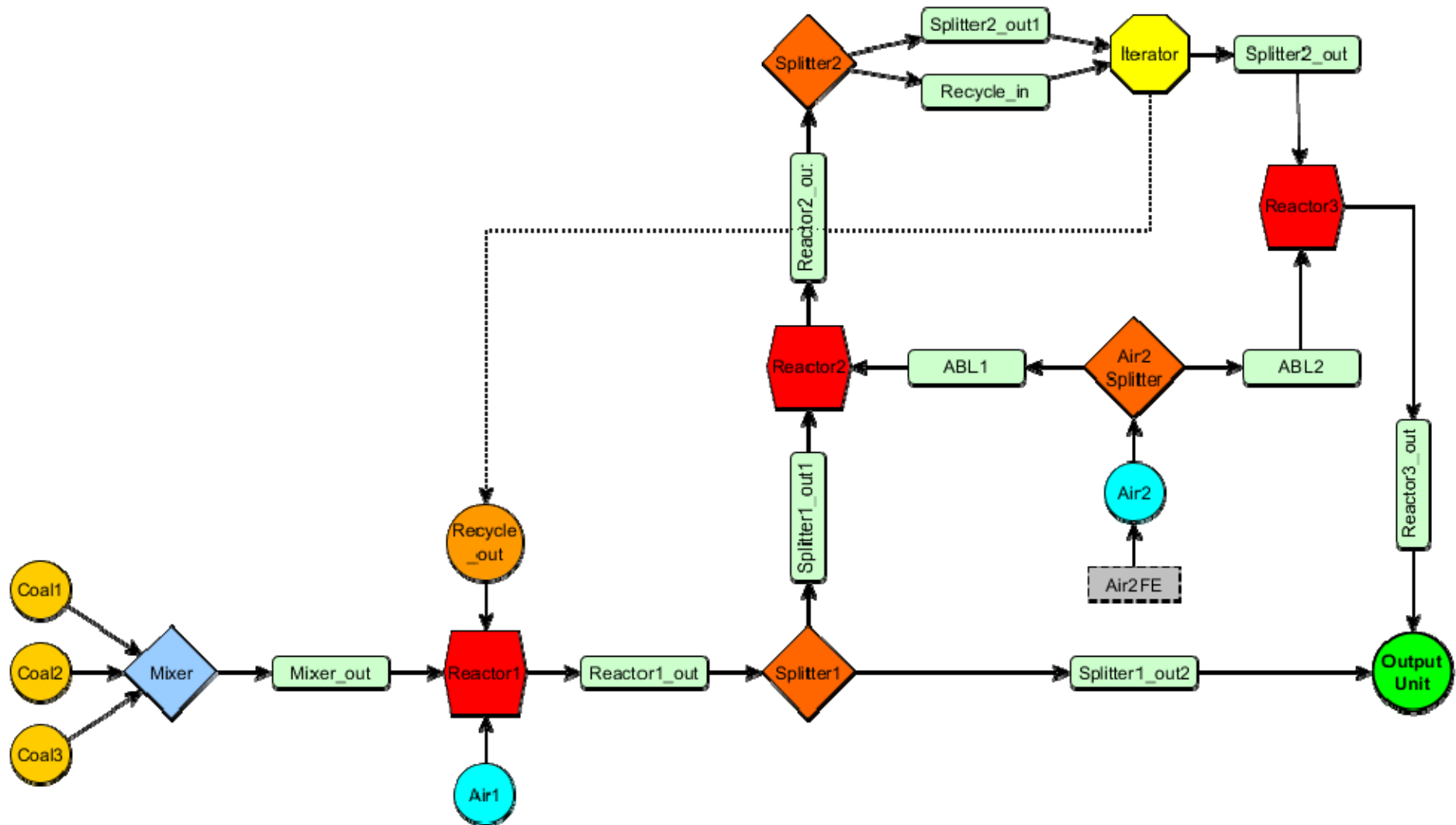
Influence of coal blends on phase formation

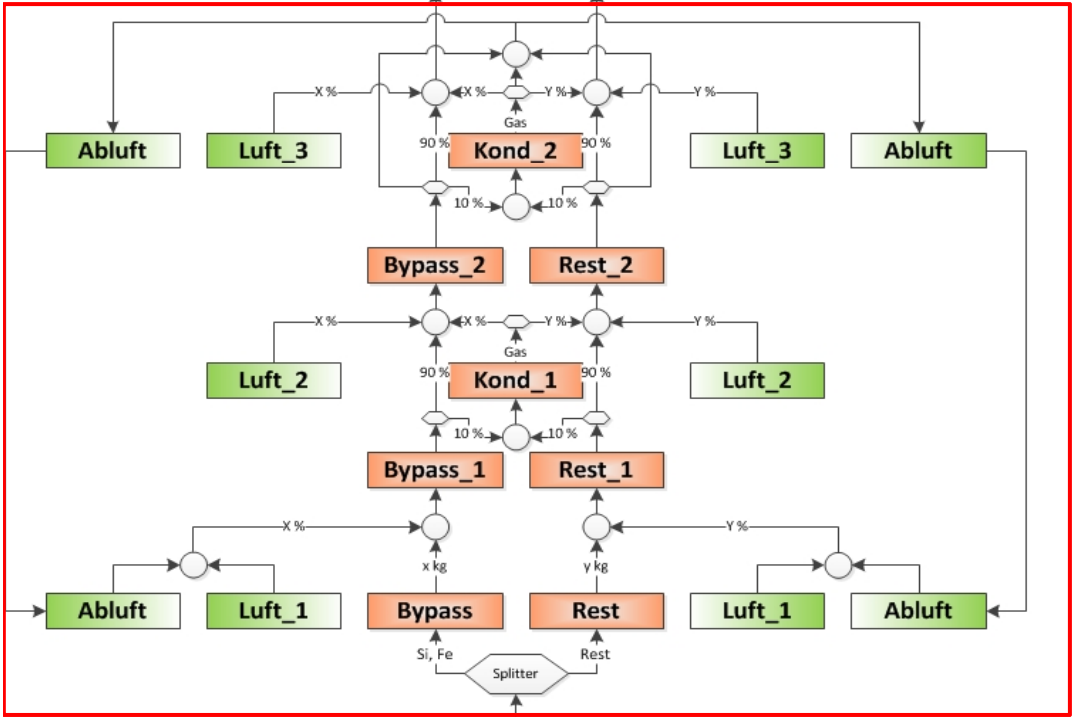
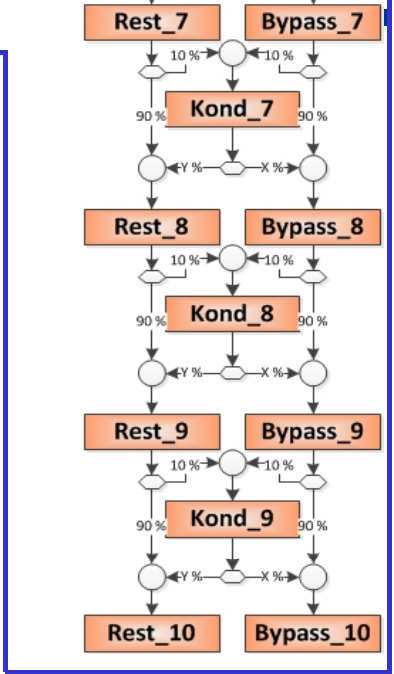
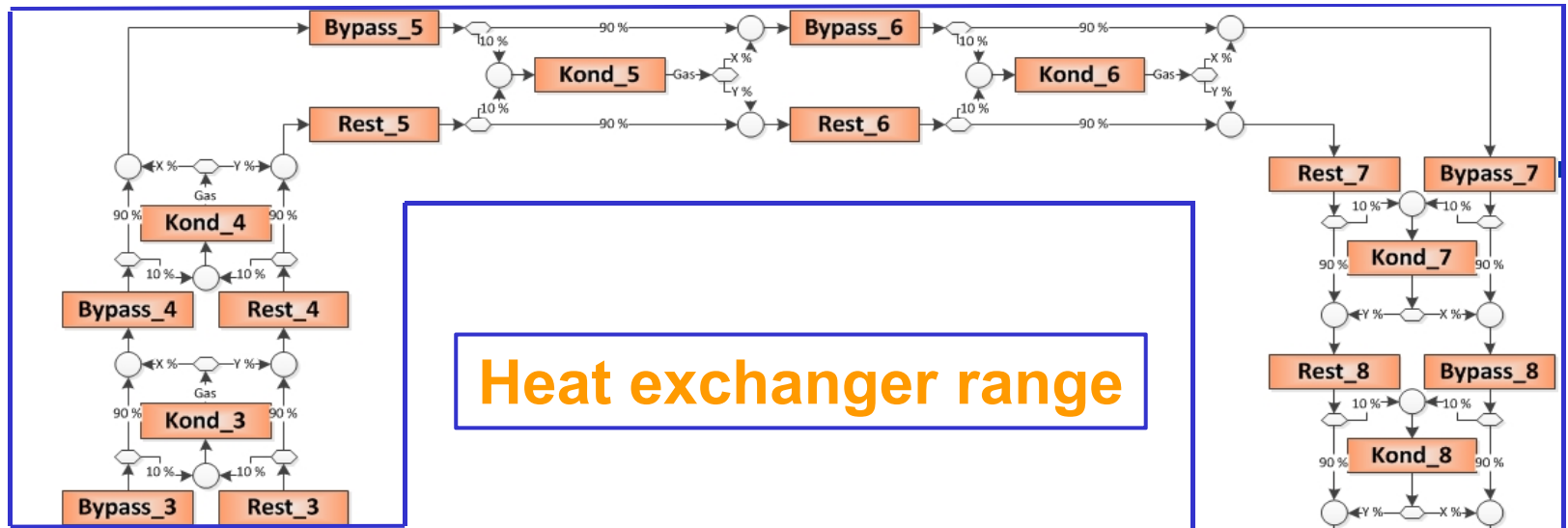
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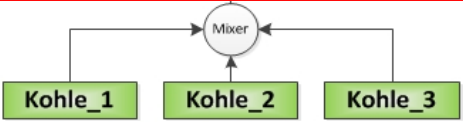
Scheme of the RWE model

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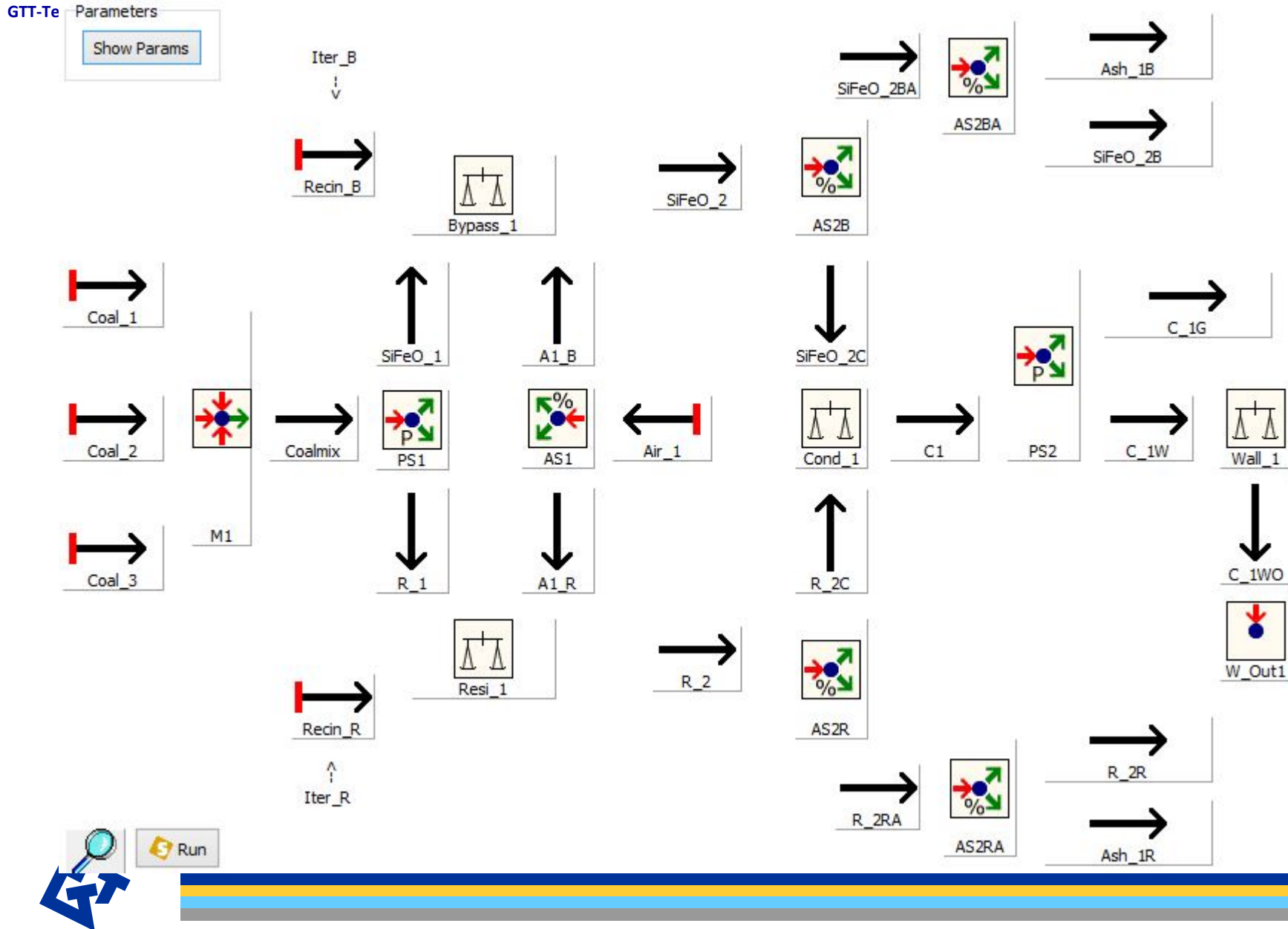
Combustion chamber



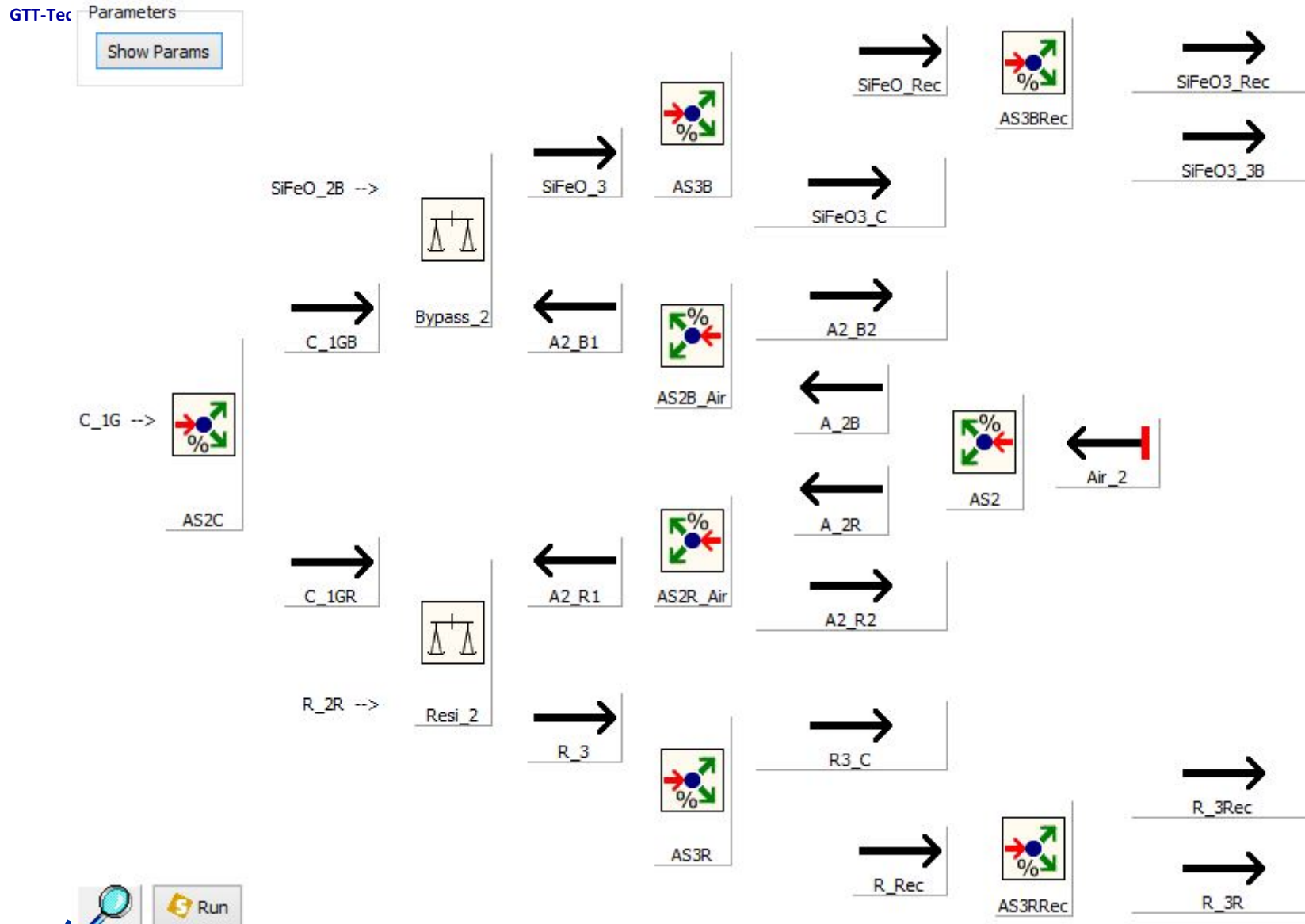
(= $x/(x+y)$
 ' = $y/(x+y)$



Realisation with SimuSage, Part 1



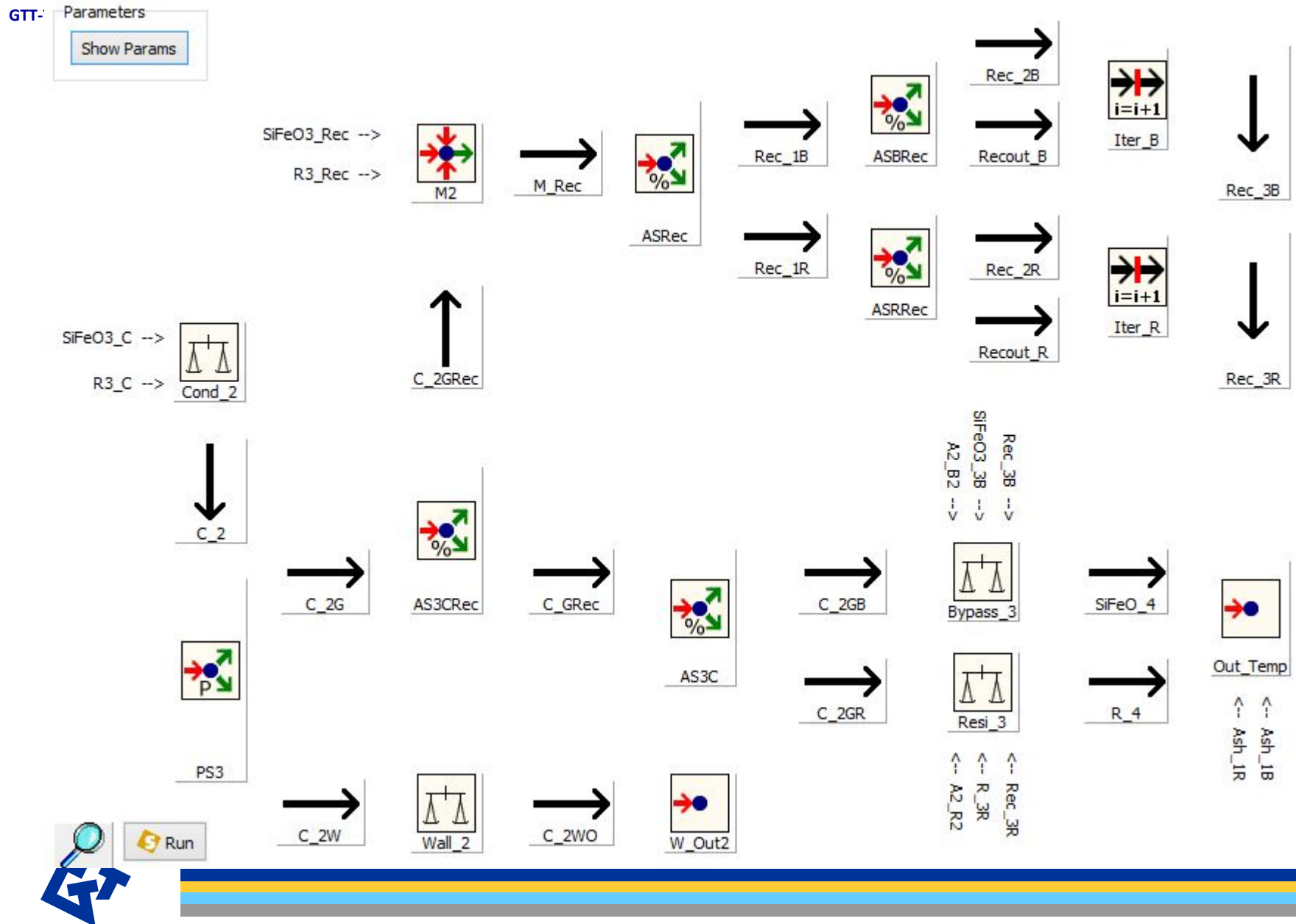
Realisation with SimuSage, Part 2



Run



Realisation with SimuSage, Part 2



Test of model compatibility

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Report Editor

-- PageControl1.Process3.R_4 -->>

| | |
|----------------|------------------|
| ChemDFI: | SIMEX |
| Rank(From,To): | (1, 1) |
| FromUnit: | Resi_3 |
| ToUnit: | Out_Temp |
| Stream Type: | ALL |
| Amount: | 21.8767 kMol |
| Enthalpy: | -1065748.0983 kJ |
| Temperature: | 1200.00 C |
| Pressure: | 1 bar |
| Volume: | 2.675E006 dm3 |

| | |
|---------------|-----------------|
| ASlag-liq#1 | |
| Amount: | 0.03719 kMol |
| Enthalpy: | -27184.3822 kJ |
| Constituents: | |
| Al2O3 | 0.00171487 kMol |
| SiO2 | 0.0132291 kMol |
| NaAlO2 | 0.00225709 kMol |
| CaO | 0.011196 kMol |
| Fe2O3 | 0.0012844 kMol |
| MgO | 0.00638229 kMol |

Threshold Amount: 1 E -3

[kg], wt% [Nm3], mol% [kMol]

Save

RWE Prozessmodell

Parameters Parameters2 **Prozess** Resultate Grafik

CO= 0.00022 %mol
O2= 3.72999 %mol

← Kessel3_aus Kessel3 ← ABL2
60 kg

Kohle1 100 %
Kohle2 0 %
Kohle3 0 %

Mixer

PS3 C_2W Wall_2 P = 1
↓
C_2WSC SF = 0
← C_2WO ASZSC

W_Out2

Report Editor

-- PageControl1.ProcessTab.Kessel3_aus -->>

| | |
|----------------|------------------|
| ChemDFI: | SIMEX |
| Rank(From,To): | (1, 2) |
| FromUnit: | Kessel3 |
| ToUnit: | OutputUnit |
| Stream Type: | ALL |
| Amount: | 21.8767 kMol |
| Enthalpy: | -1065748.0959 kJ |
| Temperature: | 1200.00 C |
| Pressure: | 1 bar |
| Volume: | 2.675E006 dm3 |

| | |
|---------------|-----------------|
| ASlag-liq#1 | |
| Amount: | 0.03719 kMol |
| Enthalpy: | -27184.3820 kJ |
| Constituents: | |
| Al2O3 | 0.00171487 kMol |
| SiO2 | 0.0132291 kMol |
| NaAlO2 | 0.00225709 kMol |

Threshold Amount: 1 E -3

[kg], wt% [Nm3], mol% [kMol]

Save Append

State of development

GTT-Technologies

- First test: re-produce RWE model by appropriate choice of split factors
→ All numerical values agree 1:1 !!!
- Now in progress: run model with split factors realising no wall-sticking and no silicate by-pass, i.e. extend RWE-model by stages related to heat exchangers
- Next step: include silicate by-pass
- Then: include wall-sticking



Summary and Outlook

GTT-Technologies

SimuSage based model using interlinked local equilibria

- Furnace chamber model with interactive user interface and direct access to RWE mineral analyses database
 - First step into development of a proper process model for coal fired power plant
 - Furnace chamber with recirculation of flue gas and input option for coal blends
- **To come: *Optimisation* calculations for coal blends as well as *extension into boiler range* and *deposit modelling***
(→VerSi project)



**THANK YOU VERY MUCH
FOR YOUR ATTENTION !**

