Importance of realistic gas atmosphere assumptions for combustion and gasification calculations

M. to Baben, J. Rezende, K. Hack

GTT-Technologies

Thermodynamic Software

Thermodynamic Databases

Consulting Services

Outline

- Motivation
- An unintentional experiment
- FactSage applications
  - Ash fusion experiments
  - Melting and oxidation of sulfides from coal ashes
  - Condensation of salts during cooling of syngas

Motivation

- Typical coal/biomass specification is based on several measurements: Caloric value, Proximate analysis, ultimate analysis, ash analysis, ash XRD, ash fusion test…
- Each test is performed under different conditions wrt. temperature and gas atmosphere.

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Mineral	1
Silicates	83.5
Quartz	49
Cristobalite	
Opal	
Kaolinite	14
Illite + Muscovite	6
Montmorillonite	0.5
Chlorite	2
Plagioclase	7
K feldspar	3
Zeolite	2
Oxides and hydroxides	2.5
Magnetite + Hematite	1
Goethite + Lepidocrocite	1
Spinel + Fe spinel	0.5
Corundum	
Diaspore + Boehmite + Gibbsite	
Brucite	
Carbonates	5.5
Calcite	3
Dolomite	1
Ankerite	0.5
Siderite	1
Magnesite	
Sulphides	2
Pyrite	2
Marcasite	
Pyrrhotite	
Sulphates	3.5
Gypsum	1
Jarosite + Melanterite	1.5
Alunite	0.5
Hexahydrite	
Barite	0.5
Phosphates	1.5
Apatite	1
Vivianite	0.5
Goyazite	
Total	98.5

Table 2
Chemical composition (wt. %) and ash-fusion temperatures (°C) of the coal samples

Sample	Proximate analysis (as received)				Ultimate analysis (daf)					High-temperature ash analysis (815 °C)											Ash-fusion test[a]		
	FC	VM	A	M	C	O	H	S	N	SiO_2	Al_2O_3	Fe_2O_3	CaO	SO_3	MgO	K_2O	TiO_2	Na_2O	SiO_2 / Al_2O_3	DAI[b]	ST	HT	FT
1. Akabira	23.8	24.6	48.9	2.7	76.4	16.0	6.1	0.4	1.1	62.96	21.16	5.58	2.37	1.28	2.11	2.33	0.80	1.42	3.0	7.8	1180	1380	1400

Vassilev, Fuel 88 (2009) 235.

Motivation

- Typical coal/biomass specification is based on several measurements: Caloric value, Proximate analysis, ultimate analysis, ash analysis, ash XRD, ash fusion test…
- Each test is performed under different conditions wrt. temperature and gas atmosphere.
- “What atmosphere should I set to compare an ash fusion test with a FactSage calculation?“
- “How do I consider slow reactions in the boiler?“
- “How do I choose the atmosphere when modelling deposit formation?“

Mineral	1
Silicates	83.5
Quartz	49
Cristobalite	
Opal	
Kaolinite	14
Illite + Muscovite	6
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1. Akabira	23.8	24.6	48.9	2.7	76.4	16.0	6.1	0.4	1.1	62.96	21.16	5.58	2.37	1.28	2.11	2.33	0.80	1.42	3.0	7.8	1180	1380	1400

Vassilev, Fuel 88 (2009) 235.

An accidental experiment

An accidental experiment

An accidental experiment – and its analysis

Turbo Power TwinTurbo 380

by Turbo Power

7 ratings

Price: $199.99 ($199.99 / Count) & FREE S

Get $50 off instantly: Pay $149.99 upon app

Item is returnable in 30 days and restocking

- Air Flow: 79 m³/h.
- Drying Power: 2100 Watts.
- Technology: Ceramic and Ionic.
- Attachments: 2 Concentrator Nozzles.
- Weight: 500 grams / 1.10 lbs.

Compare with similar items

2 new from $199.98

79 m^3/h = 1320 l/min = 54 mol N_2 / min

https://www.amazon.com/Turbo-Power-TwinTurbo-3800-Ceramic/dp/B015ETW176

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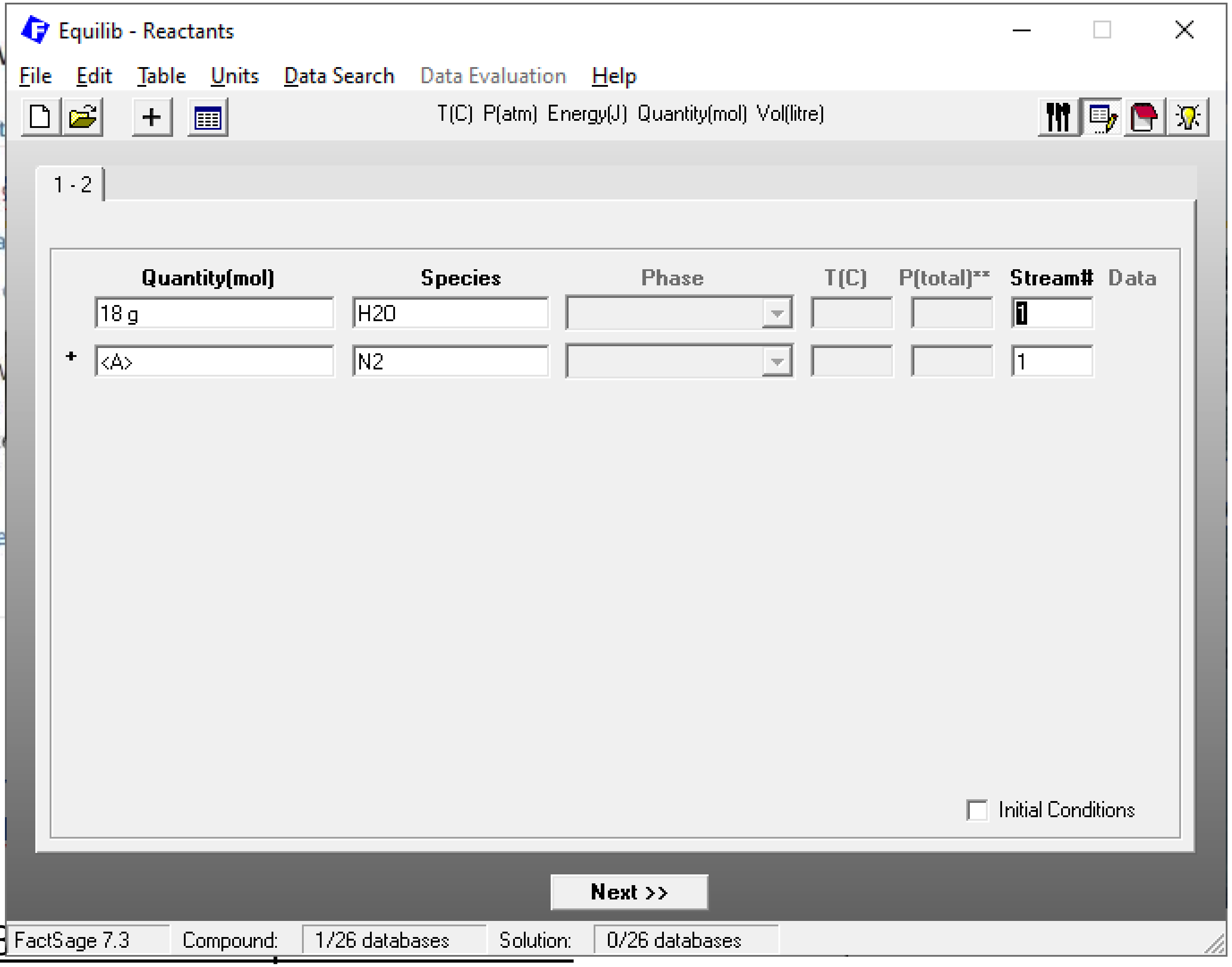
An accidental experiment – and its analysis



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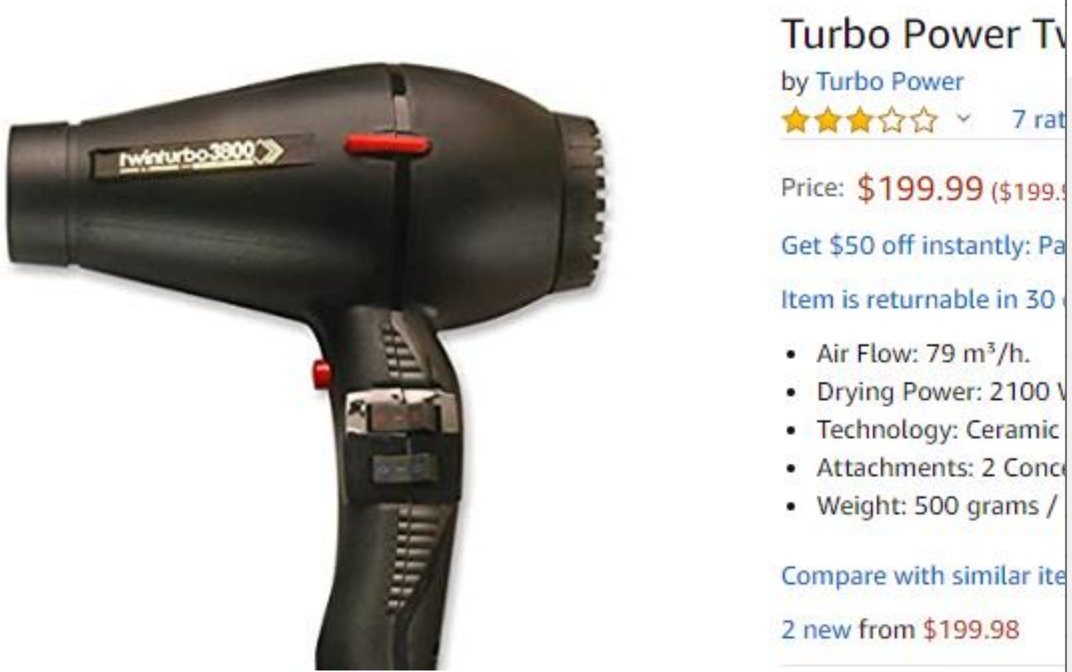

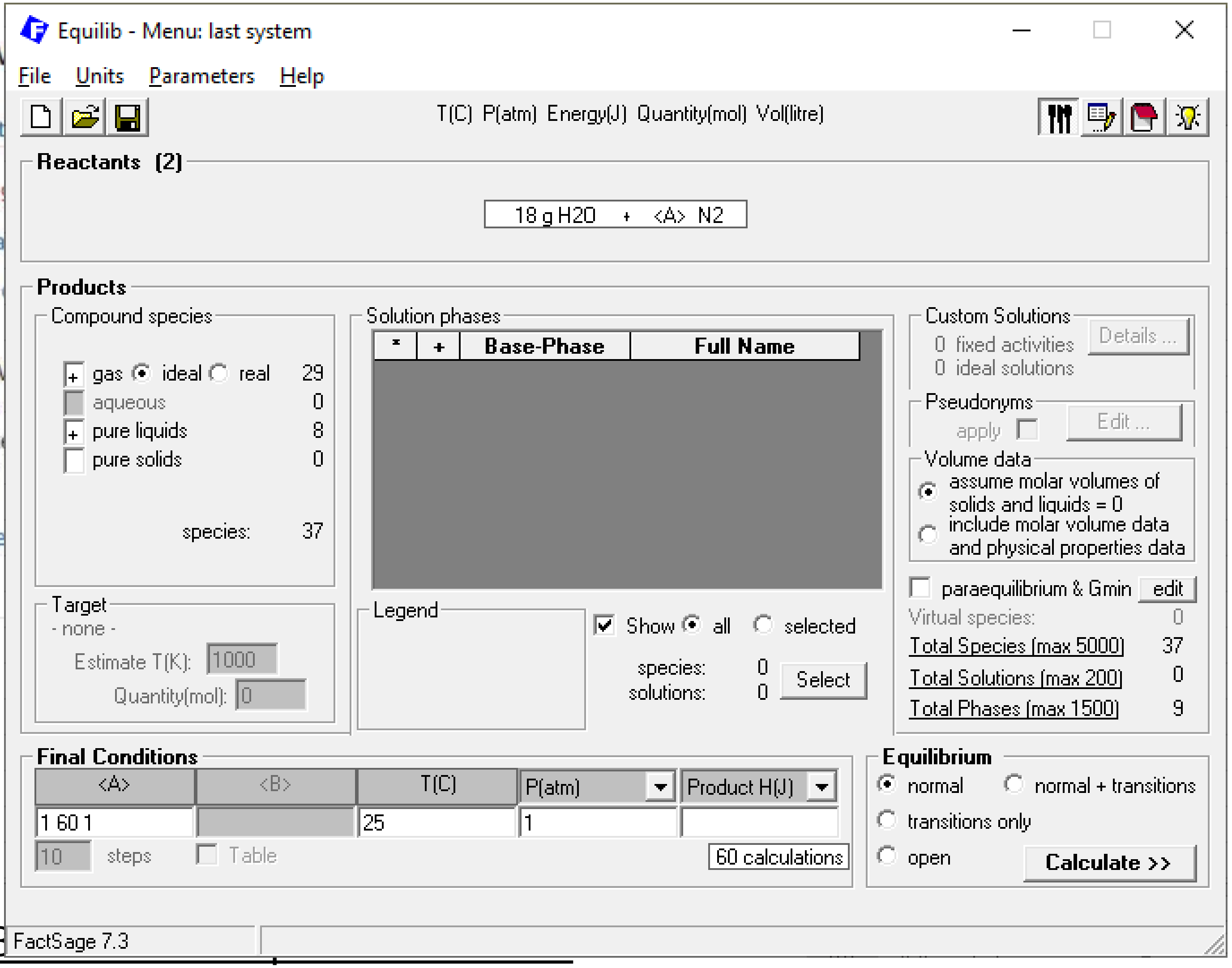

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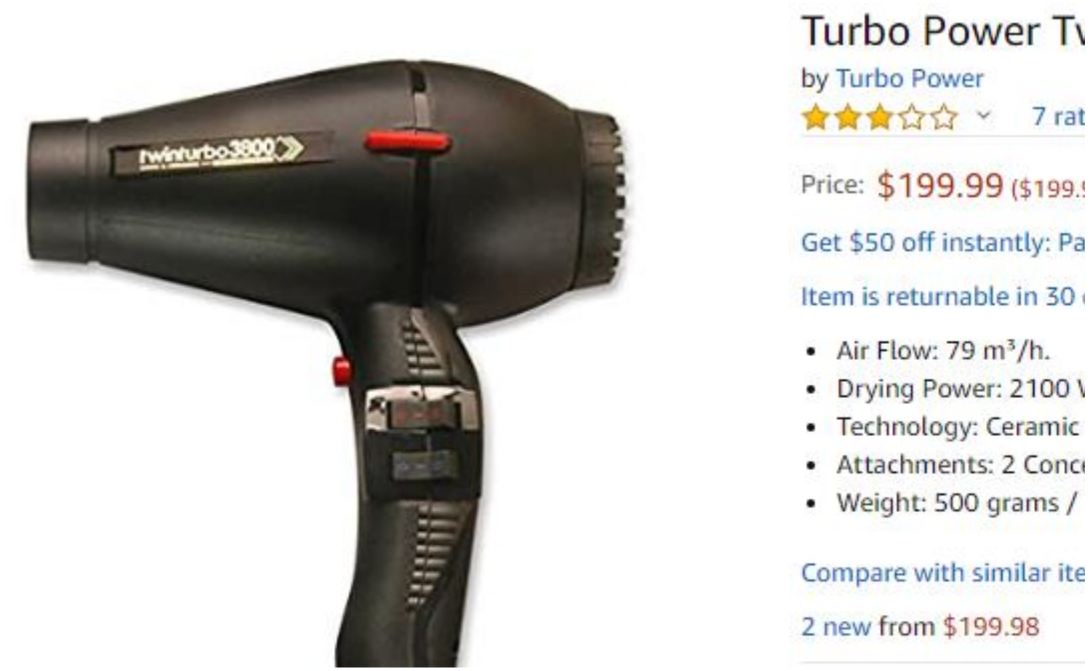

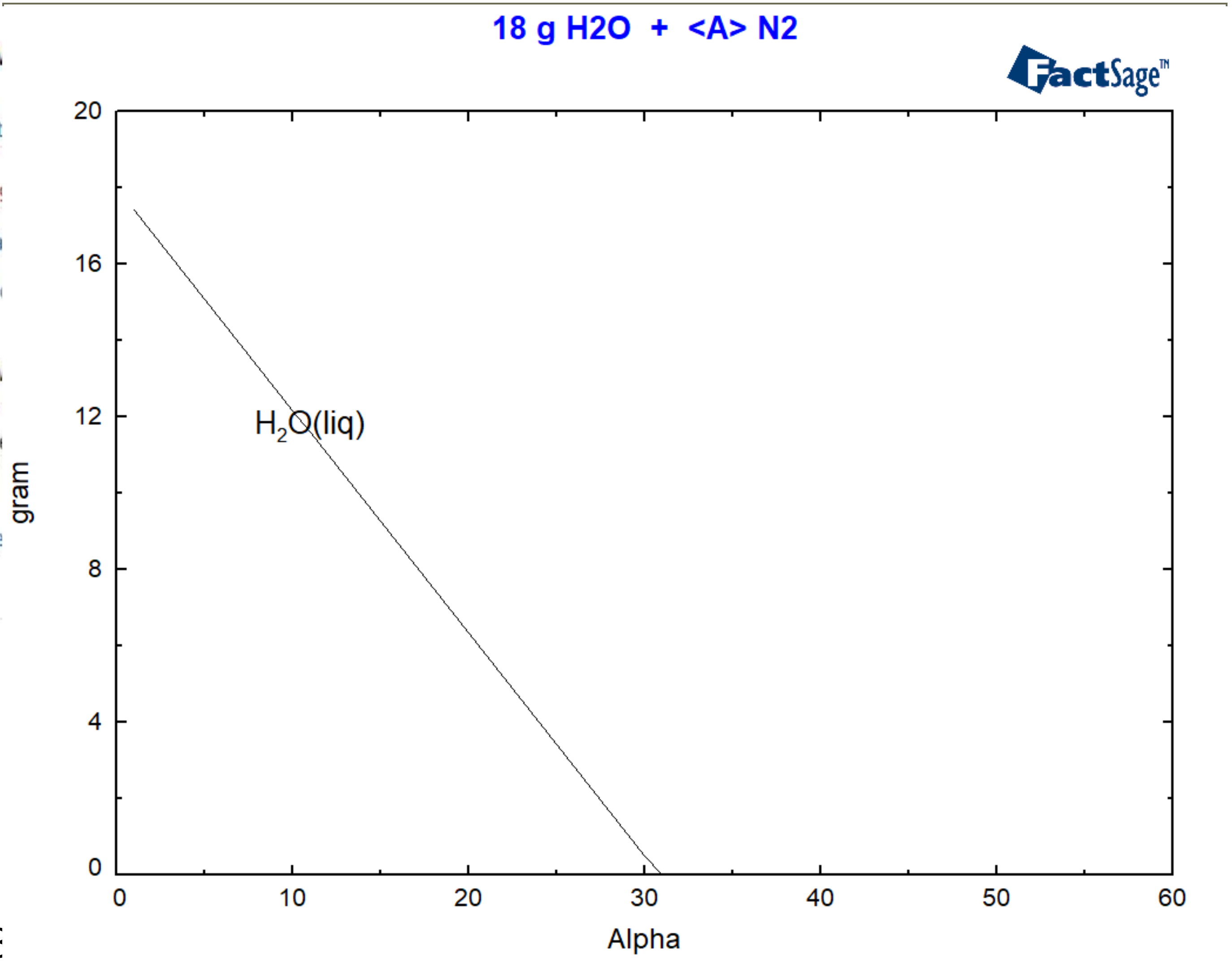

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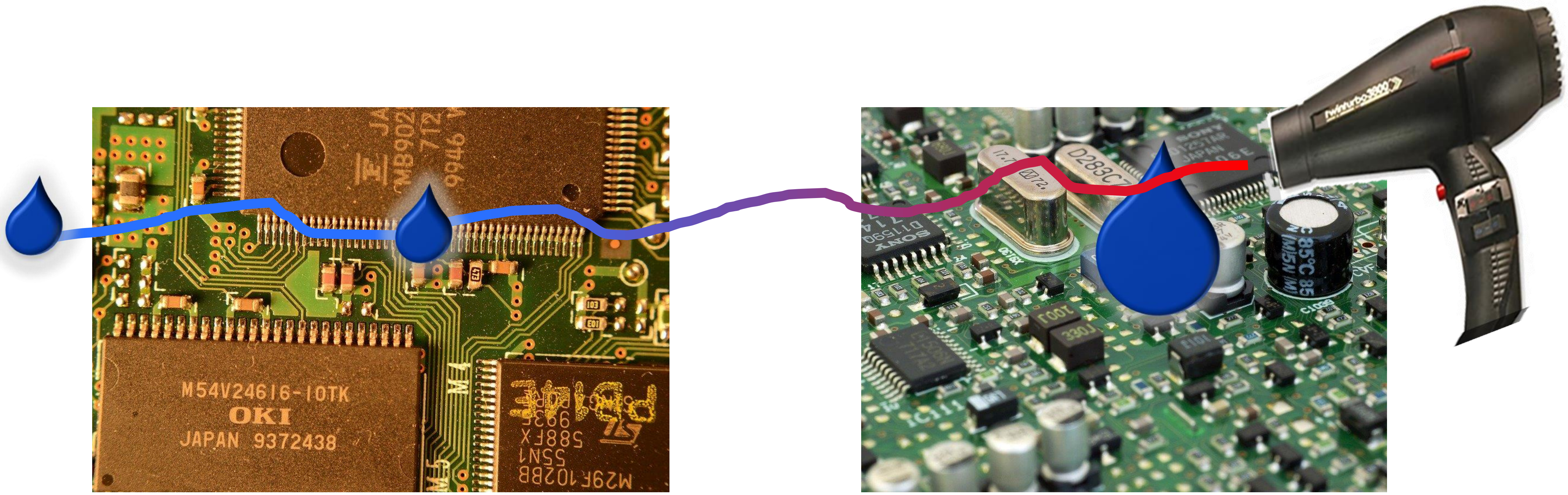
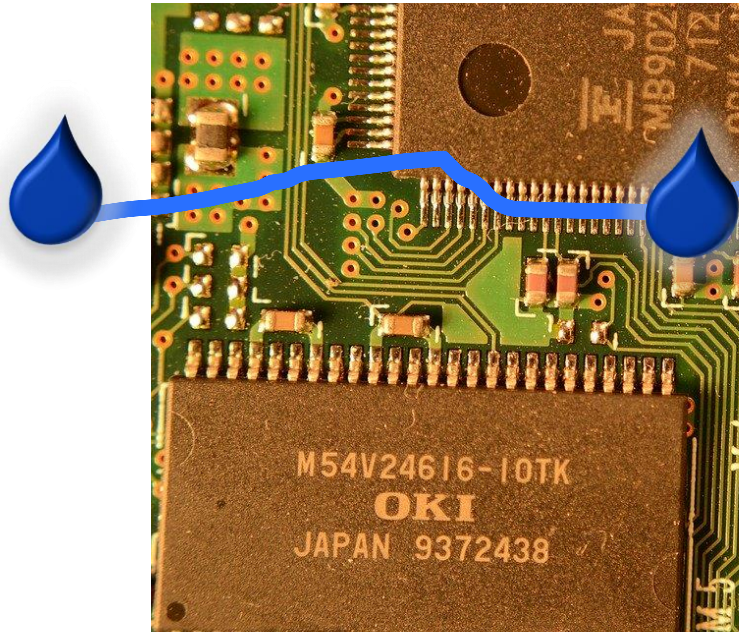
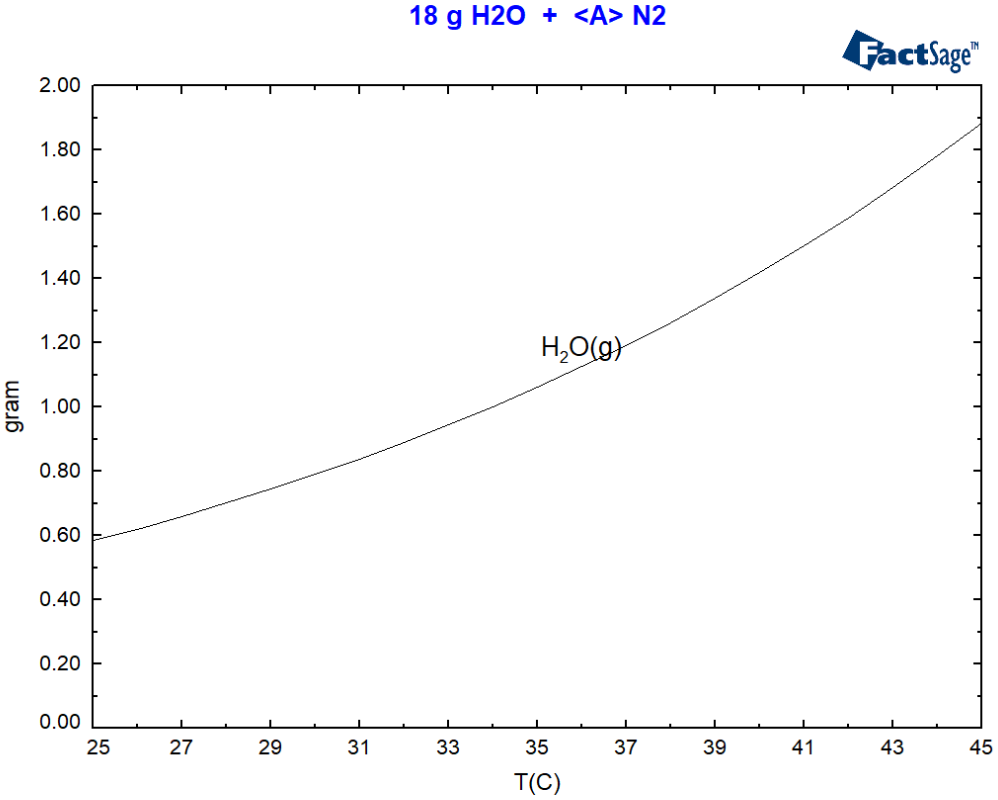


T = 25°C

T = 45°C

An accidental experiment – and its analysis





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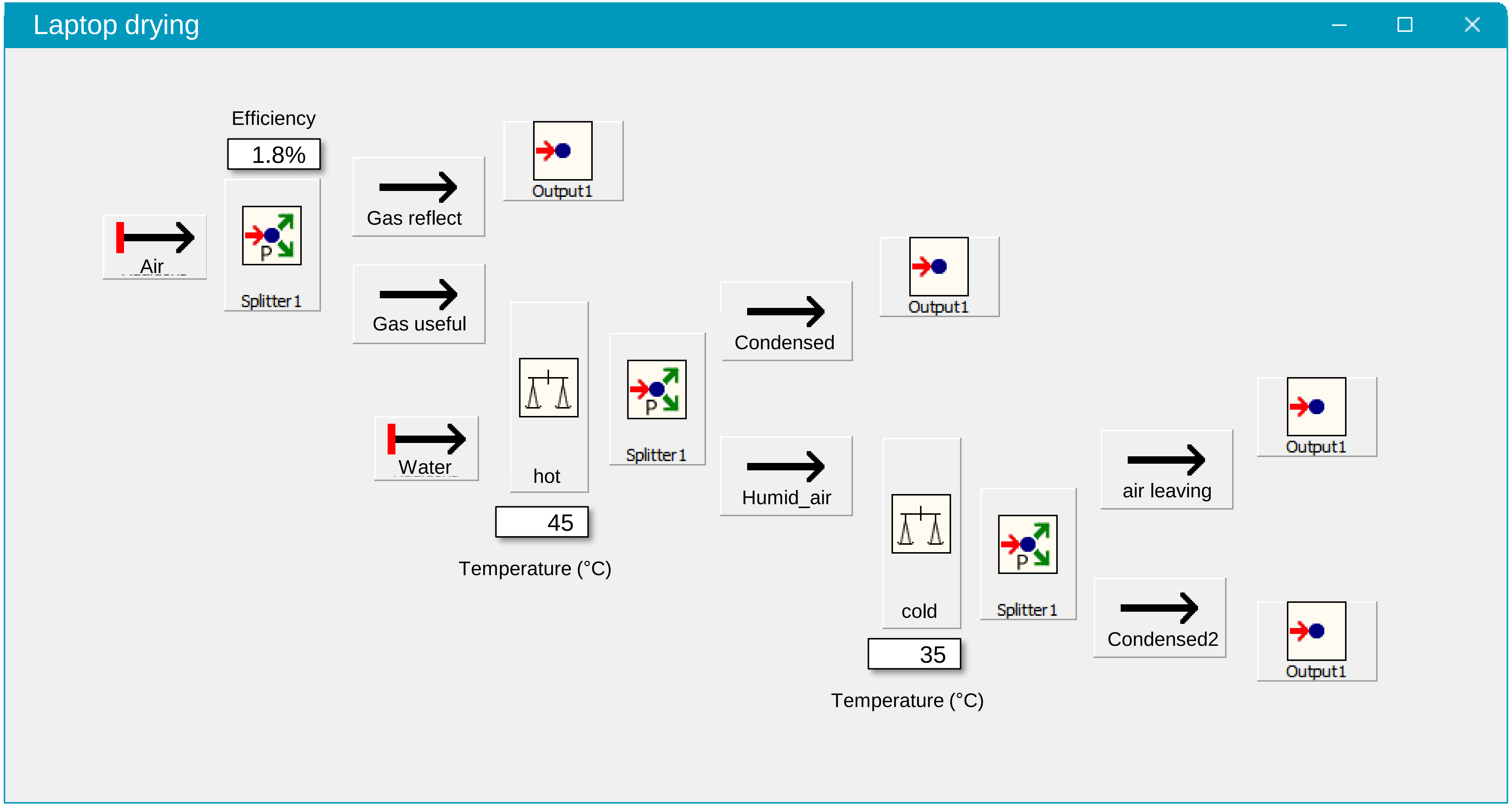

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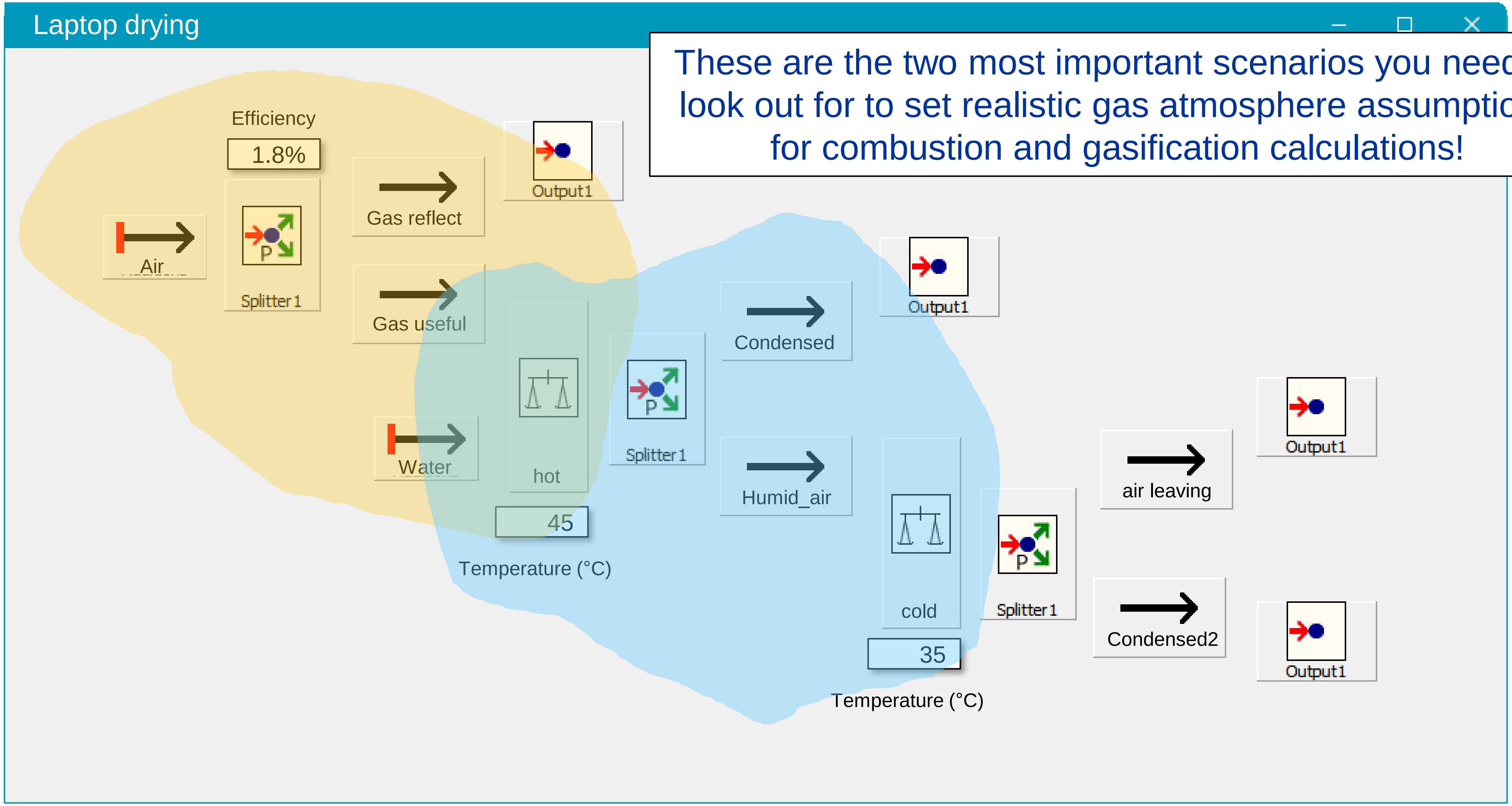

These are the two most important scenarios you need to look out for to set realistic gas atmosphere assumptions for combustion and gasification calculations!

Outline

- Motivation
- An unintentional experiment
- FactSage applications
  - **Ash fusion experiments**
  - Melting and oxidation of sulfides from coal ashes
  - Condensation of salts during cooling of syngas

Ash fusion

- Case: High-SO_3 containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:

  Insert high-T ash analysis, fix $p(O_2)$

Sample	Proximate analysis (as received)				Ultimate analysis (daf)				
	FC	VM	A	M	C	O	H	S	N
4. Balkan	46.8	14.7	38.1	0.4	85.7	4.5	4.7	4.1	1.0

High-temperature ash analysis (815 °C)											Ash-fusion test[a]		
SiO_2	Al_2O_3	Fe_2O_3	CaO	SO_3	MgO	K_2O	TiO_2	Na_2O	SiO_2 / Al_2O_3	DAI[b]	ST	HT	FT
57.81	22.87	7.34	2.66	2.70	1.35	4.15	0.80	0.32	2.5	6.1	1210	1405	1425

Vassilev, Fuel 88 (2009) 235.

Ash fusion

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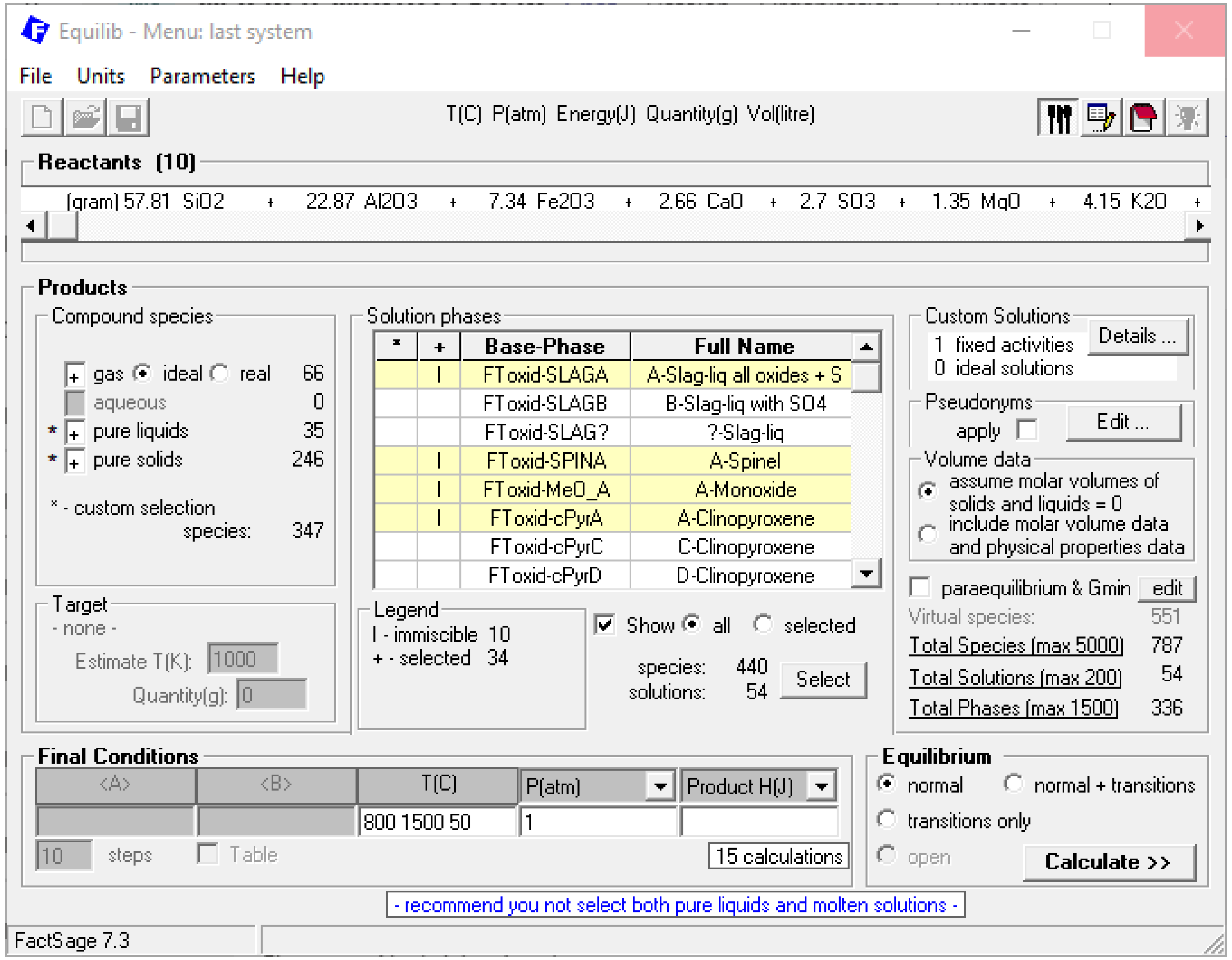
- Approach 1:

  Fix $p(O_2)$



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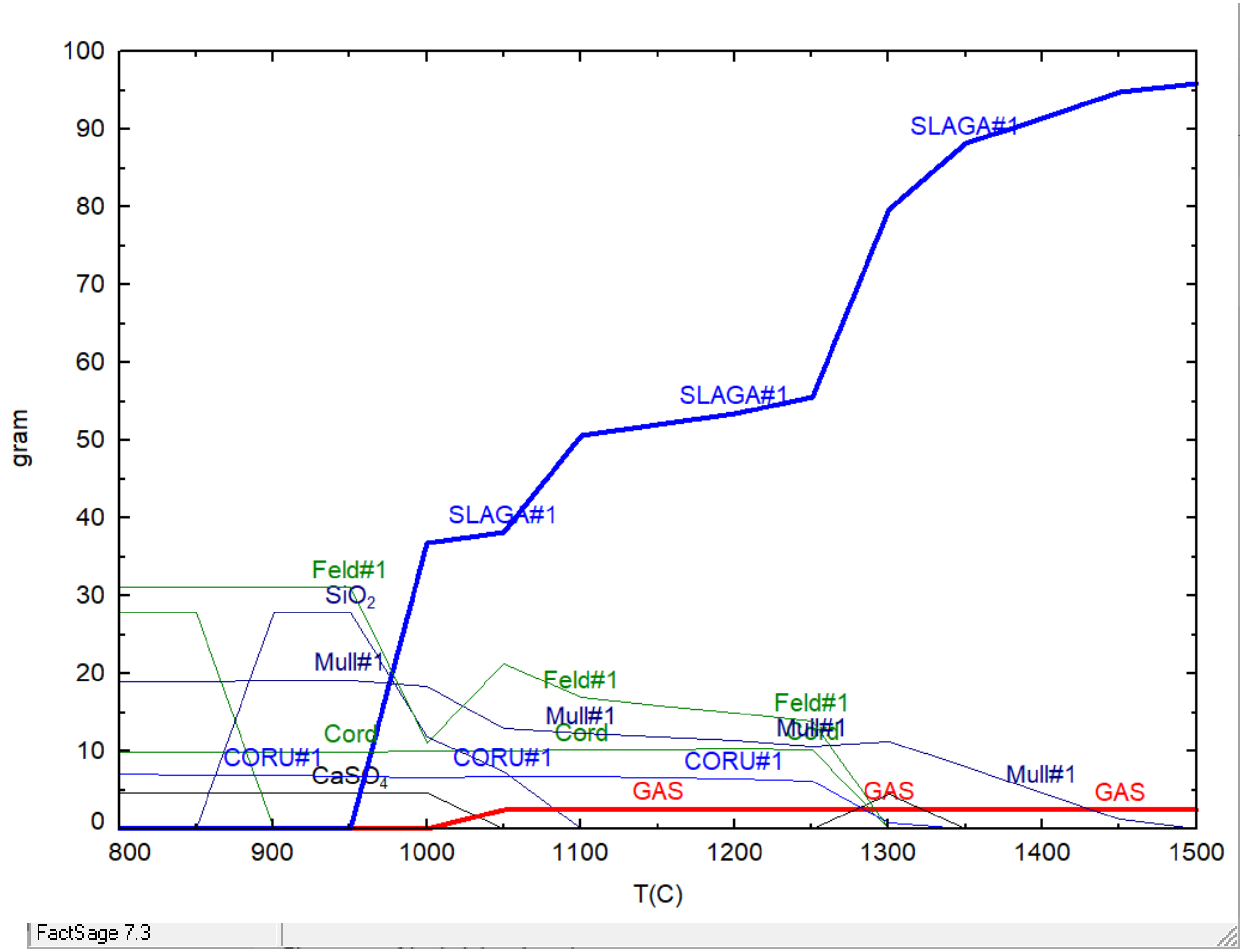

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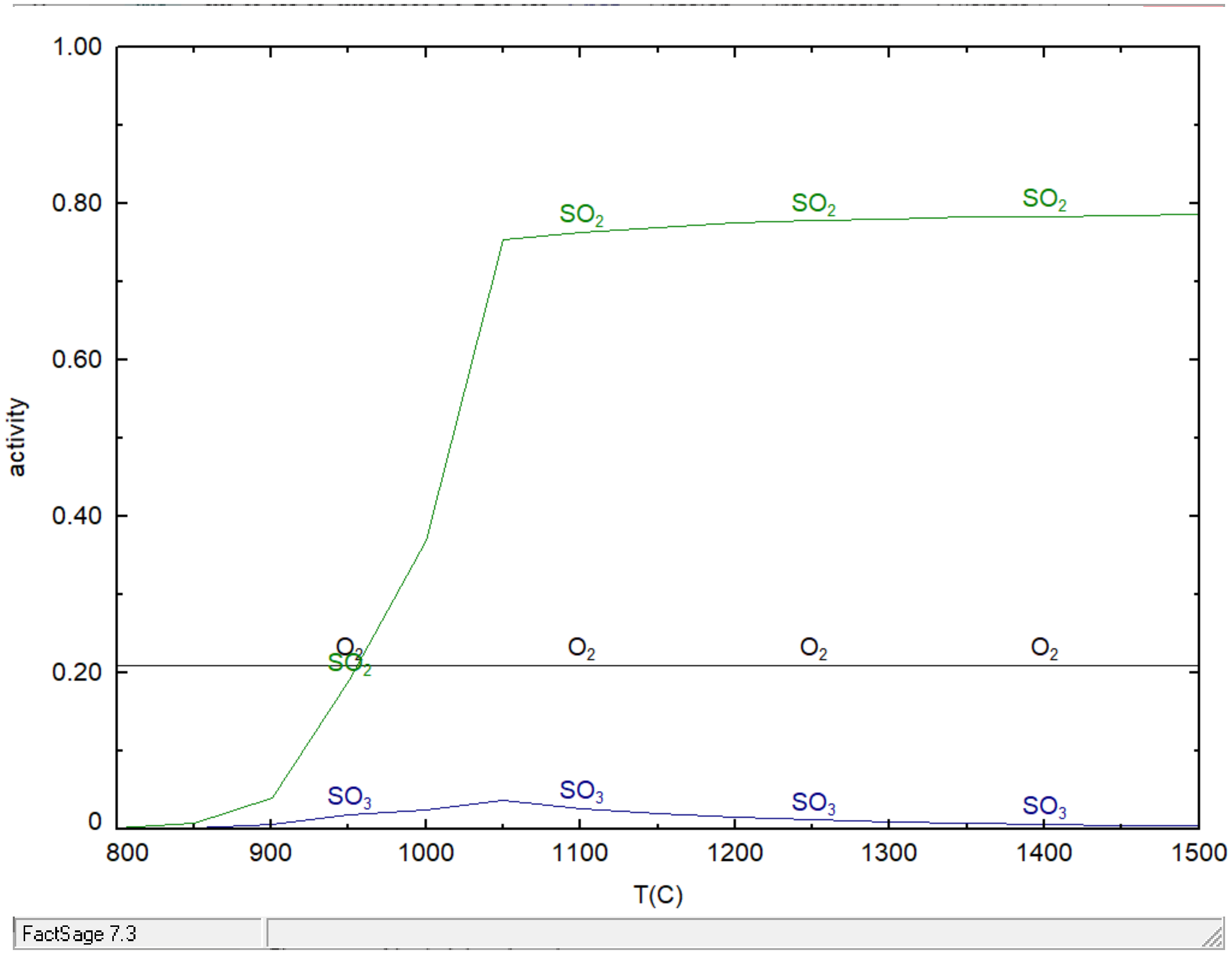
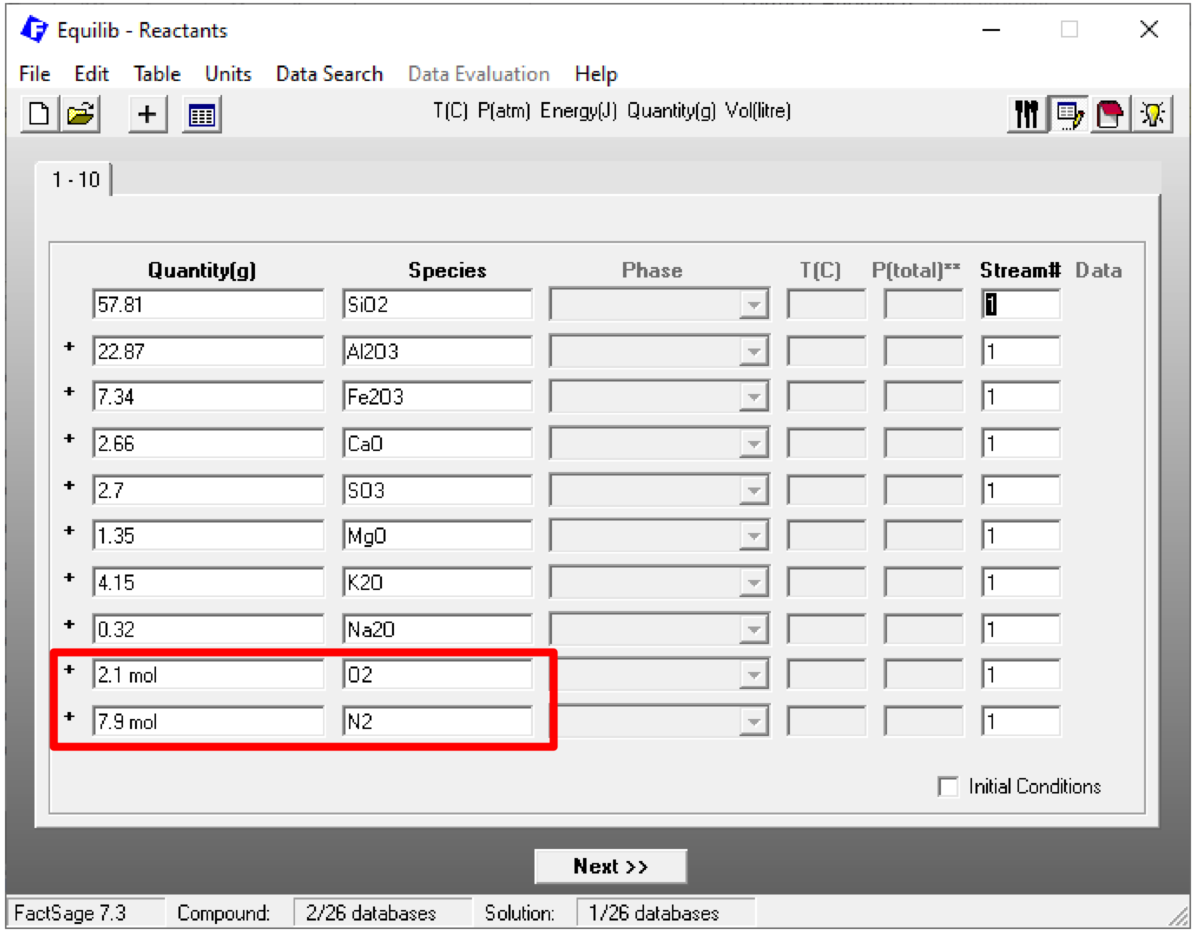


Ash fusion

- Case: High-SO_3 containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
  Fix $p(O_2)$
- Approach 2:
  Add O_2+N_2



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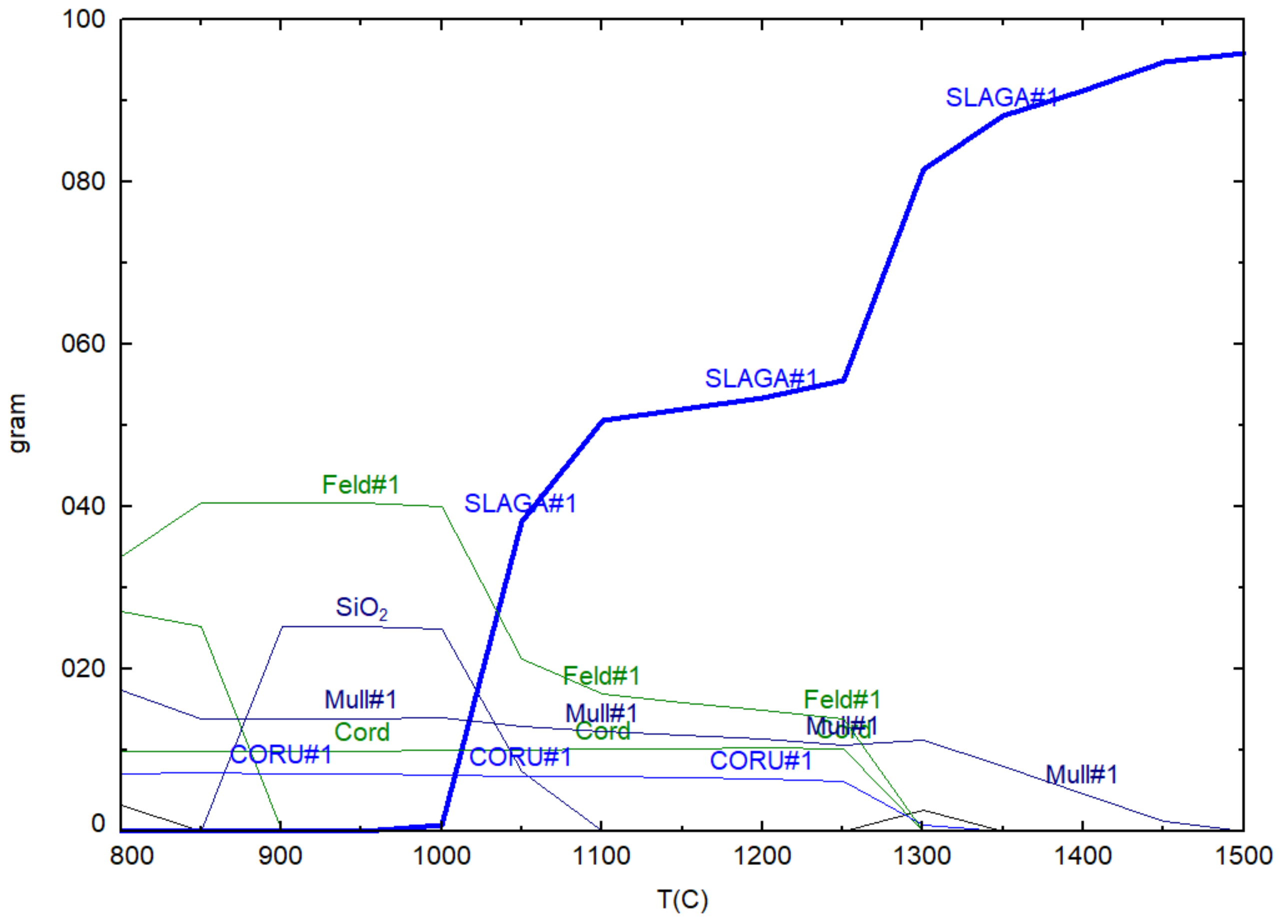

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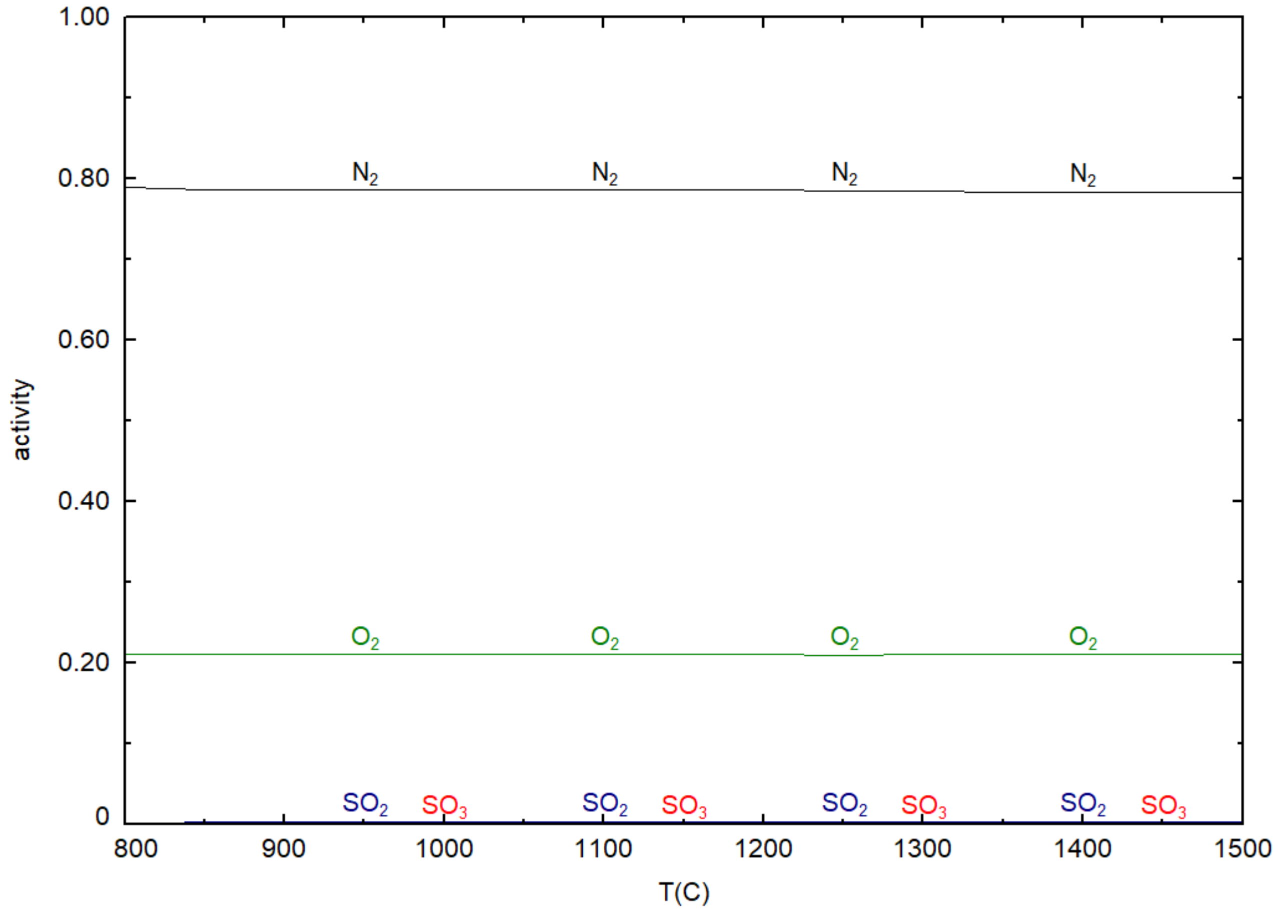
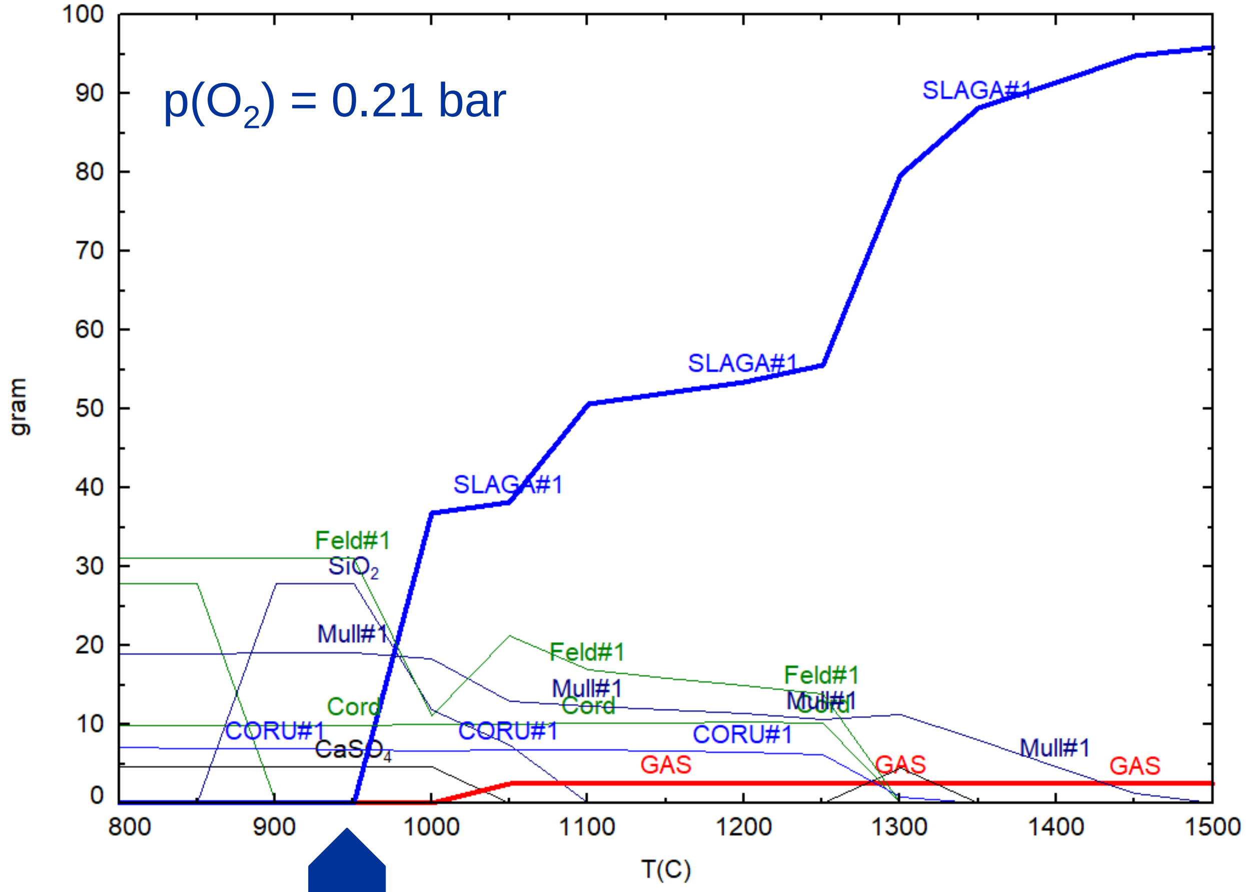
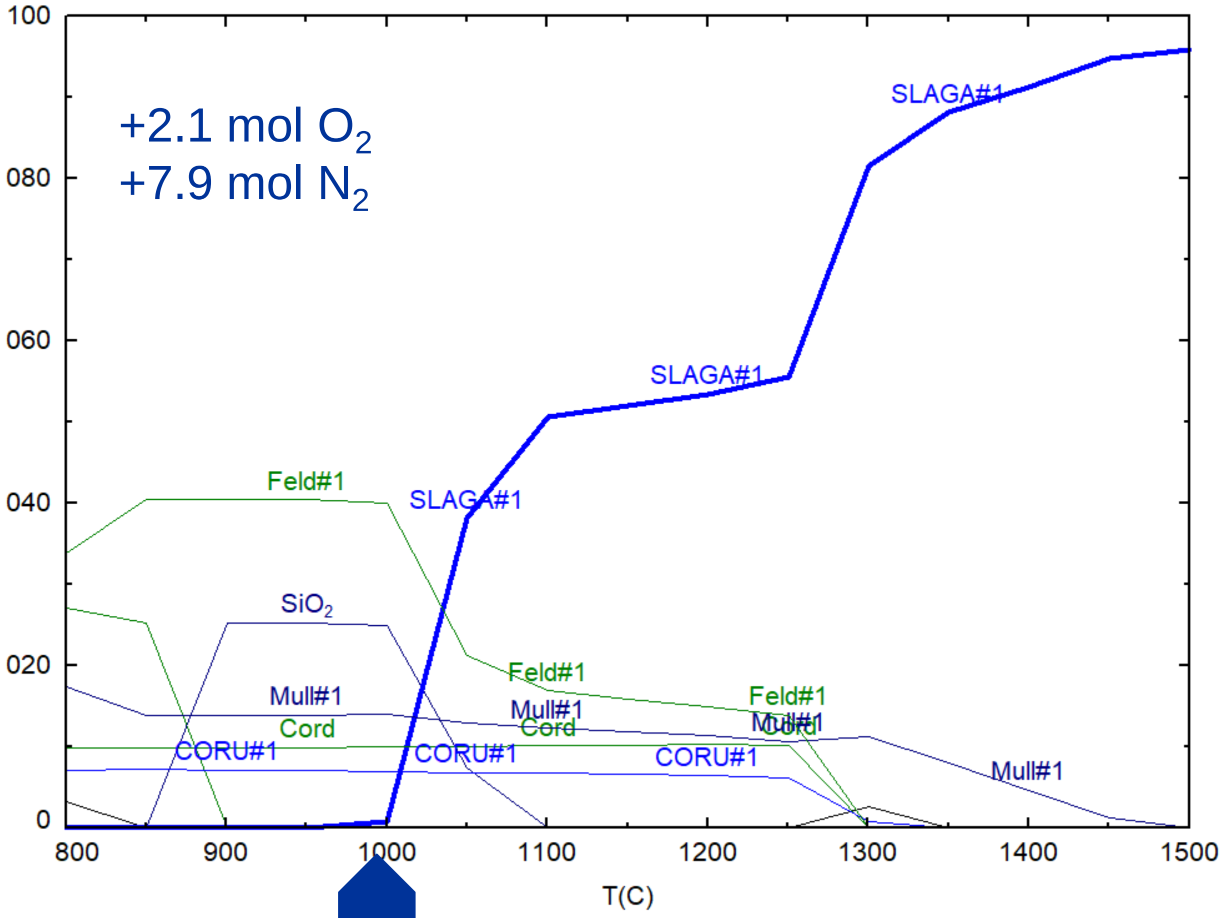


Ash fusion



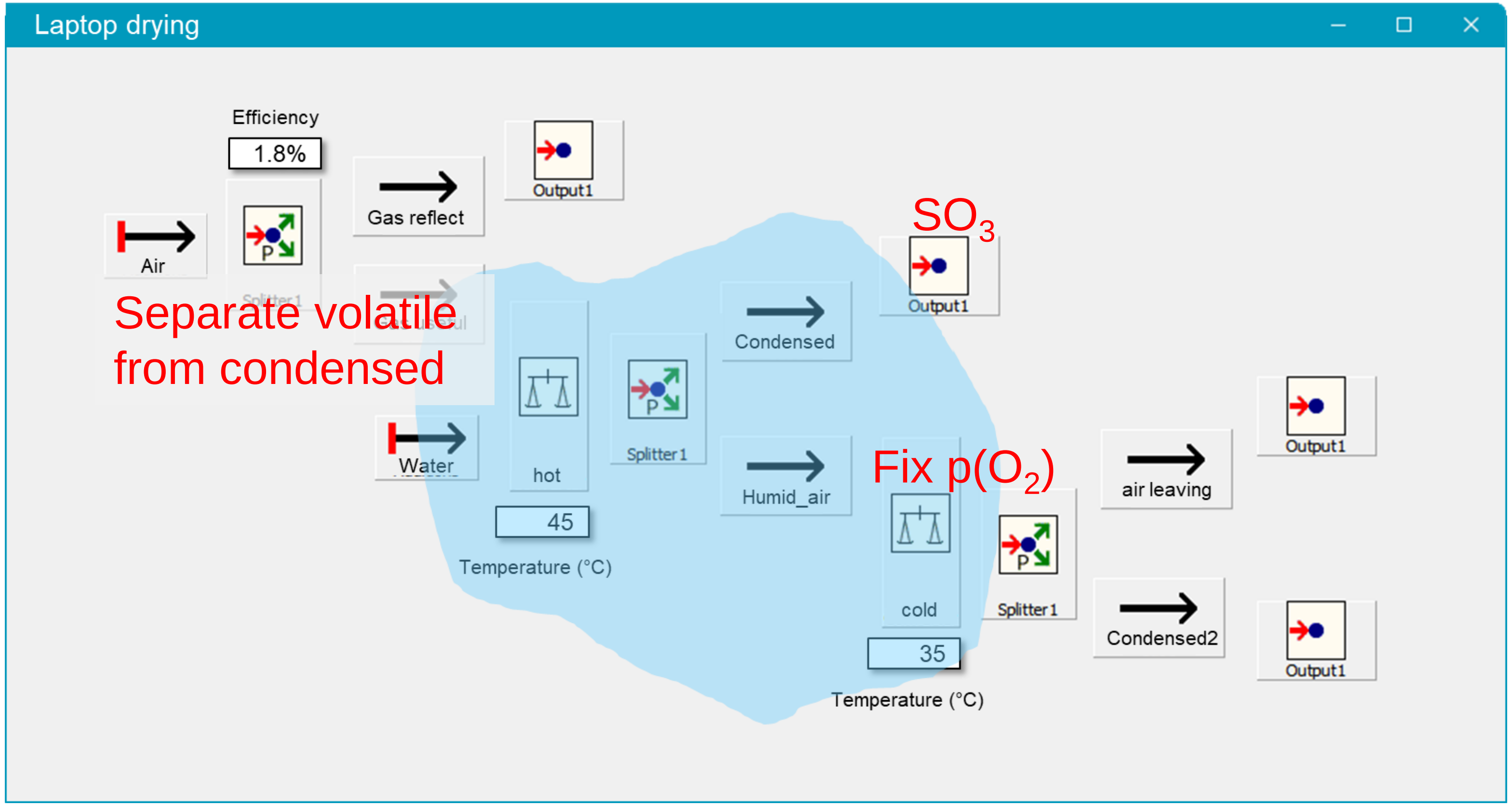
p(O_2) = 0.21 bar
gram
T(C)
SLAGA#1
Feld#1
SiO_2
Mull#1
Cord
CORU#1
$CaSO_4$
GAS



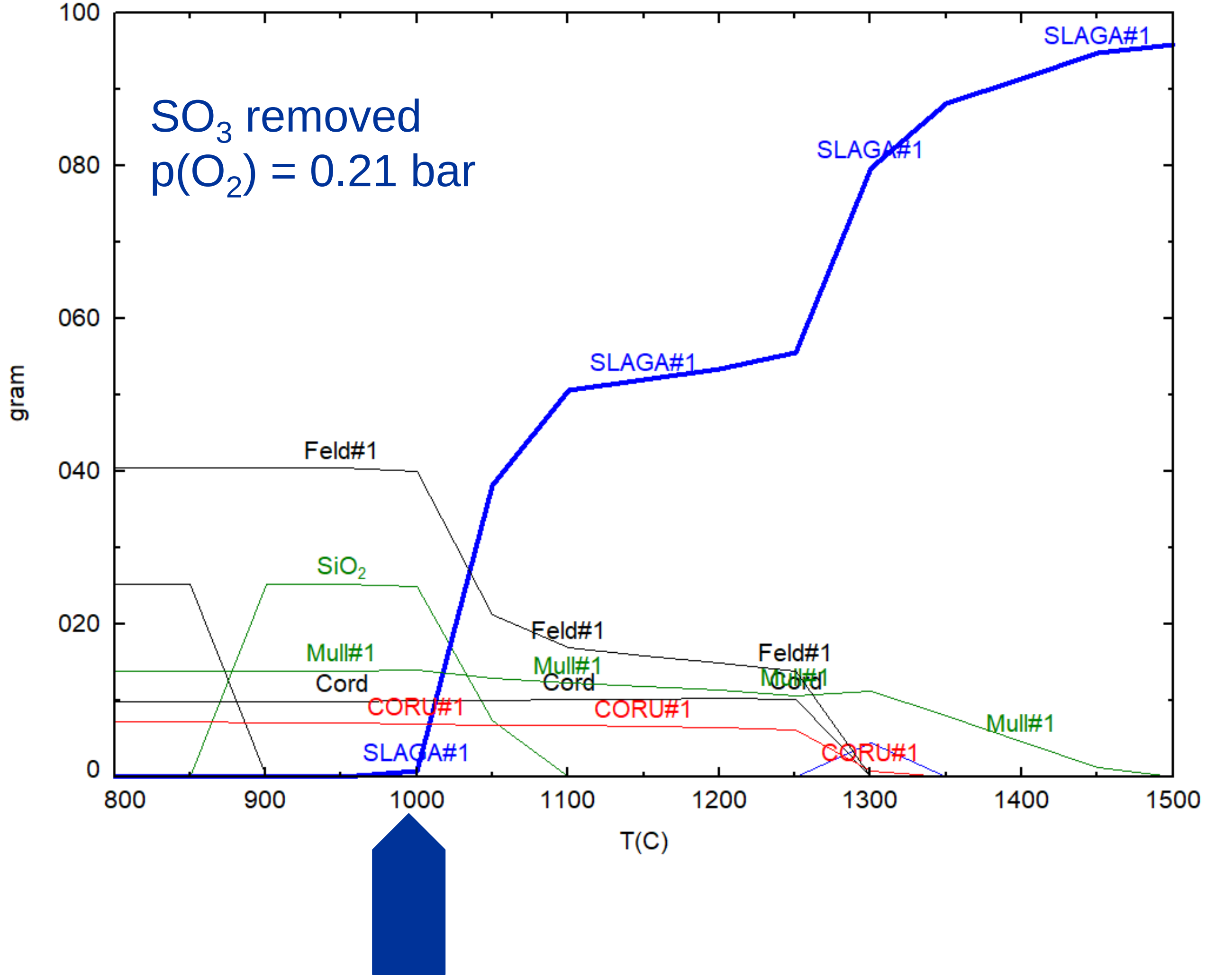
+2.1 mol O_2
+7.9 mol N_2
T(C)
SLAGA#1
Feld#1
SiO_2
Mull#1
Cord
CORU#1

Ash fusion

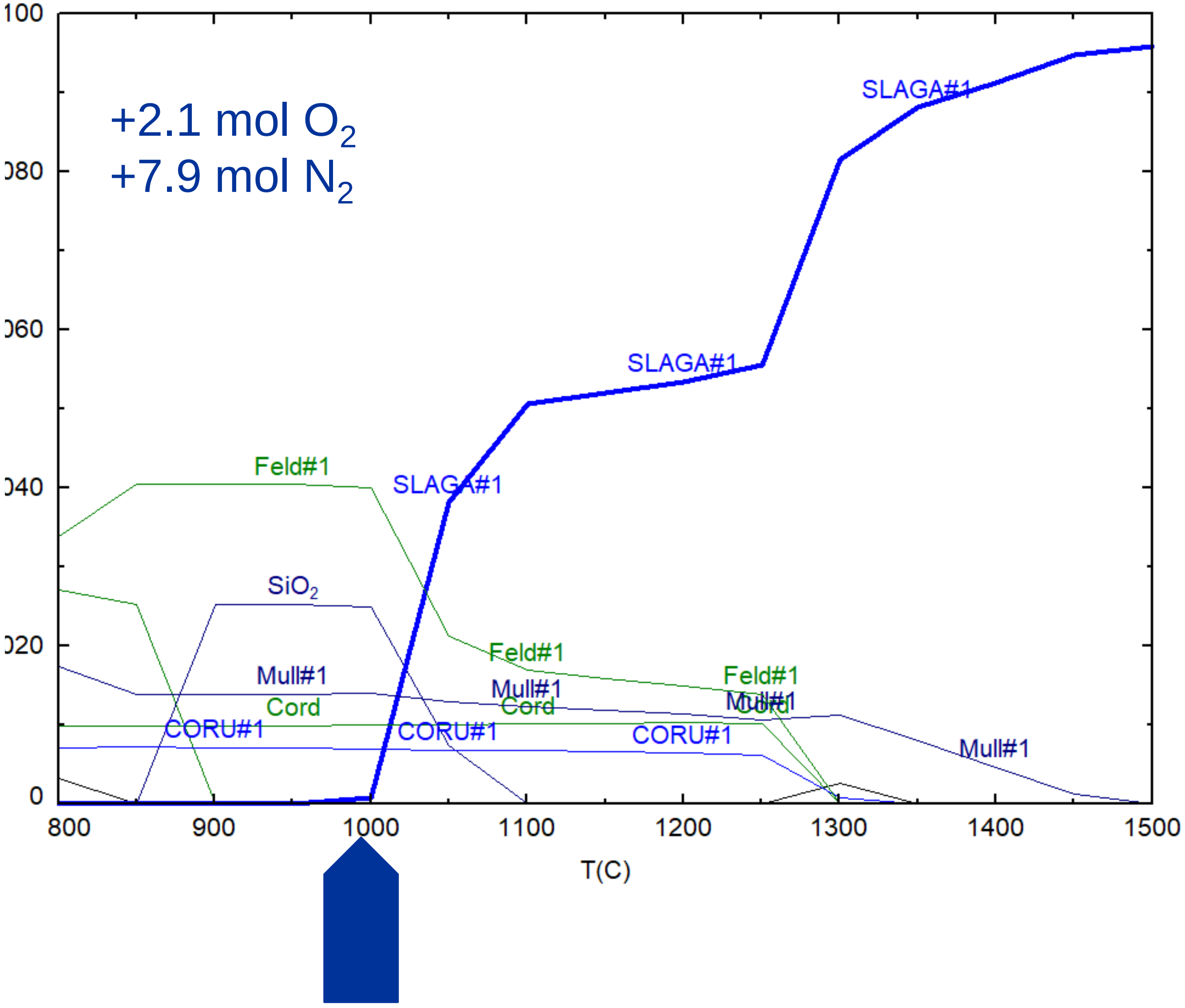
- Case: High-SO_3 containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
  Fix $p(O_2)$
- Approach 2:
  Add O_2+N_2
- Approach 3:
  Fix $p(O_2)$, omit SO_3



Ash fusion



SO_3 removed
$p(O_2) = 0.21$ bar
gram
T(C)
SLAGA#1
Feld#1
SiO_2
Mull#1
Cord
CORU#1



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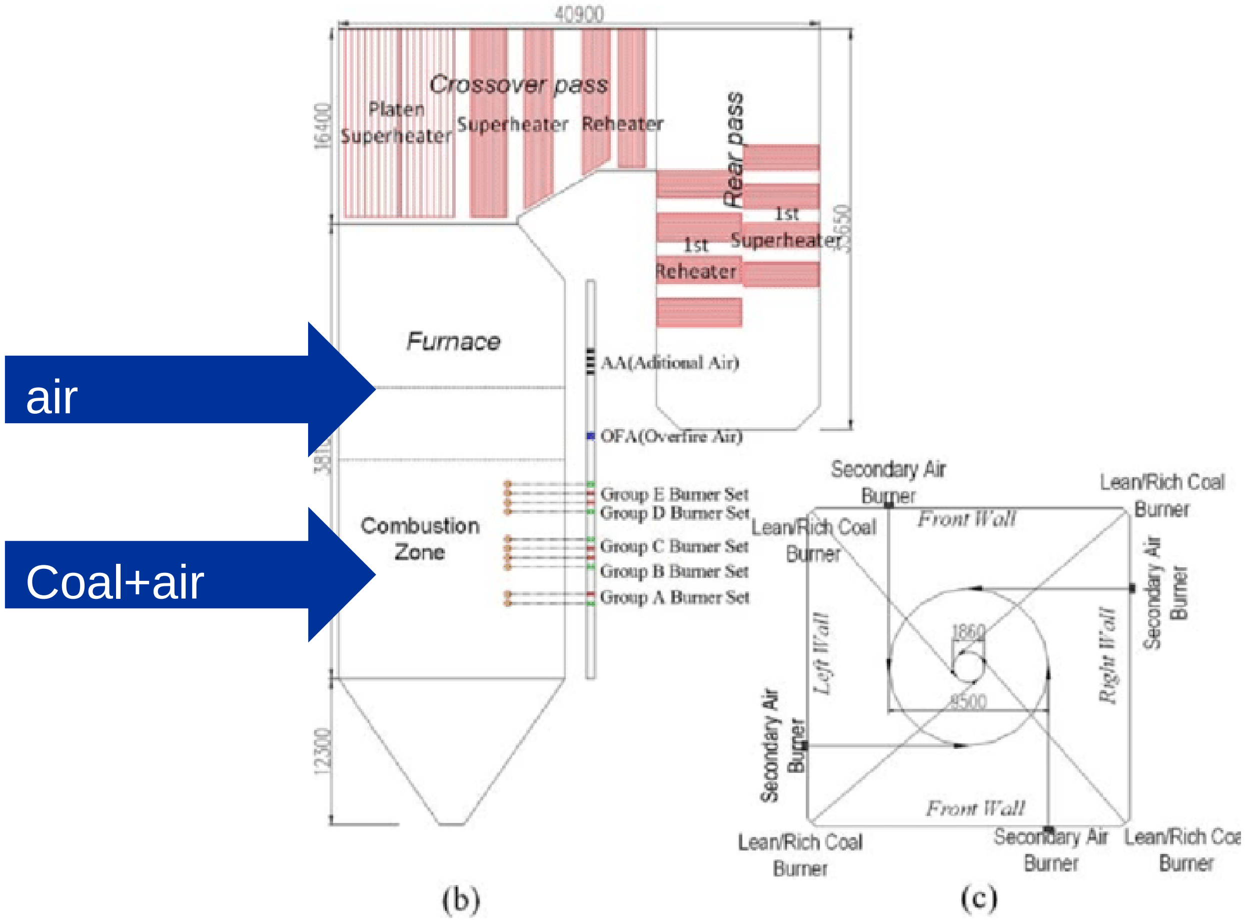
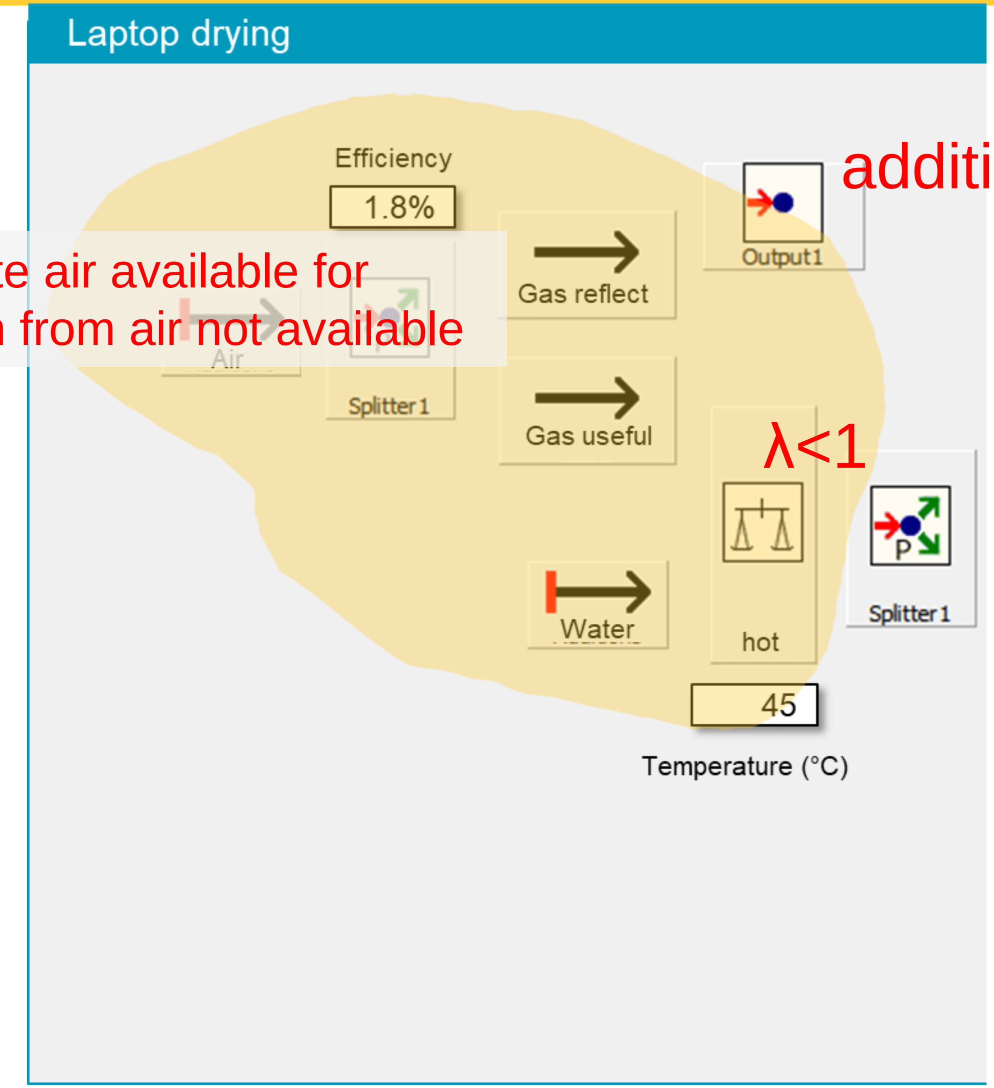
  - Condensation of salts during cooling of syngas

Melting and oxidation of sulfides from coal ashes



Sun et al., Adv. In Mech. Engin. 8 (2016) 1.

Melting and oxidation of sulfides from coal ashes



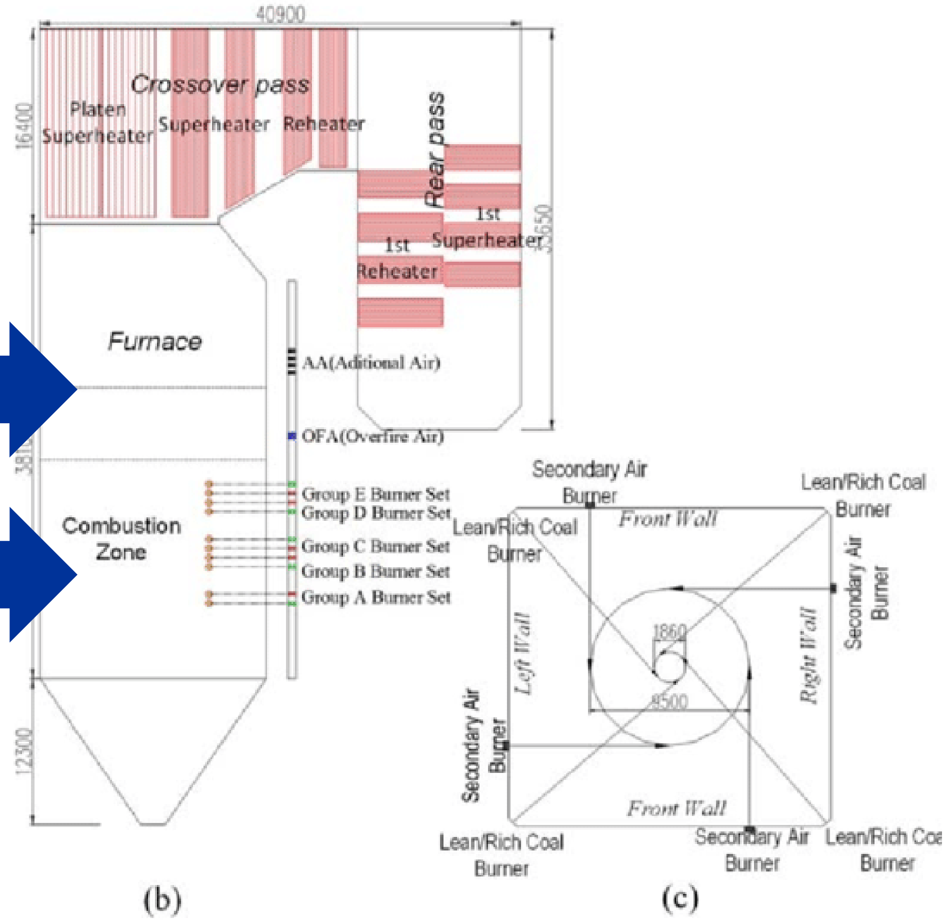
Separate air available for reaction from air not available

additional air

λ<1

air

Coal+air



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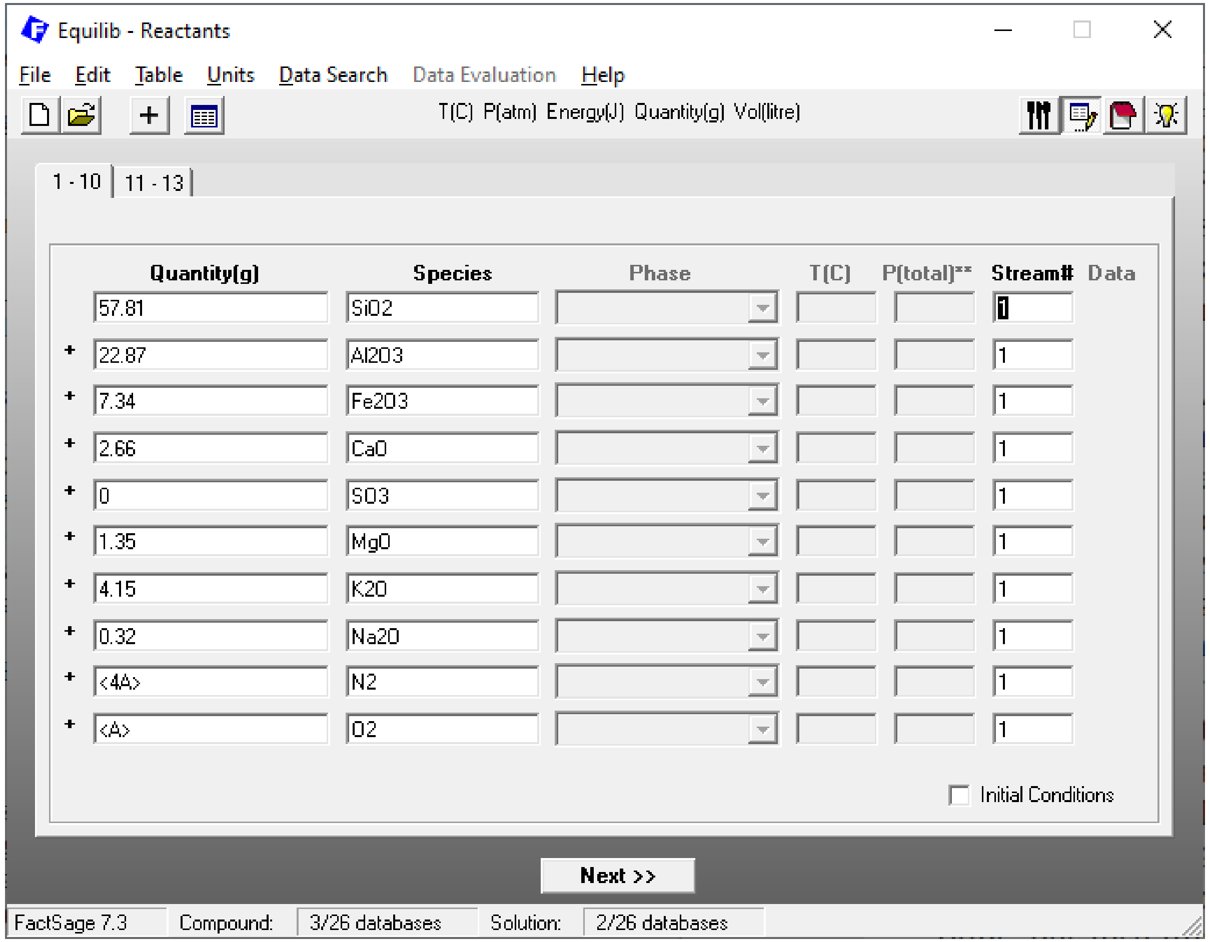
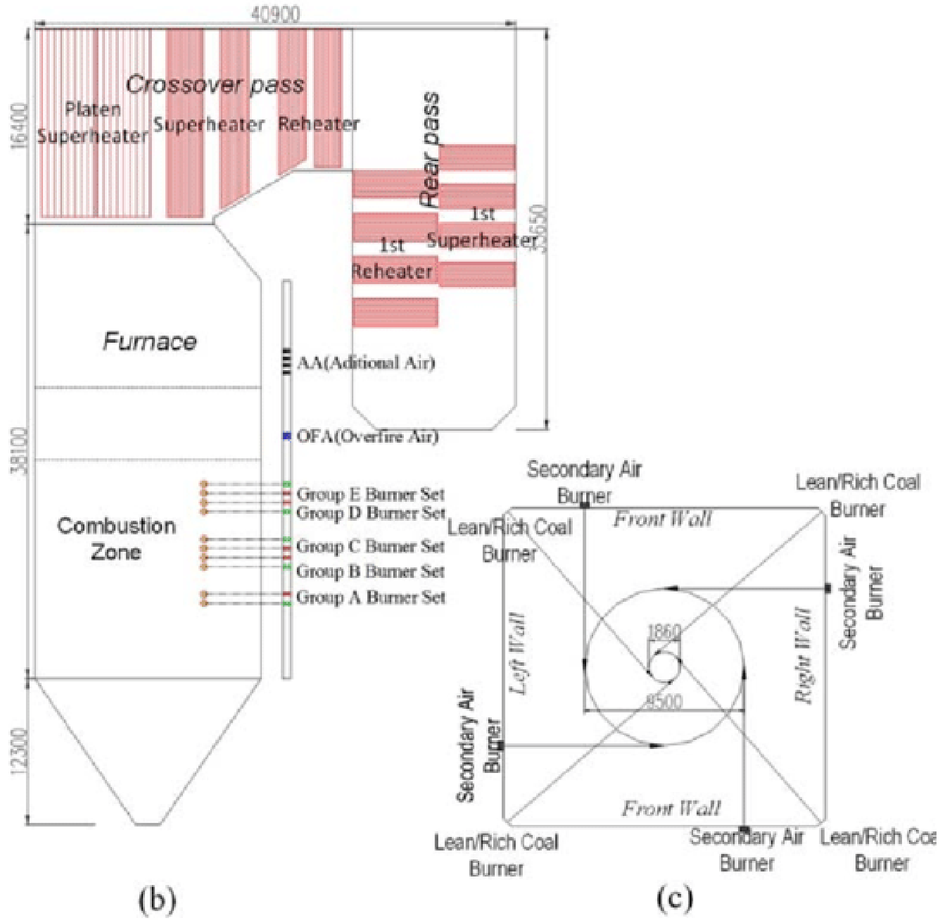
Melting and oxidation of sulfides from coal ashes





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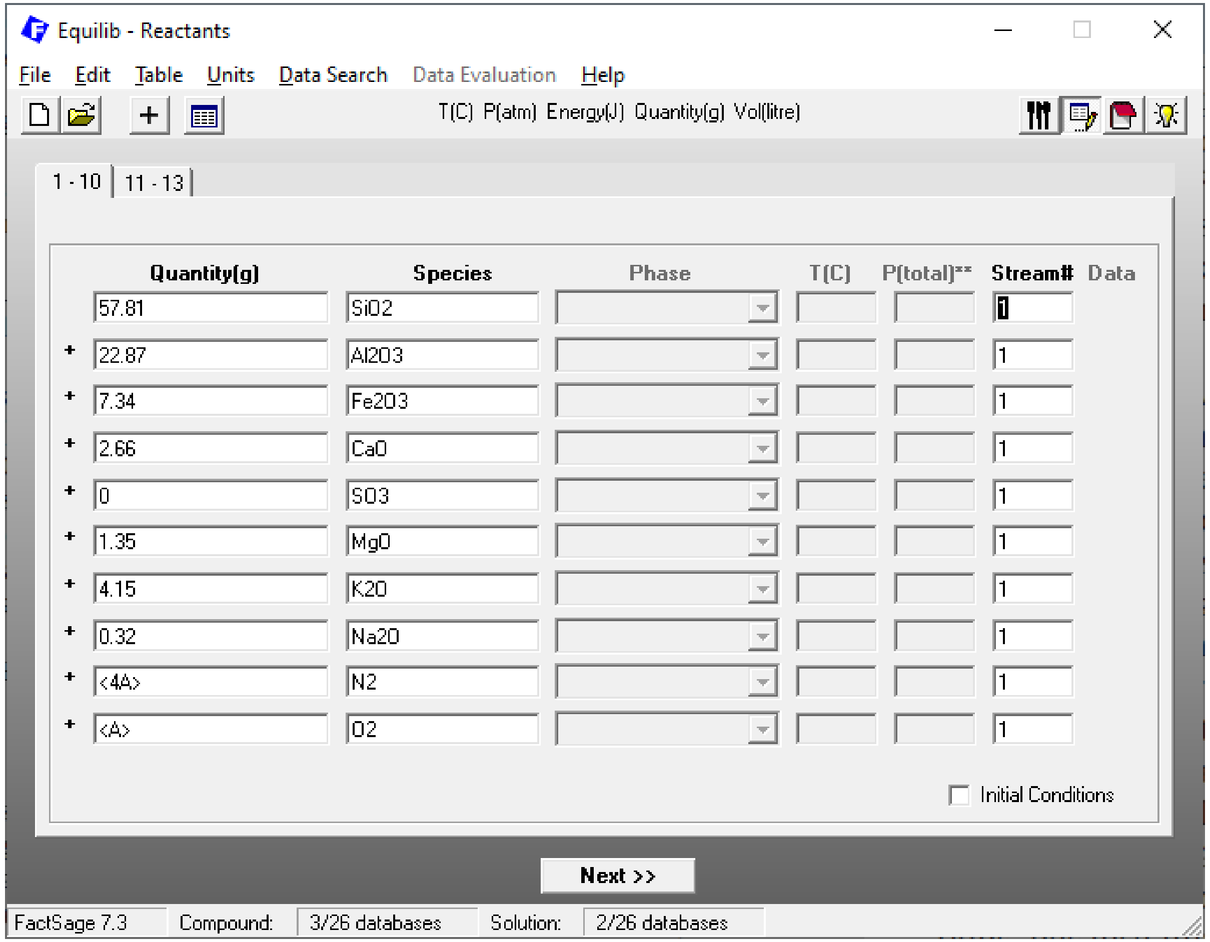

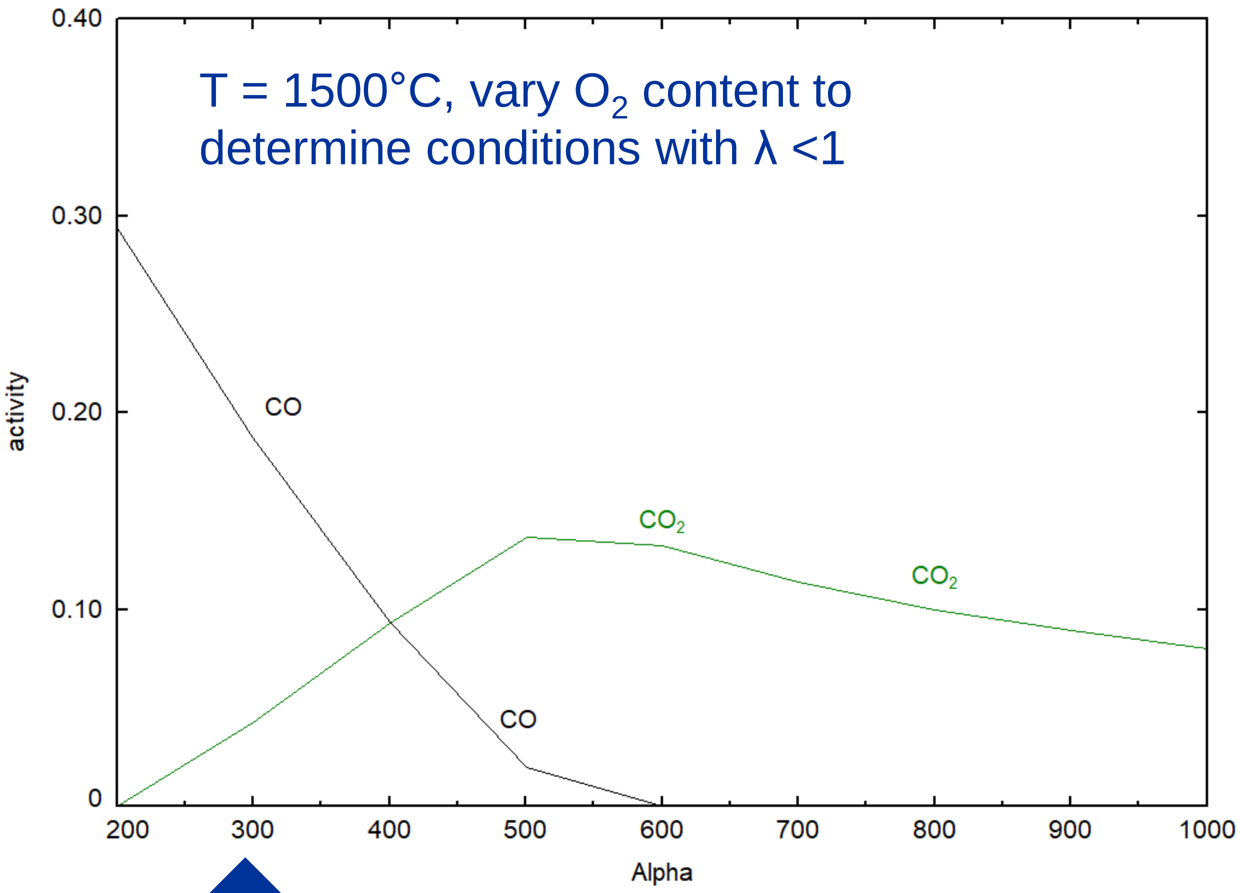

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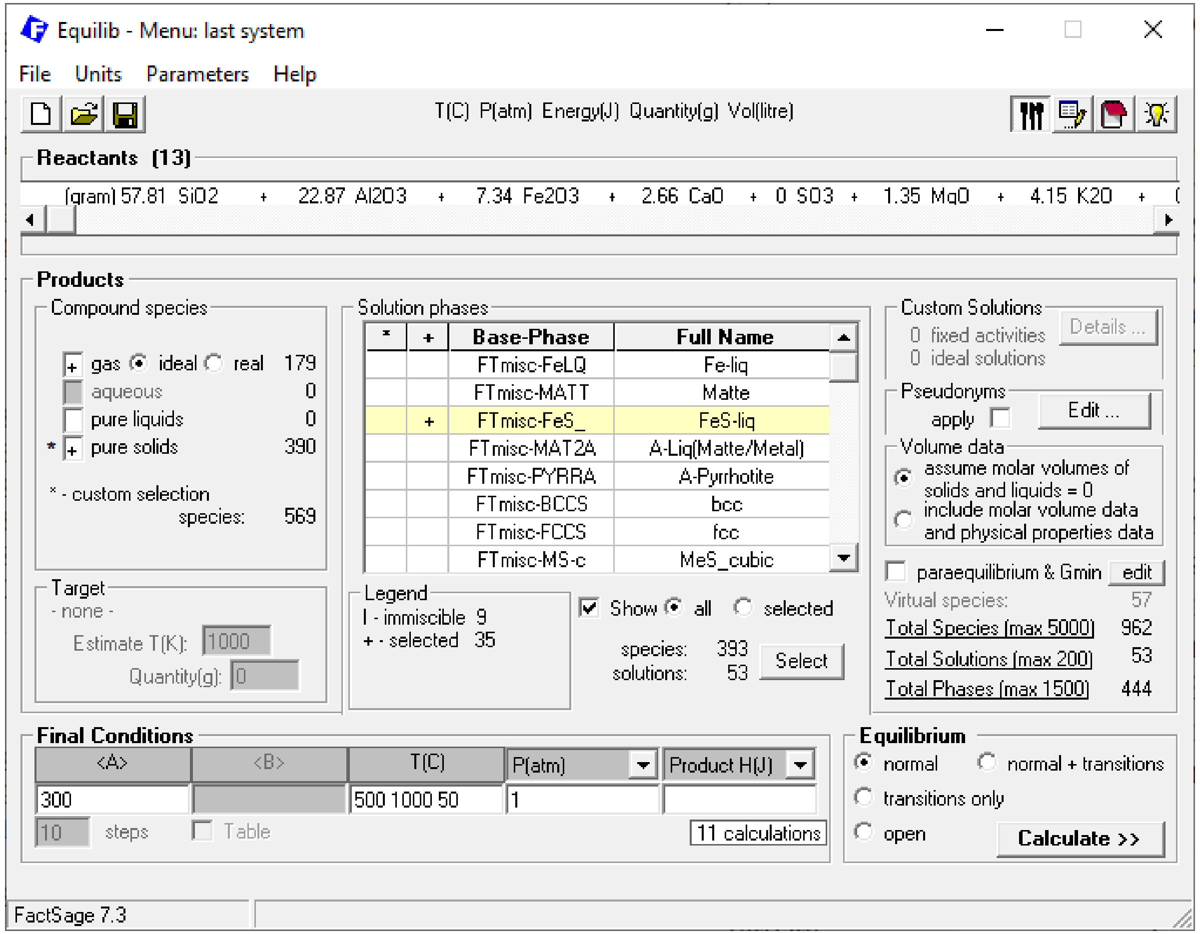

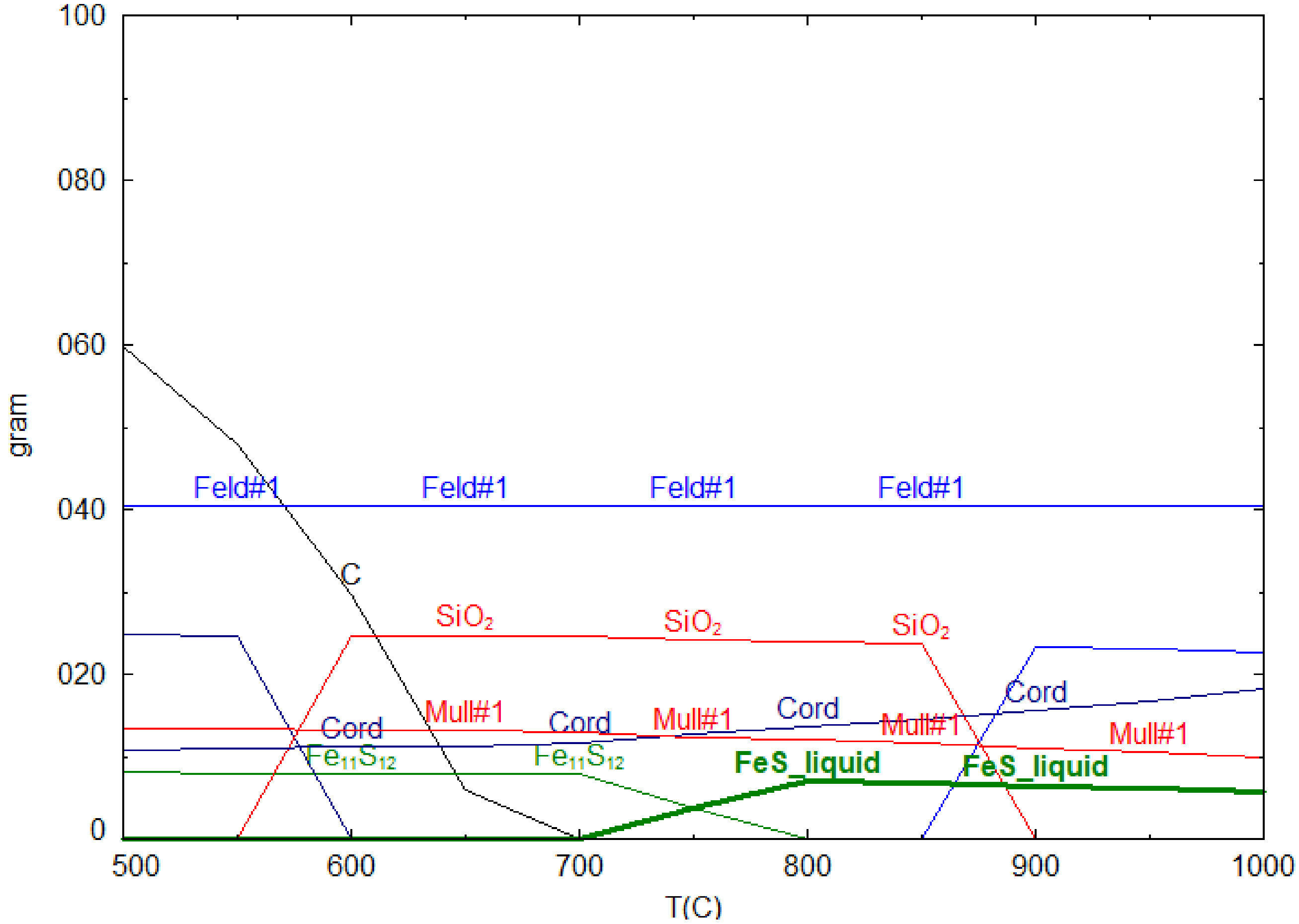

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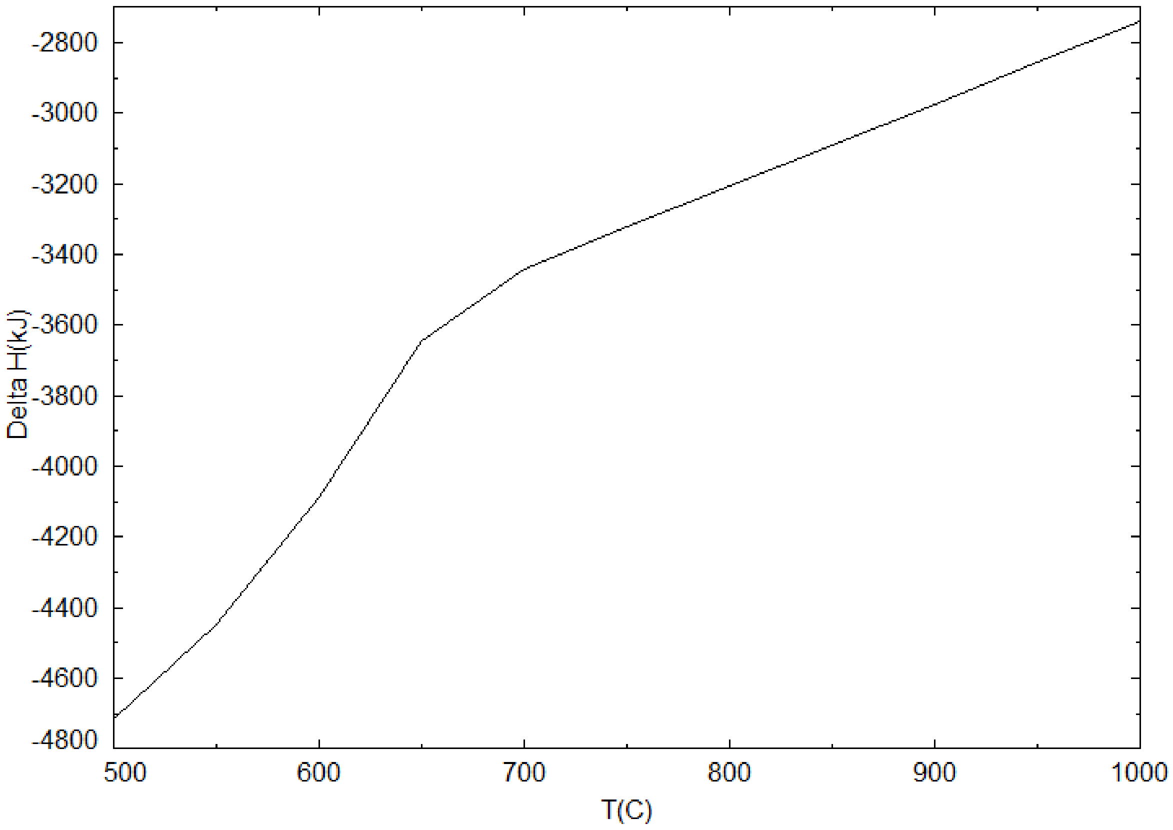

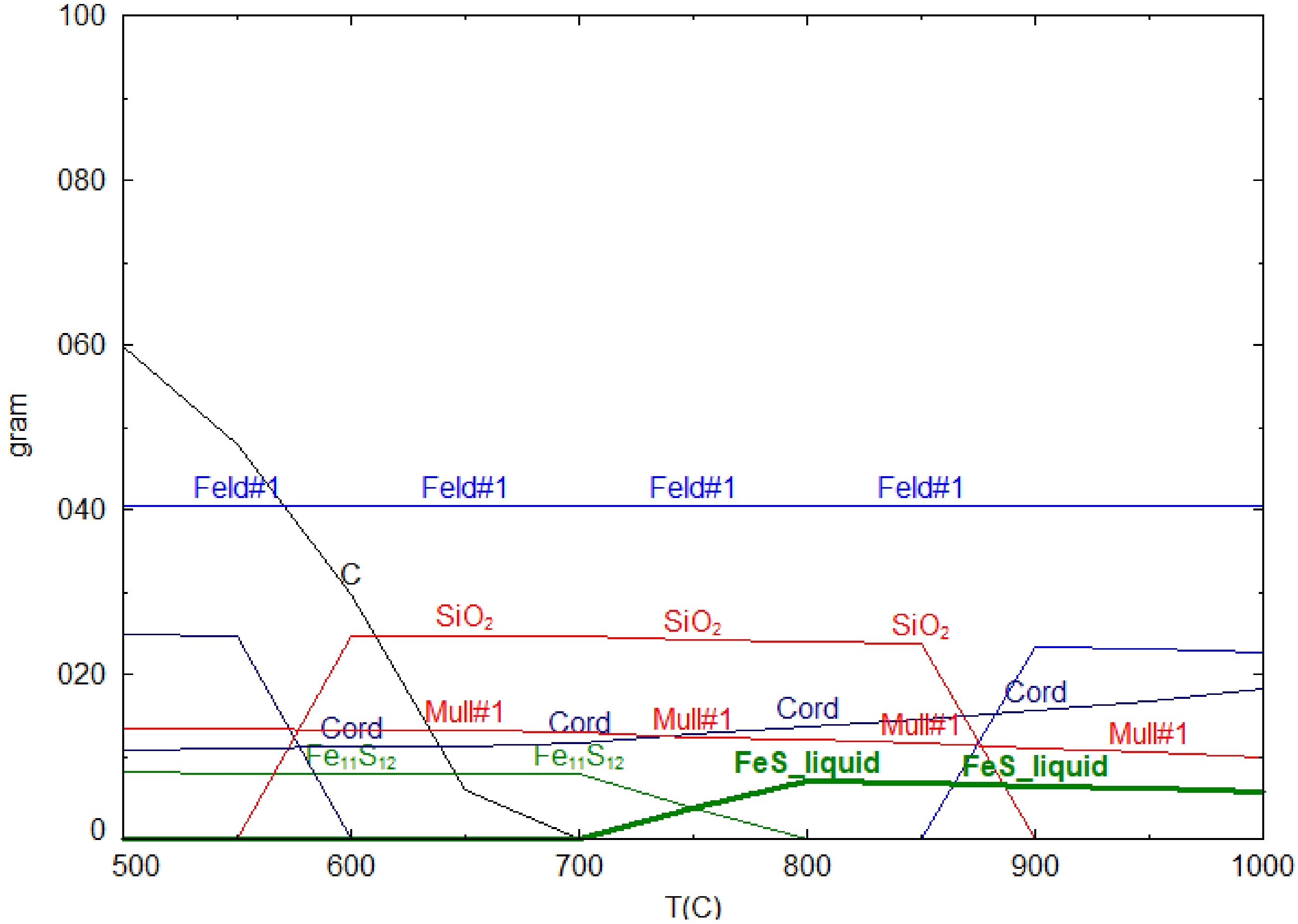

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  - **Condensation of salts during cooling of syngas**

Condensation of salts during cooling of syngas

- Case: Hazelnut shells in steam gasification

▼ Ash Properties

▼ Ash composition

SO_3	wt% (ash)	4.24
Cl	wt% (ash)	2.34
P_2O_5	wt% (ash)	5.14
SiO_2	wt% (ash)	0.98
Fe_2O_3	wt% (ash)	1.34
Al_2O_3	wt% (ash)	10.42
CaO	wt% (ash)	26.61
MgO	wt% (ash)	6.22
Na_2O	wt% (ash)	0.00
K_2O	wt% (ash)	40.34
TiO_2	wt% (ash)	0.03
Cu	mg/kg (ash)	799.0
Mn	mg/kg (ash)	1 317.0
Cr	mg/kg (ash)	1 026.0

https://phyllis.nl/Biomass/View/2875

Condensation of salts during cooling of syngas

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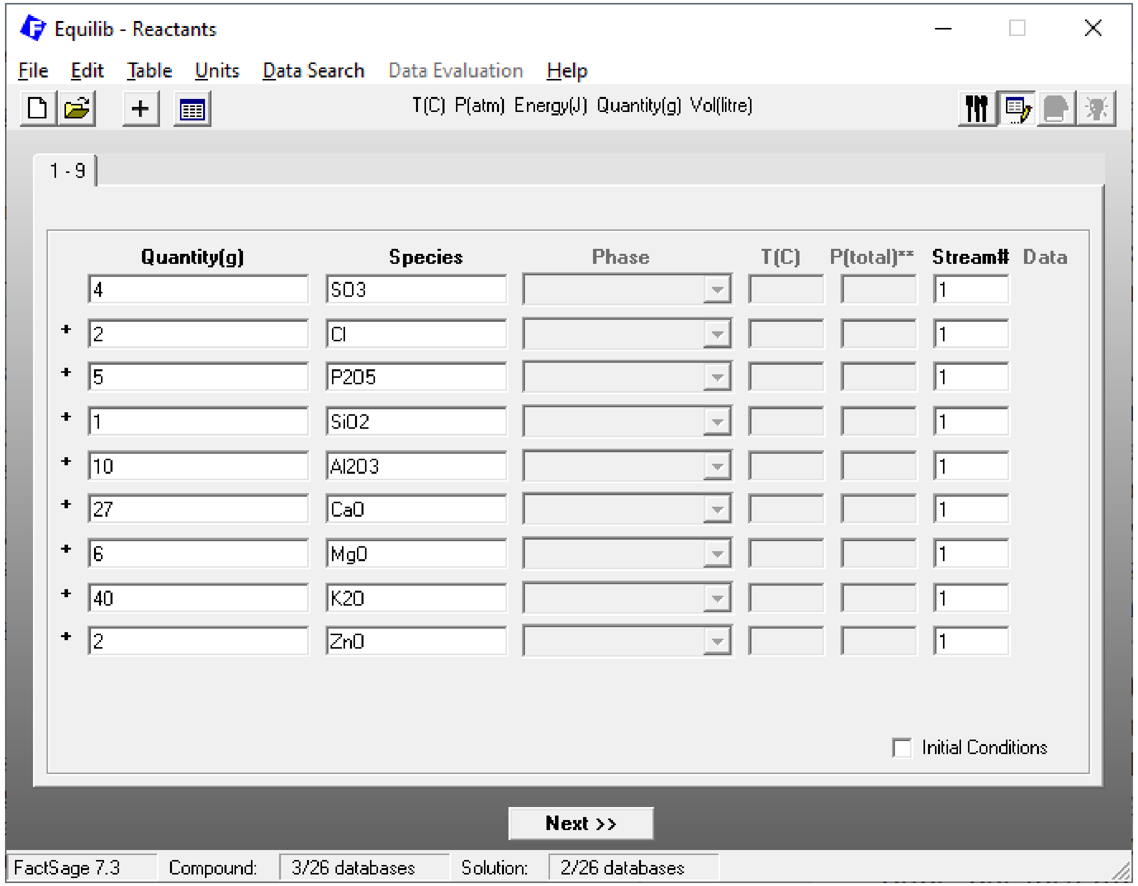
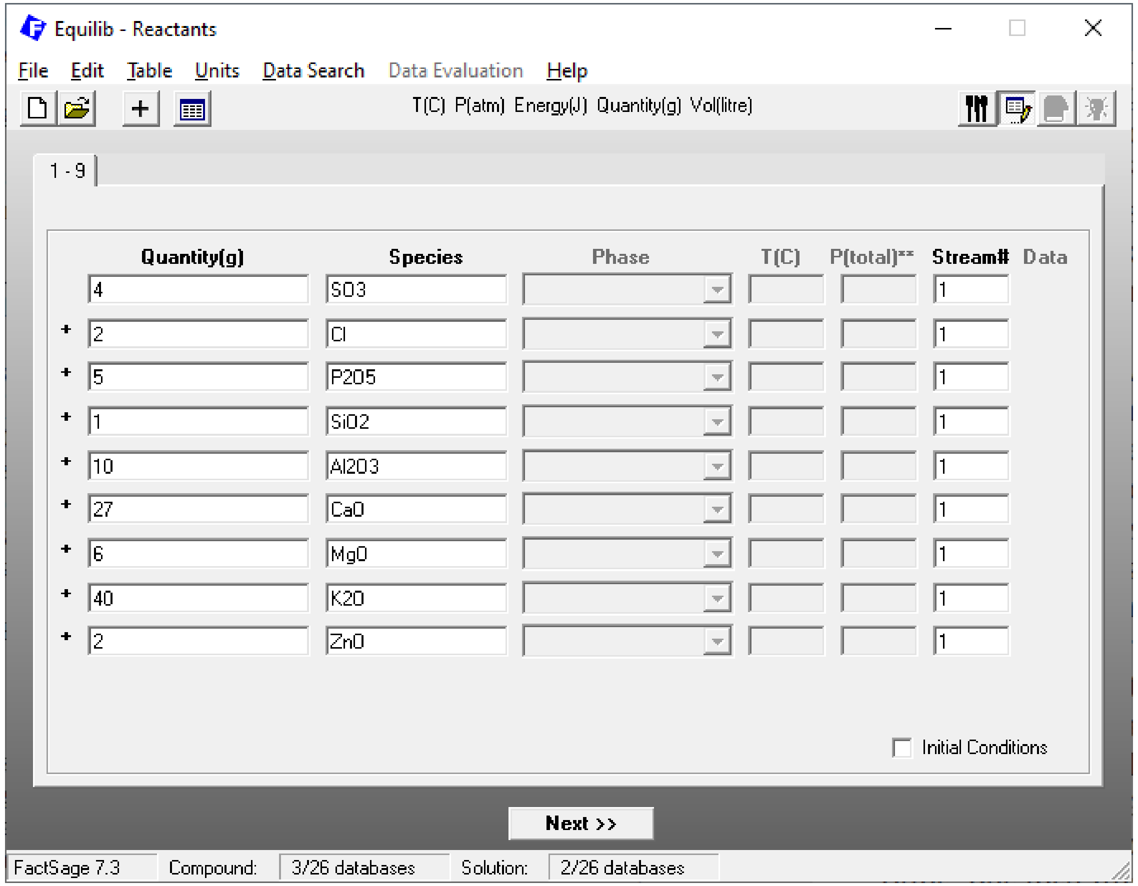


Condensation of salts during cooling of syngas

- Case: Hazelnut shells in steam gasification

TABLE 1 | Typical Composition of Dry Gas During the Oxygen and Steam Gasification of Biomass

Compound	Oxygen Gasification (Entrained Flow)	Oxygen Gasification (Fluidized Bed)	Steam Gasification
CO (vol %)	40–60	20–30	20–25
CO_2 (vol %)	10–15	25–40	20–25
H_2 (vol %)	15–20	20–30	30–45
CH_4 (vol %)	0–1	5–10	6–12
N_2 (vol %)	0–1	0–1	0–1
LHV (MJ/Nm^3)	10–12	10–12	10–14
Tar content (g/Nm^3)	<0.1	1–20	1–10



Rauch et al., WIREs Energy Environ 2013. doi: 10.1002/wene.97

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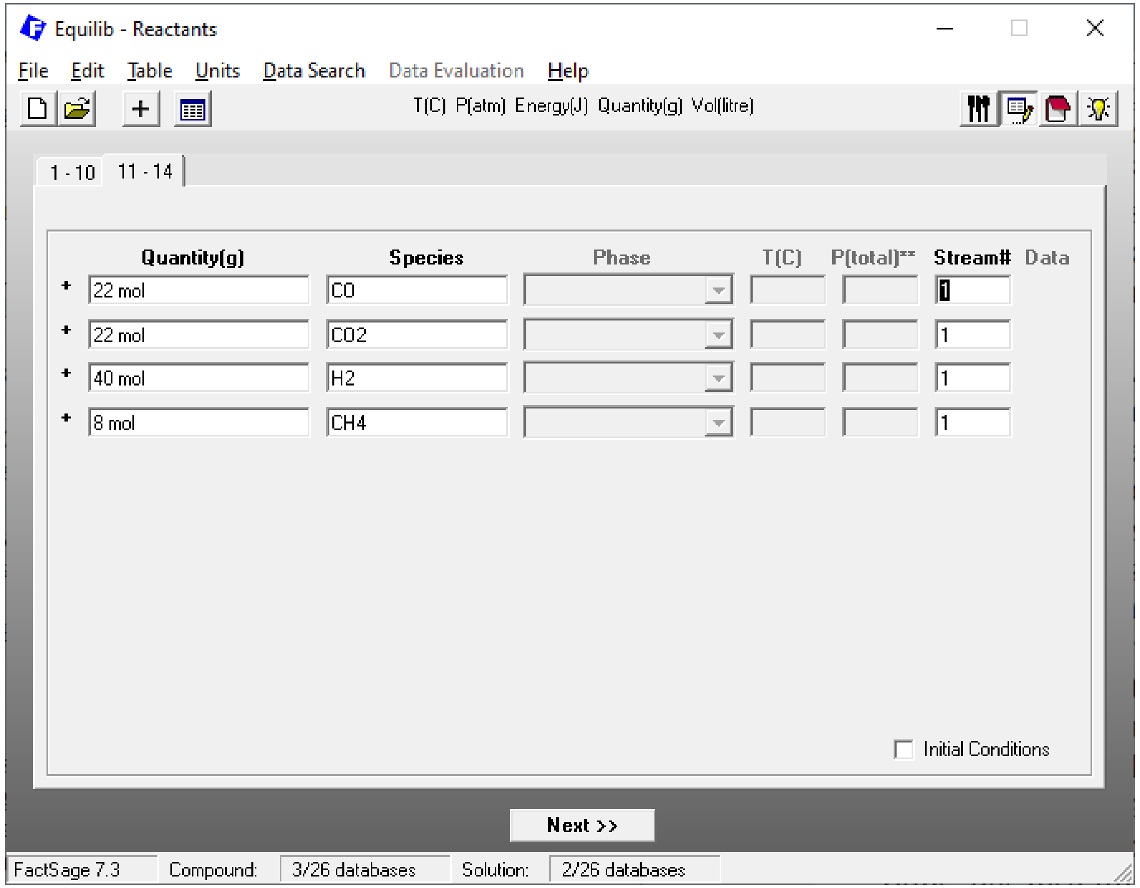
H_2 (vol %)	15–20	20–30	30–45
CH_4 (vol %)	0–1	5–10	6–12
N_2 (vol %)	0–1	0–1	0–1
LHV (MJ/Nm^3)	10–12	10–12	10–14
Tar content (g/Nm^3)	$<$0.1	1–20	1–10



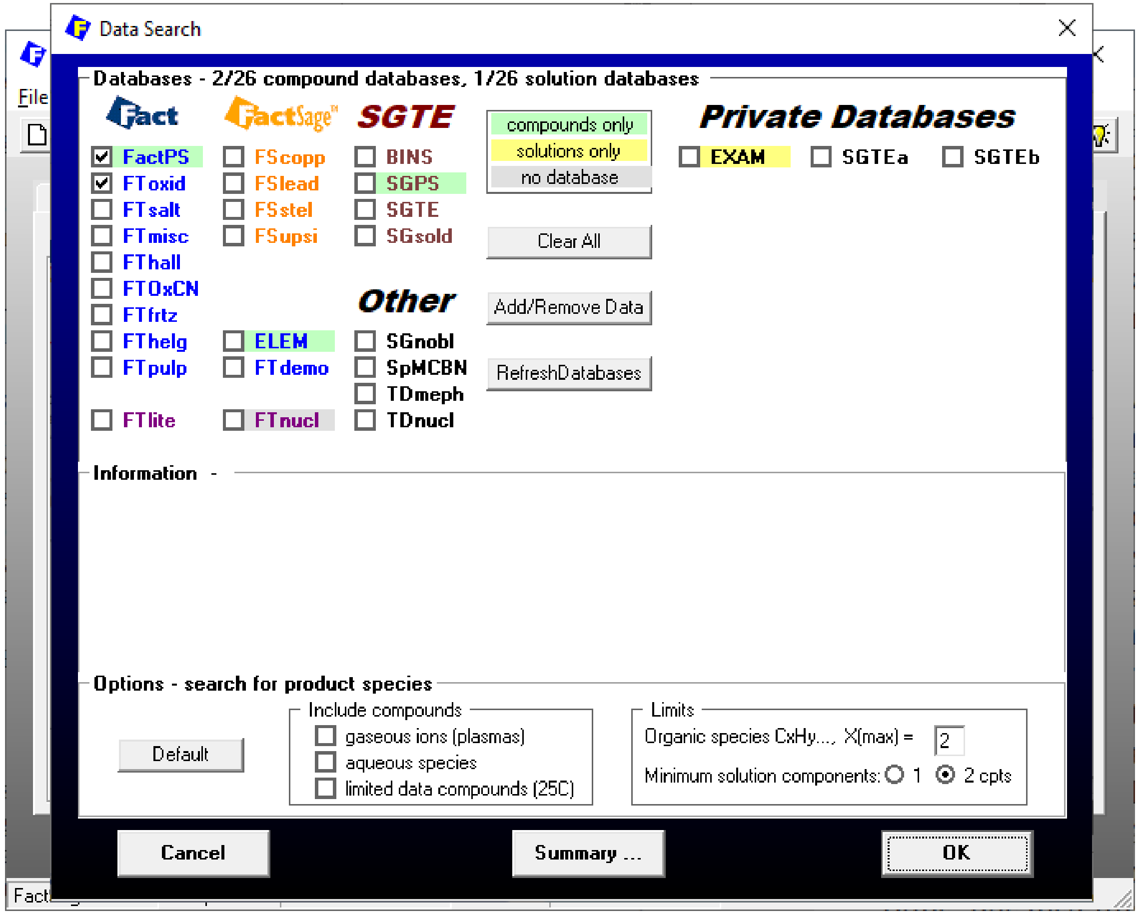
Rauch et al., WIREs Energy Environ 2013. doi: 10.1002/wene.97

Condensation of salts during cooling of syngas

- Case: Hazelnut shells in steam gasification

TABLE 1 | Typical Composition of Dry Gas During the Oxygen and Steam Gasification of Biomass

Compound	Oxygen Gasification (Entrained Flow)	Oxygen Gasification (Fluidized Bed)	Steam Gasification
CO (vol %)	40–60	20–30	20–25
CO_2 (vol %)	10–15	25–40	20–25
H_2 (vol %)	15–20	20–30	30–45
CH_4 (vol %)	0–1	5–10	6–12
N_2 (vol %)	0–1	0–1	0–1
LHV (MJ/Nm^3)	10–12	10–12	10–14
Tar content (g/Nm^3)	<0.1	1–20	1–10



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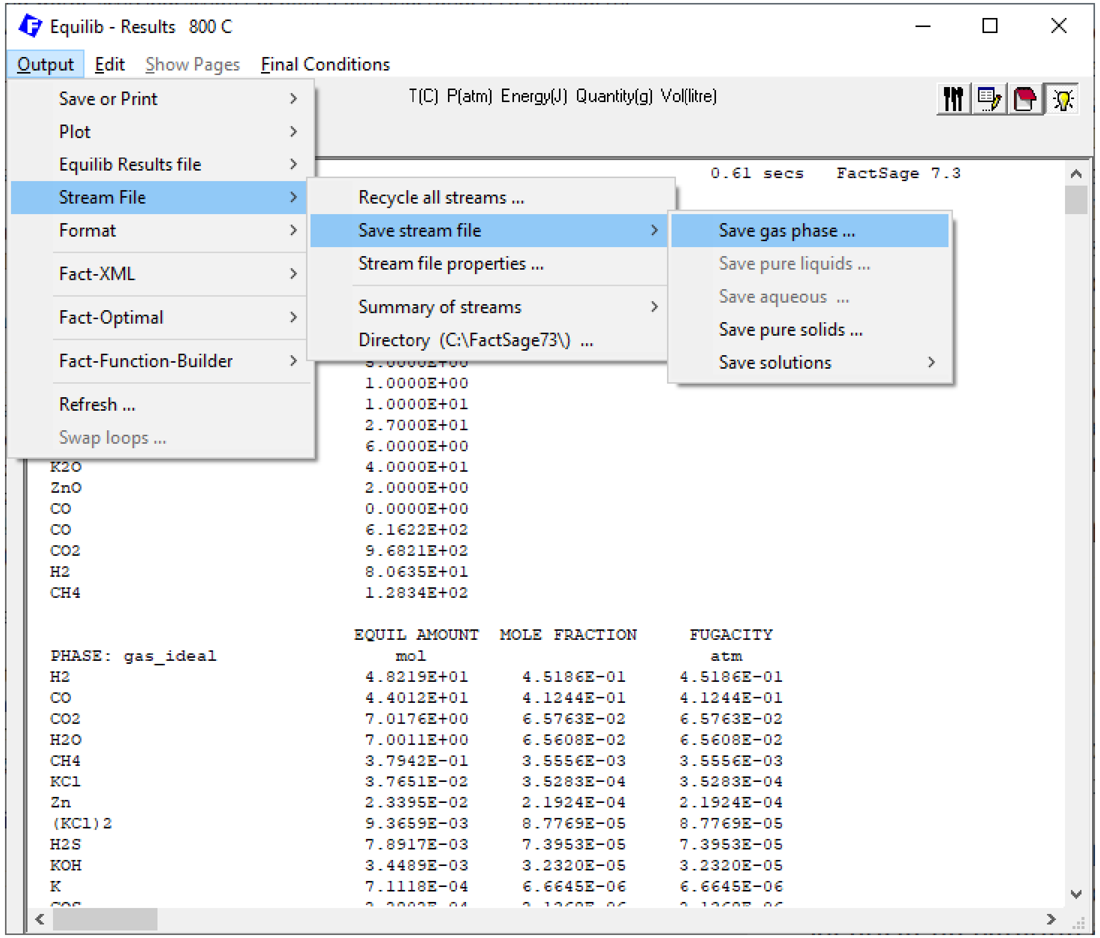
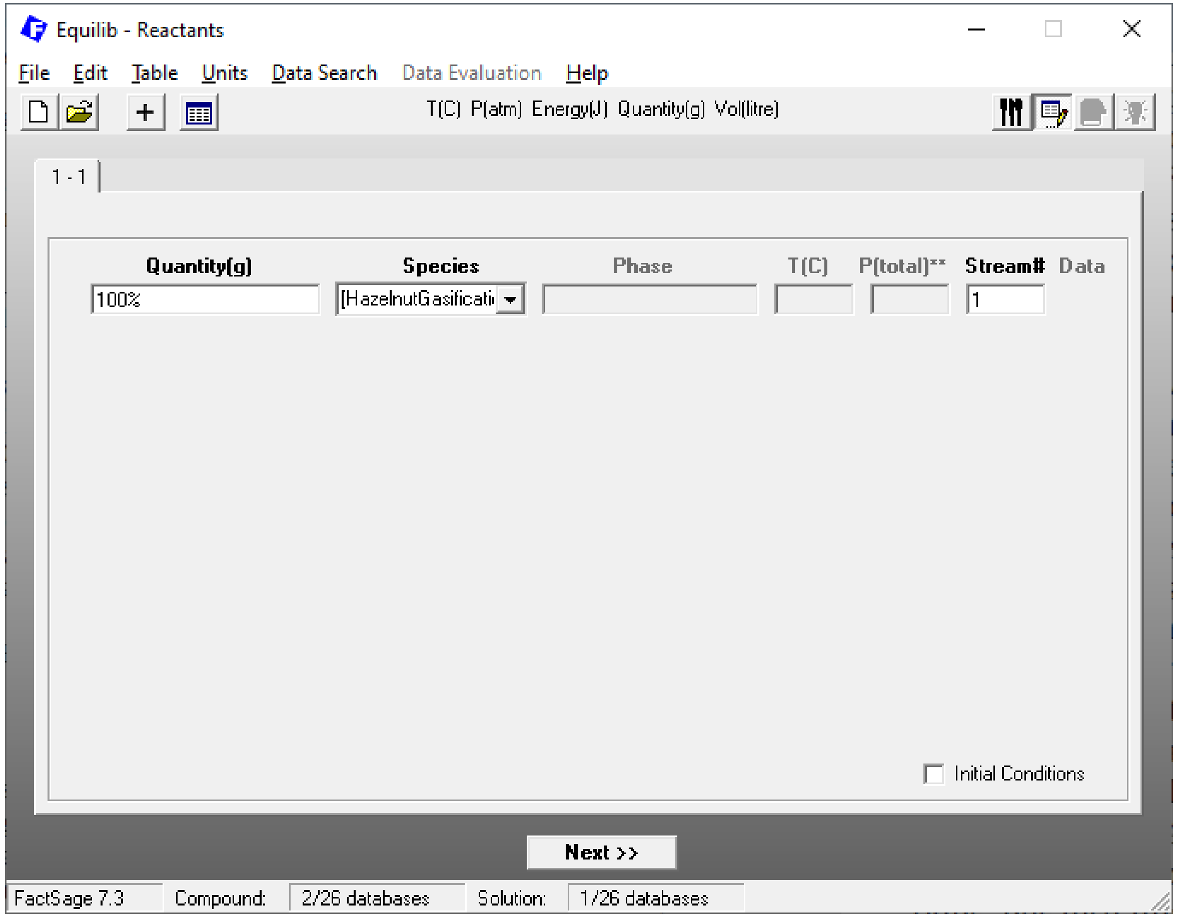
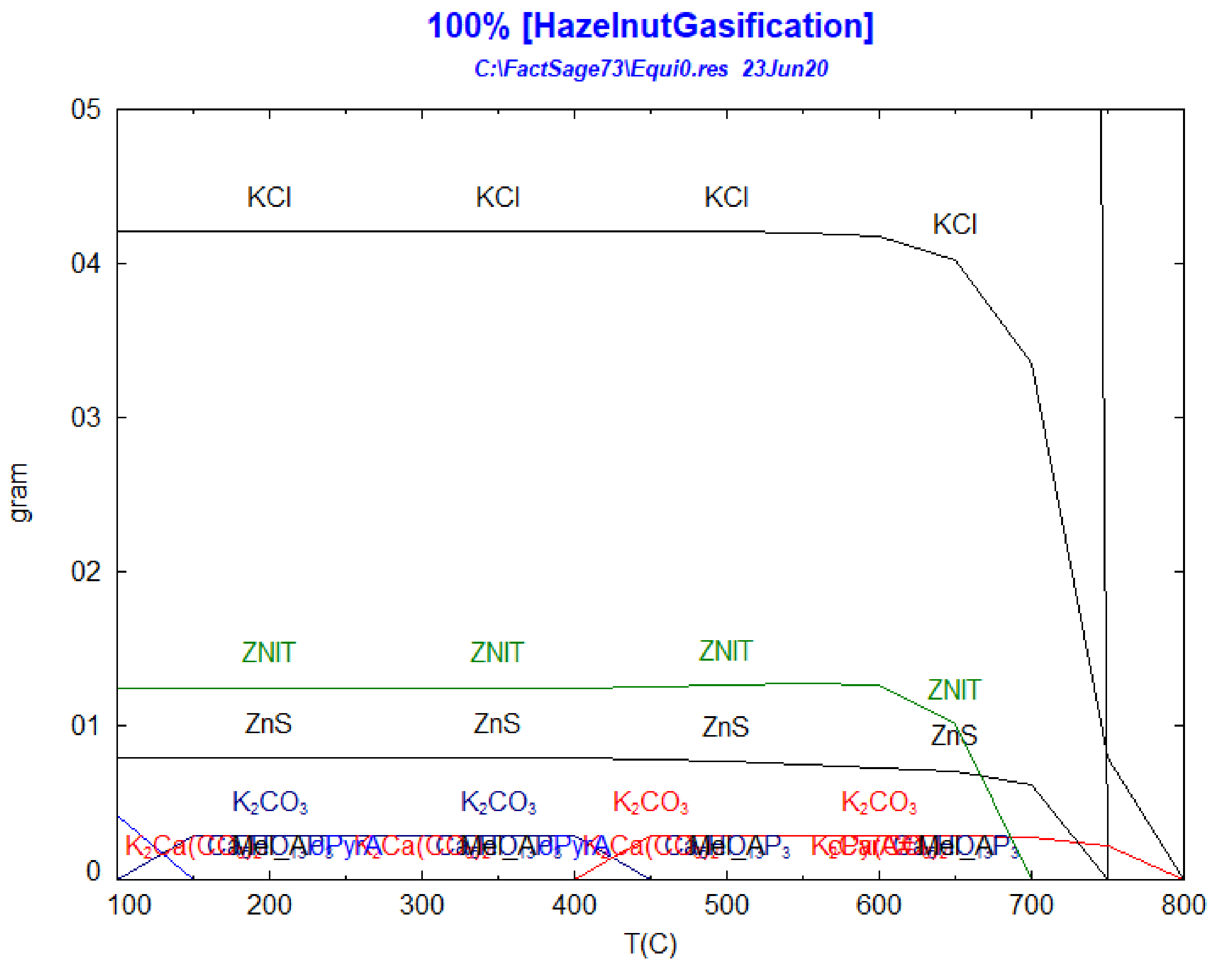




Condensation of salts during cooling of syngas

- Case: Hazelnut shells in steam gasification
- Here: One equilibrium calculation

- Better: “Scheil cooling“ from the gas phase, see Abascal et al., Ind. Eng. Chem. Res. 55 (2016) 6911.



Condensation of salts during cooling of syngas

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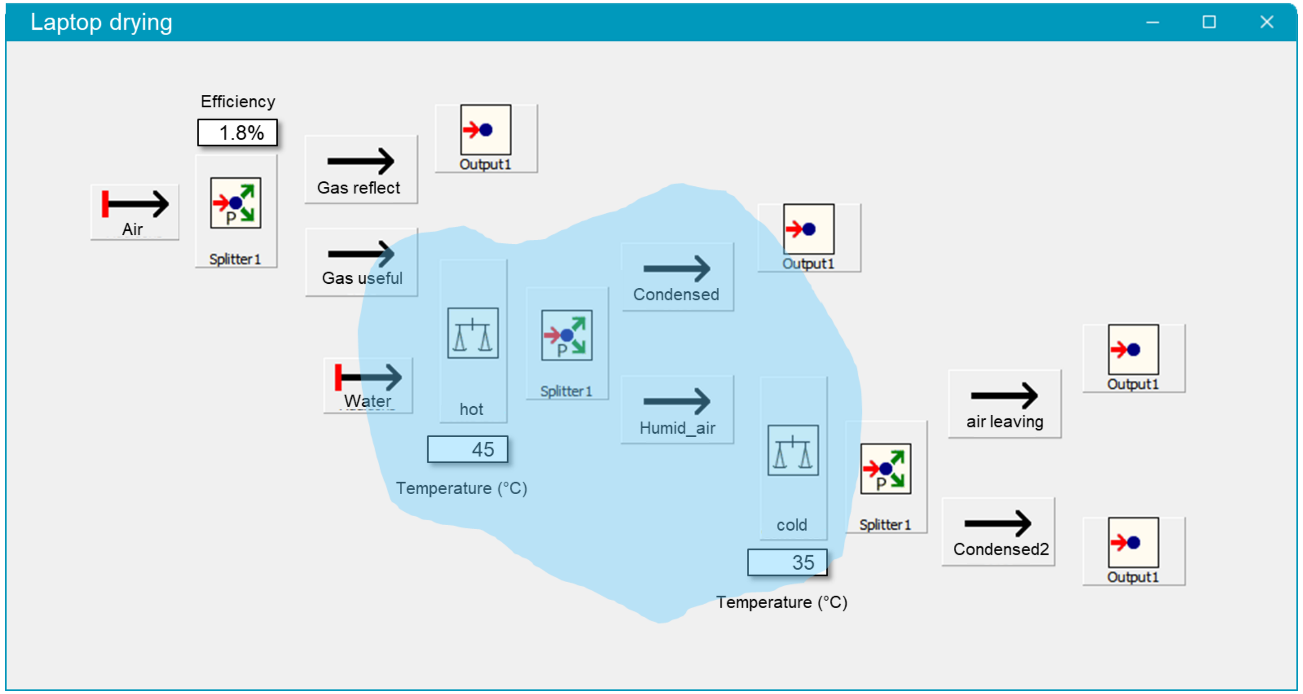

Outline

- Motivation
- An unintentional experiment
- FactSage applications
  - Ash fusion experiments
  - Melting and oxidation of sulfides from coal ashes
  - Condensation of salts during cooling of syngas

Thank you for your attention!

(no animals have been harmed during the preparation of this talk, but one laptop has suffered…)