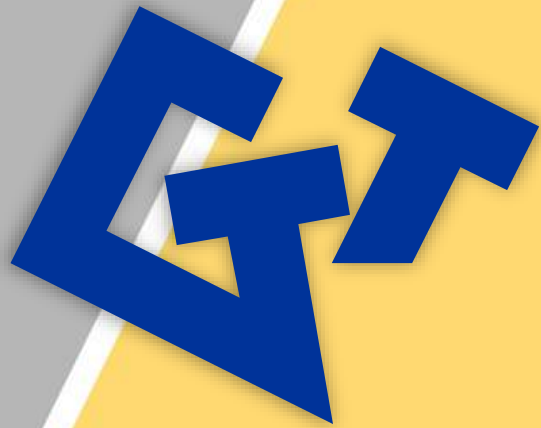




From a kitchen experiment to constrained Gibbs energy minimization

M. to Baben
GTT-Technologies

23rd GTT Users' Meeting, 23.06.2021



Thermodynamic Software



Thermodynamic Databases



Consulting Services

1. Problem statement: Experiment 1
 - Solution 1: species selection
 - Solution 2: virtual system components
2. Excursus: history and science of baking powder
3. Problem statement: Experiment 2
 - Solution: virtual system components
4. Further applications

Problem statement: Experiment 1

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

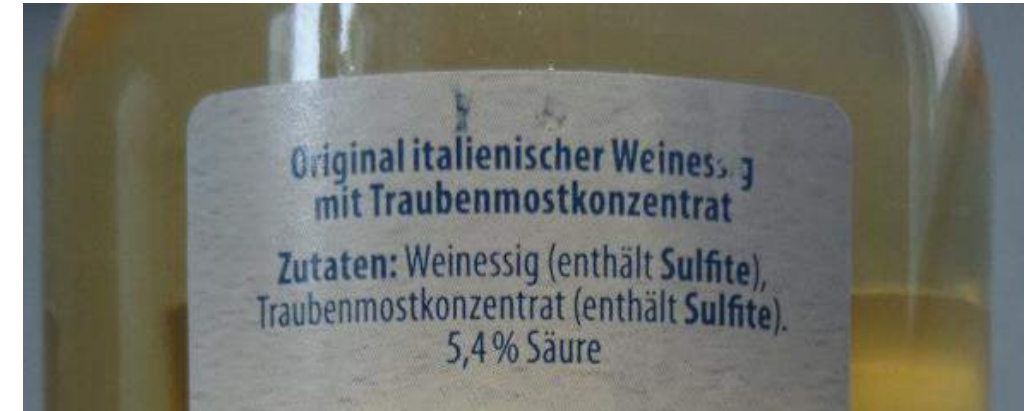
1 - 2

Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
94.6 g	H2O				1	
+ 5.4 g	CH3COOH				1	

☐ Initial Conditions

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases



[What is the pH value of vinegar? - Quora](https://www.quora.com/What-is-the-pH-value-of-vinegar)

<https://www.quora.com/What-is-the-pH-value-of-vinegar>

Most commercial vinegars contain 5% acetic acid which gives them a pH of 2.4, but specialty vinegars can be higher or lower.

Problem statement: Experiment 1

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 2

Quantity(mol)	Species	Phase	T(C)	P(total)**
94.6 g	H2O			
+ 5.4 g	CH3COOH			

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Reactants (2)

94.6 g H2O + 5.4 g CH3COOH

Products

Compound species

- + gas ☒ ideal ☐ real 41
- + aqueous 22
- + pure liquids 9
- + pure solids 3

species: 76

Target

- none -

Estimate T(K): 1000

Quantity(mol): 0

Solution phases

*	+	Base-Phase	Full Name

Custom Solutions

0 fixed activities
0 ideal solutions

Pseudonyms

apply ☐ Edit ...

Volume and physical prop data

☒ assume molar volumes of solids and liquids = 0

☐ use only molar volume data

☐ use V & phys. property data

☐ paraequilibrium & Gmin edit

Virtual species: 0

Total Species (max 5000) 76

Total Solutions (max 200) 1

Total Phases (max 1500) 14

Legend

☒ Show ☒ all ☐ selected

species: 0

solutions: 0

Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		25	1	

10 steps ☐ Table

1 calculation

Equilibrium

☒ normal ☐ normal + transitions

☐ transitions only ☐ open

- no time limit -

Calculate >>

FactSage 8.1

Problem statement: Experiment 1

	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: gas_ideal	mol		atm
CH ₃ COOH	0.0000E+00	2.2928E-15	1.0685E-16
TOTAL:	0.0000E+00	1.0000E+00	4.6603E-02
PHASE: aqueous	mol	MOLALITY	ACTIVITY
H ₂ O_liquid	5.4309E+00	5.5508E+01	1.0000E+00
H[+]	2.6617E-07	2.7205E-06	2.7205E-06
CH ₄	2.0054E-06	2.0496E-05	2.0496E-05
CO ₂	1.7397E-06	1.7781E-05	1.7781E-05
HCO ₃ [-]	2.6580E-07	2.7167E-06	2.7167E-06
CH ₃ COO[-]	1.5756E-14	1.6103E-13	1.6103E-13
CH ₃ COOH	2.3268E-15	2.3781E-14	2.3781E-14
TOTAL:	5.4309E+00		1.0000E+00
pH = 5.5654			
	mol		ACTIVITY
C_Graphite(s)	1.7984E-01		1.0000E+00

Problem statement: Experiment 1

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 2

Quantity(mol)	Species	Phase	T(C)	P(total)**
94.6 g	H2O			
+ 5.4 g	CH3COOH			

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Reactants (2)

94.6 g H2O + 5.4 g CH3COOH

Products

Compound species

- ☒ gas ☒ ideal ☐ real 41
- ☒ aqueous 22
- ☒ pure liquids 9
- ☐ pure solids 0

species: 73

Target

- none -

Estimate T(K): 1000

Quantity(mol): 0

Solution phases

*	+	Base-Phase	Full Name

Legend

☒ Show ☒ all ☐ selected

species: 0

solutions: 0

Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
10	steps	25	1	

1 calculation

Equilibrium

☒ normal ☐ normal + transitions

☐ transitions only ☐ open

- no time limit -

Calculate >>

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply ☐ Edit ...

Volume and physical prop data

☒ assume molar volumes of solids and liquids = 0

☐ use only molar volume data

☐ use V & phys. property data

☐ paraequilibrium & Gmin edit

Virtual species: 0

Total Species (max 5000) 73

Total Solutions (max 200) 1

Total Phases (max 1500) 11

FactSage 8.1

Problem statement: Experiment 1

	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: gas_ideal	mol		atm
CH ₄	8.9858E-02	4.8831E-01	4.8831E-01
CO ₂	8.8391E-02	4.8034E-01	4.8034E-01
CH ₃ COOH	5.9167E-13	3.2153E-12	3.2153E-12
TOTAL:	1.8402E-01	1.0000E+00	1.0000E+00
PHASE: aqueous	mol	MOLALITY	ACTIVITY
H ₂ O_liquid	5.2453E+00	5.5508E+01	9.9969E-01
H[+]	7.7352E-06	8.1858E-05	8.1858E-05
CH ₄	6.4266E-05	6.8009E-04	6.8009E-04
CO ₂	1.5239E-03	1.6126E-02	1.6126E-02
CH ₃ COO[-]	1.5218E-11	1.6105E-10	1.6105E-10
CH ₃ COOH	6.7625E-11	7.1564E-10	7.1564E-10
TOTAL:	5.2469E+00		1.0000E+00
pH = 4.0869			

1. Problem statement: Experiment 1
Solution 1: species selection
Solution 2: virtual system components
2. Excursus: history and science of baking powder
3. Problem statement: Experiment 2
Solution: virtual system components
4. Further applications

Problem statement: Experiment 1 - Solution: species selection

F Selection - Equilib Page 1/1 : T(C) = 25, P(atm) = 1

File Edit Show Sort

Selected: 3/22 **AQUEOUS**

Page 1/1 : T(C) = 25, P(atm) = 1

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	51	H ⁺ (aq)	FactPS	aqueous			8.1858E-05	8.1858E-05	8.1858E-05
	52	H ₂ (aq)	FactPS	aqueous			1.5978E-09	1.5978E-09	1.5978E-09
	53	CH ₄ (aq)	FactPS	aqueous			6.8009E-04	6.8009E-04	6.8009E-04
	54	C ₂ H ₂ (aq)	FactPS	aqueous			5.4321E-40	5.4321E-40	5.4321E-40
	55	C ₂ H ₄ (aq)	FactPS	aqueous			6.3104E-22	6.3104E-22	6.3104E-22
	56	C ₂ H ₆ (aq)	FactPS	aqueous			2.0559E-10	2.0559E-10	2.0559E-10
	57	O ₂ (aq)	FactPS	aqueous			2.9984E-75	2.9984E-75	2.9984E-75
	58	OH ⁻ (aq)	FactPS	aqueous			1.2069E-10	1.2069E-10	1.2069E-10
	59	HO ₂ ⁻ (aq)	FactPS	aqueous			3.1211E-62	3.1211E-62	3.1211E-62
	60	HOOH(aq)	FactPS	aqueous			1.2701E-54	1.2701E-54	1.2701E-54
	61	CO(aq)	FactPS	aqueous			2.5744E-13	2.5744E-13	2.5744E-13
	62	CO ₂ (aq)	FactPS	aqueous			1.6126E-02	1.6126E-02	1.6126E-02
	63	CO ₃ ²⁻ (aq)	FactPS	aqueous			4.6868E-11	4.6868E-11	4.6868E-11
	64	C ₂ O ₄ ²⁻ (aq)	FactPS	aqueous			5.0549E-19	5.0549E-19	5.0549E-19
	65	CH ₃ OH(aq)	FactPS	aqueous			5.0422E-15	5.0422E-15	5.0422E-15
	66	CH ₃ CH ₂ OH(aq)	FactPS	aqueous			2.0970E-17	2.0970E-17	2.0970E-17
	67	HCOO ⁻ (aq)	FactPS	aqueous			2.9402E-10	2.9402E-10	2.9402E-10
	68	HCOOH(aq)	FactPS	aqueous			1.2494E-10	1.2494E-10	1.2494E-10
+	69	CH ₃ COO ⁻ (aq)	FactPS	aqueous			1.6105E-10	1.6105E-10	1.6105E-10
+	70	CH ₃ COOH(aq)	FactPS	aqueous			7.1564E-10	7.1564E-10	7.1564E-10
	71	HCO ₃ ⁻ (aq)	FactPS	aqueous			8.1857E-05	8.1857E-05	8.1857E-05

☐ permit selection of 'X' species Help Suppress Duplicates Edit priority list :

Show Selected Select All Select/Clear... Clear OK

Parameters Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

94.6 g H₂O + 5.4 g CH₃COOH

Species: 5

Legend

☒ Show ☒ all ☐ selected

species: 0 solutions: 0

Equilibrium

☒ normal ☐ normal + transitions

☐ transitions only ☐ open

- no time limit -

Problem statement: Experiment 1 - Solution: species selection

	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: gas_ideal	mol		atm
CH3COOH	0.0000E+00	1.0000E+00	4.2520E-03 ✓
TOTAL:	0.0000E+00	1.0000E+00	4.2520E-03
PHASE: aqueous	mol	MOLALITY	ACTIVITY
H2O_liquid	5.2511E+00	5.5508E+01	9.8295E-01
H[+]	3.9499E-04	4.1753E-03	4.1753E-03
CH3COO[-]	3.9499E-04	4.1753E-03	4.1753E-03
CH3COOH	8.9527E-02	9.4638E-01	9.4638E-01
pH = 2.3793 ✓			

What is the pH value of vinegar? - Quora

<https://www.quora.com/What-is-the-pH-value-of-vinegar>

Most commercial vinegars contain 5% acetic acid which gives them a pH of 2.4, but specialty vinegars can be higher or lower.

Problem statement: Experiment 1 - Solution: species selection

Phase	Species	H	C	O	e ⁻ (aq)
Gas	CH ₄	4	1		
	CO ₂		1	2	
	CH ₃ COOH	4	2	2	
Aqueous	H ₂ O	2		1	
	H ⁺				-1
	CH ₄	4	1		
	CO ₂		1	2	
	CH ₃ COOH	4	2	2	
	CH ₃ COO ⁻	3	2	2	1
Graphite	C		1		

Problem statement: Experiment 1 - Solution: species selection

Phase	Species	H	C	O	e ⁻ (aq)
Gas	CH₄	4	1		
	CO₂		1	2	
	CH ₃ COOH	4	2	2	
Aqueous	H ₂ O	2		1	
	H ⁺				-1
	CH₄	4	1		
	CO₂		1	2	
	CH ₃ COOH	4	2	2	
	CH ₃ COO ⁻	3	2	2	1
Graphite	C		1		

$$\rightarrow \sum n(\text{acetic acid}) = \frac{1}{2} n(\text{C})$$

Problem statement: Experiment 1 - Solution: virtual system components



Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 3

Quantity(mol)	Species	Phase	T(C)	P{total}**	Stream#	Data
94.6 g	H2O				1	
+ 8.9922127E-02	CH3COOHQa				1	
+ 0	CH3COOQa[-]					

☐ Initial Conditions

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases

Problem statement: Experiment 1 - Solution: virtual system components



F Selection - Equilib - no results -

File Edit Show Sort

Selected: 41/42 **GAS**

- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	22	H2O(g)	FactPS	Steam					
+	23	HOO(g)	FactPS	gas					
+	24	HOOH(g)	FactPS	gas					
+	25	CO(g)	FactPS	gas					
+	26	C2O(g)	FactPS	gas					
+	27	CO2(g)	FactPS	gas					
+	28	C3O2(g)	FactPS	gas					
+	29	HCO(g)	FactPS	gas					
+	30	H2CO(g)	FactPS	gas					
+	31	CH3O(g)	FactPS	Methoxy					
+	32	CH3O(g2)	FactPS	Hydroxymethyl					
+	33	CH3OH(g)	FactPS	gas					
+	34	CH2CO(g)	FactPS	gas					
+	35	C2H4O(g)	FactPS	Oxirane_gas					
+	36	C2H4O(g2)	FactPS	Acetaldehyde_g					
+	37	CH3CH2OH(g)	FactPS	gas					
+	38	CH3CH2OH(g2)	FactPS	(CH3)2O					
+	39	COOH(g)	FactPS	gas					
+	40	HCOOH(g)	FactPS	gas					
	41	CH3COOH(g)	FactPS	gas					
+	42	CH3COOHQa(g)	FactPS	gas					

☐ permit selection of 'X' species Help Suppress Duplicates Edit priority list:

Show Selected Select All Select/Clear... Clear OK

F Selection - Equilib - no results -

File Edit Show Sort

Selected: 22/24 **AQUEOUS**

- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	56	C2H2(aq)	FactPS	aqueous					
+	57	C2H4(aq)	FactPS	aqueous					
+	58	C2H6(aq)	FactPS	aqueous					
+	59	O2(aq)	FactPS	aqueous					
+	60	OH(-)(aq)	FactPS	aqueous					
+	61	HO2(-)(aq)	FactPS	aqueous					
+	62	HOOH(aq)	FactPS	aqueous					
+	63	CO(aq)	FactPS	aqueous					
+	64	CO2(aq)	FactPS	aqueous					
+	65	CO3(2-)(aq)	FactPS	aqueous					
+	66	C2O4(2-)(aq)	FactPS	aqueous					
+	67	CH3OH(aq)	FactPS	aqueous					
+	68	CH3CH2OH(aq)	FactPS	aqueous					
+	69	HCOO(-)(aq)	FactPS	aqueous					
+	70	HCOOH(aq)	FactPS	aqueous					
	71	CH3COO(-)(aq)	FactPS	aqueous					
	72	CH3COOH(aq)	FactPS	aqueous					
+	73	HCO3(-)(aq)	FactPS	aqueous					
+	74	HC2O4(-)(aq)	FactPS	aqueous					
+	75	CH3COOQa(-)(aq)	FactPS	aqueous					
+	76	CH3COOHQa(aq)	FactPS	aqueous					

☐ permit selection of 'X' species Help Suppress Duplicates Edit priority list:

Show Selected Select All Select/Clear... Clear OK

Problem statement: Experiment 1 - Solution: virtual system components



	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: gas_ideal	mol		atm
CH3COOHQa	0.0000E+00	1.0000E+00	4.2520E-03 ✓
TOTAL:	0.0000E+00	1.0000E+00	3.5070E-02
PHASE: aqueous	mol	MOLALITY	ACTIVITY
H2O_liquid	5.2511E+00	5.5508E+01	9.8295E-01
H[+]	3.9499E-04	4.1753E-03	4.1753E-03
CH3COOQa [-]	3.9499E-04	4.1753E-03	4.1753E-03
CH3COOHQa	8.9527E-02	9.4638E-01	9.4638E-01
pH = 2.3793 ✓			

[What is the pH value of vinegar? - Quora](https://www.quora.com/What-is-the-pH-value-of-vinegar)

<https://www.quora.com/What-is-the-pH-value-of-vinegar>

Most commercial vinegars contain 5% acetic acid which gives them a pH of 2.4, but specialty vinegars can be higher or lower.

Problem statement: Experiment 1 - Solution: virtual system components



Phase	Species	H	C	O	e ⁻ (aq)
Gas	CH ₄	4	1		
	CO ₂		1	2	
	CH ₃ COOH	4	2	2	
Aqueous	H ₂ O	2		1	
	H ⁺				-1
	CH ₄	4	1		
	CO ₂		1	2	
	CH ₃ COOH	4	2	2	
	CH ₃ COO ⁻	3	2	2	1
Graphite	C		1		

Problem statement: Experiment 1 - Solution: virtual system components



Phase	Species	H	C	O	e ⁻ (aq)	Qa
Gas	CH ₄	4	1			
	CO ₂		1	2		
	CH ₃ COOHQa	4	2	2		1
Aqueous	H ₂ O	2		1		
	H ⁺				-1	
	CH ₄	4	1			
	CO ₂		1	2		
	CH ₃ COOHQa	4	2	2		1
	CH ₃ COOQa ⁻	3	2	2	1	1
Graphite	C		1			

$$\rightarrow \sum n(\text{acetic acid}) = n(Qa)$$

1. Problem statement: Experiment 1
 - Solution 1: species selection
 - Solution 2: virtual system components
- 2. Excursus: history and science of baking powder**
3. Problem statement: Experiment 2
 - Solution: virtual system components
4. Further applications

History and science of baking powder

- **Ingredients:** **Baking powder** is a dry chemical **leavening agent**, a mixture of a **carbonate** or **bicarbonate** and a weak **acid**. The base and acid are prevented from reacting prematurely by the inclusion of a buffer such as **cornstarch**.
https://en.wikipedia.org/wiki/Baking_powder
- Alfred Bird (1843): NaHCO_3
- Justus Liebig and Eben Norton Horsford (1863): $\text{NaHCO}_3 + \text{Na}_2\text{H}_2\text{P}_2\text{O}_7$
- Oetker (1903): $\text{NaHCO}_3 + (\text{Na}_2\text{H}_2\text{P}_2\text{O}_7 \cdot \text{starch})$

History and science of baking powder



84 kg Natriumbikarbonat
261 kg Backpulver



4.8 g NaHCO_3
15 g baking powder

1. Problem statement: Experiment 1
 - Solution 1: species selection
 - Solution 2: virtual system components
2. Excursus: history and science of baking powder
- 3. Problem statement: Experiment 2**
 - Solution: virtual system components
4. Further applications

Problem statement: Experiment 2

100 ml Water + 1 package of baking powder + 2 cl vinegar → ?

100 ml H_2O + 4.8 g NaHCO_3 + 2 cl vinegar → ?

→ I may not unselect $\text{CO}_2(\text{g})$, $\text{HCO}_3^-(\text{aq})$, ...!

Problem statement: Experiment 2 - Solution: virtual system components



Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 2

Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
94.6 g	H2O				1	
+ 5.4 g	CH3COOH				1	

CH3COOH: 5.4 g = 8.992213E-02 mol = 1.190496E-02 lb

- Convert this reactant amount to >
- Balance this reactant amount to a total ...
- Convert ALL reactant amounts to >
- Scale ALL reactant amounts to >
- Set ALL reactant quantities to 5.4 g
- Help ...

fraction - quantities will add up to 1
pct - quantities will add up to 100
total - quantities will add up to

☐ Initial Conditions

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases

Problem statement: Experiment 2 - Solution: virtual system components



Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 5

Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
18.92 g	H2O				1	
+ 1.7984425E-02	CH3COOHQa				1	
+ 0	CH3COOQa[-]					
+ 100 g	H2O				1	
+ 4.8 g	NaHCO3				1	

☐ Initial Conditions

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases

Problem statement: Experiment 2 - Solution: virtual system components



Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 5

Quantity(mol)	Species	Phase	T(C)	P(total)**	Str
18.92 g	H2O				1
+ 1.7984425E-02	CH3COOHQa				1
+ 0	CH3COOQa[-]				
+ 100 g	H2O				1
+ 4.8 g	NaHCO3				1

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Reactants (5)

18.92 g H2O + 1.7984425E-02 CH3COOHQa + 0 CH3COOQa[-] + 100 g H2O + 4.8 g NaHCO3

Products

Compound species

- * + gas ☒ ideal ☐ real 47
- * + aqueous 24
- pure liquids 0
- pure solids 0
- * - custom selection species: 71

Target

- none -

Estimate T(K): 1000

Quantity(mol): 0

Solution phases

*	+	Base-Phase	Full Name
---	---	------------	-----------

Legend

☒ Show ☒ all ☐ selected

species: 0

solutions: 0

Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
10	steps	25	1	

1 calculation

Equilibrium

☒ normal ☐ normal + transitions

☐ transitions only ☐ open

- no time limit -

Calculate >>

FactSage 8.1

Problem statement: Experiment 2 - Solution: virtual system components



	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: gas_ideal	mol		atm
CO2	1.4063E-02	9.6914E-01	9.6914E-01
CH3COOHQa	3.3369E-08	2.2996E-06	2.2996E-06
TOTAL:	1.4511E-02	1.0000E+00	1.0000E+00
PHASE: aqueous	mol	MOLALITY	ACTIVITY
H2O_liquid	6.6186E+00	5.5508E+01	9.8436E-01
H[+]	7.4789E-09	6.2724E-08	6.2724E-08
OH[-]	1.8493E-08	1.5509E-07	1.5509E-07
HCO3[-]	2.5305E-02	2.1223E-01	2.1223E-01
Na[+]	4.3267E-02	3.6287E-01	3.6287E-01
NaHCO3	1.3872E-02	1.1634E-01	1.1634E-01
CH3COOQa[-]	1.7923E-02	1.5032E-01	1.5032E-01
CH3COOHQa	6.1028E-05	5.1183E-04	5.1183E-04
pH = 7.2026			

1. Problem statement: Experiment 1
 - Solution 1: species selection
 - Solution 2: virtual system components
2. Excursus: history and science of baking powder
3. Problem statement: Experiment 2
 - Solution: virtual system components
- 4. Further applications**

Further applications

Using Virtual Elements to Impose Constraints

- FactSage permits the use of “virtual elements” with chemical symbols Qa, Qb, Qc,, Qz with atomic weights of 0.0. Virtual elements may be used in the modules **EQUILIB**, **PHASE DIAGRAM**, **COMPOUND** and **SOLUTION** in the same way as real elements.
- The use of virtual elements provides a useful means of applying constraints to certain equilibrium calculations as will be illustrated in the examples in this Section.
- For many of these examples you will need to activate the databases **VIRT** and **SURF** which can be found in the **FACTBASE** sub-folder of your FactSage folder.
- For additional examples, see:
R. Pajarre, P. Koukkari and P. Kangas, Chem. Eng. Sci., 146 (2016) 244-258 and
P. Koukkari, VTT Technology Bulletin 160 (2014), VTT Tech. Res. Ctr of Finland, Espoo, Finland. <https://www.vttresearch.com/sites/default/files/pdf/technology/2014/T160.pdf>



Equilib Advanced 15.1

www.factsage.com

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity

Equilib - Regular Features ...

Equilib - Advanced Features ...

Equilib - XML output ...

Equilib - Fact-Optimal ...

Equilib - Fact-Function-Builder ...

Equilib - Physical properties calculations ...

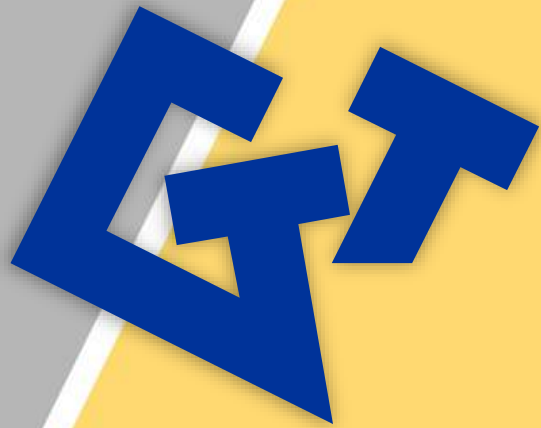
Equilib - Thermal conductivity of microstructures ...

100 g H2O

4.8 g NaHCO3

Next >>

FactSage 8.1 Compound: 1/42 databases Solution: 0/39 databases



Thank you very much for the attention!

Any question? Contact me!
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Thermodynamic Software



Thermodynamic Databases



Consulting Services