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.

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.

	Mineral	1
	Silicates	83.5
	Quartz	49
	Cristobalite	
1212.	Opal	
/	Kaolinite	14
	Illite + Muscovite	6
	Montmorillonite	0.5
	Chlorite	2
	Plagioclase	7
bnc a	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	
ision test ^a	Barite	0.5
	Phosphates	1.5
HT FT	Apatite	1
	Vivianite	0.5
1380 1400	Govazite	
1500 1400	Total	98.5

Г	abl	e 2	
	-	-	

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

Sample	Proxim	nate analys	sis (as rece	eived)	Ultim	ate anal	ysis (da	ıf)		High-te	High-temperature ash analysis (815 °C)									Ash-fusion test ^a			Barite	
	FC	VM	А	М	С	0	Н	S	N	SiO ₂	Al_2O_3	Fe ₂ O ₃	CaO	SO ₃	MgO	K ₂ 0	TiO ₂	Na ₂ O	SiO ₂ / Al ₂ O ₃	DAI ^b	ST	HT	FT	Phosphates Apatite Vivianite
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	Goyazite Total

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?"

Table 2 Chemical comp	able 2 Themical composition (wt. %) and ash-fusion temperatures (°C) of the coal samples														Jarosite + N Alunite Hexabydrit									
Sample	Proxin	nate analy	sis (as rec	eived)	Ultima	ate analy	ysis (da	ıf)		High-te	emperatui	re ash ana	lysis (815	5 °C)							Ash-fus	sion test ^a		Barite
	FC	VM	А	М	С	0	Н	S	N	SiO ₂	Al_2O_3	Fe ₂ O ₃	CaO	SO ₃	MgO	K ₂ 0	TiO ₂	Na ₂ O	SiO ₂ / Al ₂ O ₃	DAI ^b	ST	HT	FT	Phosphates Apatite Vivianite
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	Goyazite Total

Vassilev, Fuel 88 (2009) 235.

Mineral	1
Silicates	83.5
Quartz	49
Cristobalite	
Opal	
Kaolinite	14
llite + Muscovite	6
Montmorillonite	0.5
Chlorite	2
Plagioclase	7
K feldspar	3
Zeolite	2
Dxides and hydroxides	2.5
Magnetite + Hematite	1
Goethite + Lepidocrocite	1
pinel + 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
arosite + Melanterite	1.5
Alunite	0.5
lexahydrite	
Barite	0.5
Phosphates	1.5
Apatite	1
/ivianite	0.5
Goyazite	
lotal	00 5

An accidental experiment





An accidental experiment









 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

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 • 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

$79 \text{ m}^3/\text{h} = 1320 \text{ l/min} = 54 \text{ mol } \text{N}_2 \text{ / min}$



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





 Turbo Power TwinTurbo 380

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79 m³/h = 1320 l/min = 54 mol N₂ / min Estimated efficiency of 1.8% \rightarrow 1 mol N₂ / min



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





Turbo Power ★★☆☆☆ ~ Price: \$199.99 (s	Print Print File Edit Table Units Dim Image: The sector of the	
Get \$50 off instant Item is returnable i Air Flow: 79 m ³ / Drying Power: 2 Technology: Cer Attachments: 2 Weight: 500 gra Compare with simil 2 new from \$199.9	Quantity(mol) Species Phase T(C) P(total in a gradient of a gradi	al)** Stream# Data
79 m ³ /h = 1320 l/min = 54 mol N ₂ / min Estimated efficiency of 1.8% \rightarrow 1 mol N ₂ / min		Initial Conditions
https://www.amazon.com/Turbo-Power-TwinTurbo	-38 FactSage 7.3 Compound: 1/26 databases Solution: 0/26 databases	//.

$79 \text{ m}^3/\text{h} = 1320 \text{ l/min} = 54 \text{ mol } \text{N}_2 \text{ / min}$ Estimated efficiency of $1.8\% \rightarrow 1 \text{ mol } N$

Gr

An accidental experiment – and its analysis



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by Turbo Power ★★★☆☆ ~ 7 rat	T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)	M 📑 🐼
Price: \$199.99 (\$199.9 Get \$50 off instantly: Pa	Reactants (2) 18 g H20 + <a> N2	
tem is returnable in 30 (• Air Flow: 79 m³/h.	Products Compound species * + Base-Phase	Custom Solutions 0 fixed activities Details
 Drying Power: 2100 V Technology: Ceramic Attachments: 2 Conce Weight: 500 grams / Compare with similar ite 	Figas (• ideal () real 29 aqueous 0 Figure liquids 8 pure solids 0 species: 37	0 ideal solutions Pseudonyms apply Edit Volume data solids and liquids = 0 c include molar volume data and physical properties data
2 new from \$199.98	Target Legend - none - Estimate T(K): Quantity(mol): 0	paraequilibrium & Gmin edit Virtual species: 0 <u>Total Species (max 5000)</u> 37 <u>Total Solutions (max 200)</u> 0 <u>Total Phases (max 1500)</u> 9
n N ₂ / min	Final Conditions <a> T(C) P(atm) Product H(J) 1 60 1 25 1 10 steps Table 60 calculations	rormal C normal + transitions transitions only open Calculate >>
TuinTurha 20	F	

79 m³/h = 1320 l/min = 54 mol N₂ / min Estimated efficiency of 1.8% \rightarrow 1 mol N₂ / min

https://www.amazon.com/Turbo-Power-TwinTurbo-38 FactSage 7.3







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 - Melting and oxidation of sulfides from coal ashes
 - Condensation of salts during cooling of syngas

- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 - Insert high-T ash analysis, fix $p(O_2)$

Sample	Proximat	e analysis	(as receiv	ed)	Ultimate analysis (daf)							
	FC	VM	А	М	С	0	Н	S	Ν			
4. Balkan	46.8	14.7	38.1	0.4	85.7	4.5	4.7	4.1	1.0			

High-te	mperatur	Ash-fusion test ^a											
SiO ₂	Al_2O_3	Fe ₂ O ₃	CaO	SO ₃	MgO	K ₂ 0	TiO ₂	Na ₂ O	SiO ₂ / Al ₂ O 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.



- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 Fix p(O₂)

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	T	C) P(atm) Energy(J	l) Quantity(g) Vol(litre)	🚻 📑 💌
Reactants (10)				
(gram) 57.81 SiO2 + 22.8	7 Al2O3 +	7.34 Fe2O3	+ 2.66 CaO + 2.7 SO3	+ 1.35 MgO + 4.15 K2O +
4				•
- Producte				
	- Solution ph	ases		Custom Solutions
	× +	Base-Phase	Full Name 🔺	1 fixed activities Details
두 gas 🕫 ideal 🔿 real 🛛 66		FT oxid-SLAGA	A-Slag-liq all oxides + S	0 ideal solutions
📕 aqueous 🛛 🛛 🖉		FT oxid-SLAGB	B-Slag-liq with SO4	Pseudonyms
* ∓ pure liquids 35		FToxid-SLAG?	?-Slag-liq	apply 🗖 🔡 Edit
* + pure solids 246		FToxid-SPINA	A-Spinel	Volume data
* - custom selection		FToxid-MeO_A	A-Monoxide	solids and liquids = 0
species: 347		FT oxid-cPyrA	A-Clinopyroxene	C include molar volume data
		FT oxid-cPyrC	C-Clinopyroxene	and physical properties data
		F I oxid-cPyrD	D-Uinopyroxene	🔲 🗖 paraequilibrium & Gmin 🔄 edit
- none -	Legend	la 10	Show 🔍 all 🔿 selected	Virtual species: 551
Estimate T(K): 1000	+ - selecter	d 34		Total Species (max 5000) 787
Quantity(a): 0			species: 440 solutions: 54 Select	Total Solutions (max 200) 54
quantity(g). jo			solutions. 04	Total Phases (max 1500) 336
- Final Conditions				Fauilibrium
<a> 	T(C)	P(atm)	▼ Product H(J) ▼	normal O normal + transitions
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	- recom	mend you not select	both pure liquids and molten s	colutions -
FactSage 7.3				

- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 Fix p(O₂)



- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 Fix p(O₂)



- Gr
- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 Fix p(O₂)
- Approach 2: Add O₂+N₂

存 Equilib - I	Reactants						_	×
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1.10								1
	Quantity(g)	Spe	cies	Phase	T(C) P(total)**	Stream#	Data
57.81		Si02			<u> </u>		1	
+ 22.87		AI203			-		1	
+ 7.34		Fe203			-		1	
+ 2.66		CaO			-		1	
+ 2.7			—				1	
+ 1.35		MaQ					1	
+ 415		[K:30					1	
4.13		K20						
* 0.32		Na20					1	
⁺ 2.1 m	ol	02			<u> </u>		1	
► 7.9 m	ol	N2			-		1	
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				Next >>				
FactSage 7.3	Compound	: 2/26 databases	Solution:	1/26 databases				

- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 Fix p(O₂)
- Approach 2: Add O₂+N₂



- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210°C)
- Approach 1:
 Fix p(O₂)
- Approach 2: Add O₂+N₂







- Case: High-SO₃ containing bituminous, high ash coal (ST= 1210° C)
- Approach 1:
 Fix p(O₂)

- Approach 2: Add O₂+N₂
- Approach 3: Fix p(O₂), omit SO₃





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







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1	- 10 11 - 1	13									
	Q	uantity(g)		Species	Phase		(C)	P(total)**	Stream#	Data	
	57.81		SiO2			Ψ.			1		
	• 22.87		Al203			Ŧ			1		
	• 7.34		Fe203			-			1		
1	• 2.66		CaO			-			1		
	• 0		503		,				1		
	+ 1.25		MaQ				·		1		
	1.00										
	• 4.15		K2U			T					
	• 0.32		Na20			$\overline{\nabla}$			1		
	• <4A>		N2			Ŧ			1		
1	• <a>		02			-			1		
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FactSa	age 7.3	Compound:	3/26 databa	ases Solutio	on: 2/26 databa	ises					1



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



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🗅 🖻 + 🔳	T(C) P(atm) Energy(J) Quantity(g	Vol(litre)	III 📑 🔁	0.10	
1 10 11 10					$T = 1500^{\circ}C$, vary O_2 content to
1.10 [11.13]					determine conditions with $\lambda < 1$
Quantitu(a)	Consist Phase	T(C)	P(total)** Choam# Data		
57.81	Si02			0.30 -	
+ 22.87	AI203				\setminus
+ 7.34	Fe203		1		
+ 2.66	CaO			2	
+ 0	 S03			0.20 -	Со
+ 1.35	MaD		1	ä	
+ 4.15	K20		1		CO ₂
+ 0.32	Na20		1		
+ <4A>	N2		1	0.10 -	
+ <a>	02	-	1		
	Nevt			0	<u> </u>
FeelQeen 7.2 Commun. 1				200	300 400 500 600 700 800
FactSage 7.3 Compound: 3	3726 databases Solution: 2726 database	3			Alpha









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• Case: HazeInut shells in steam gasification

1		5 47	
▼ Ash Prope	rties		
▼ Ash con	position		
SO3		wt% (ash)	4.24
CL		wt% (ash)	2.34
P ₂ O ₅		wt% (ash)	5.14
SiO ₂		wt% (ash)	0.98
Fe ₂ O ₃		wt% (ash)	1.34
Al ₂ O ₃		wt% (ash)	10.42
CaO		wt% (ash)	26.61
MgO		wt% (ash)	6.22
Na ₂ O		wt% (ash)	0.00
K ₂ O		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



• Case: HazeInut shells in steam gasification

Ash Properties		
▼ Ash composition		
50 ₃	wt% (ash)	4.24
CL	wt% (ash)	2.34
P ₂ O ₅	wt% (ash)	5.14
SiO2	wt% (ash)	0.98
Fe ₂ O ₃	wt% (ash)	1.34
Al ₂ O ₃	wt% (ash)	10.42
CaO	wt% (ash)	26.61
MgO	wt% (ash)	6.22
Na ₂ O	wt% (ash)	0.00
K ₂ O	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

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		Qua	ntity(g)		Spec	cies	Phase		T(C)	P(total)**	Stream#	Data	
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	+ 27				CaO			-			1		
	+ 6			M	MgO	[-			1		
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	+ 2			Z	ZnO	[-			1		
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Each	Saga 7 3		ompourse	. <u>272</u> 6	databases	Solution:	2/26 database						



Case: HazeInut shells in steam gasification

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

	Oxygen	Oxygen	
	Gasification	Gasification	
	(Entrained	(Fluidized	Steam
Compound	Flow)	Bed)	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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) 🛋 🕂 🚺		T(C)	P(atm) Ene	rgy(J) Quantity(g) V	ol(litre)			111	🦻 🖹 🤋
1-9									
Quar	ntity(g)	Speci	es	Phase		T(C)	P(total)**	Stream#	Data
4		S03						1	
+ 2		CI						1	
+ 5		P205						1	
+ 1		Si02	— F		ΞΓ			1	
+ 10		AI203	— `		Ţ			1	
+ 27		CaO	— '		Ξi			1	
+ 6		MaQ	— 'r		Ξí			1	
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Rauch et al., WIREs Energy Environ 2013. doi: 10.1002/wene.97



• Case: HazeInut shells in steam gasification

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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
N2 (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

存 Equil	ib - Reactants						- [×
<u>F</u> ile <u>E</u> di	t <u>T</u> able <u>U</u> nit	s <u>D</u> ata Search	Data Evaluation	<u>H</u> elp					
0 🖻	+ 🔳		T(C) P(atm) En	ergy(J) Quantity(g) ^v	Vol(litre)		111	🦻 🕞	₽.
1 - 10	11 - 14								
	Quantity(g	9)	Species	Phase	T(C)	P(total)**	Stream#	Data	1
+ 2	22 mol	CO			_		1		
+ 2	22 mol	C02	[-		1		
+ 7	40 mol	H2	—— í			·	1		
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Rauch et al., WIREs Energy Environ 2013. doi: 10.1002/wene.97



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Compound	Flow)	Bed)	Gasification
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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
N2 (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



Case: HazeInut shells in steam gasification

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M. to Baben, GTT-Technologies

Condensation of salts during cooling of syngas

- Case: HazeInut 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.





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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...)

Thermodynamic Software

Thermodynamic Databases

Consulting Services