MEPHISTA
A thermodynamic database for new generation nuclear fuels

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MEPHISTA : « Multiphase Equilibria in Fuels via Standard Thermodynamic Analysis » is a self-consistent database designed for thermochemical equilibria calculation codes, specially developed for new generation nuclear fuels. The Calphad approach [1970Kaufman], [1998Saunders], [2007Zinkevich], [2007Schmid-Fetzer], (Figure 1), was used to obtain the assessed parameters of the Gibbs Energies of all the phases in the chemical system. MEPHISTA is consistent with the previous NUCLEA [2007Cheynet]1 and MOX [2007Cheynet]2 databases. 15 chemical elements are included in the database :

Ba-C-Cs-Fe-La-Mo-O-Pu-Ru-Si-Sr-U-Zr + Ar-H

This database covers the entire field from metal to oxide domains, and the temperature range up to 3500 K. 78 binary, 34 quasi-binary, 18 ternary, 2 quasi-ternary systems, 219 condensed stoechiometric compounds and 151 gaseous species are included in the database.

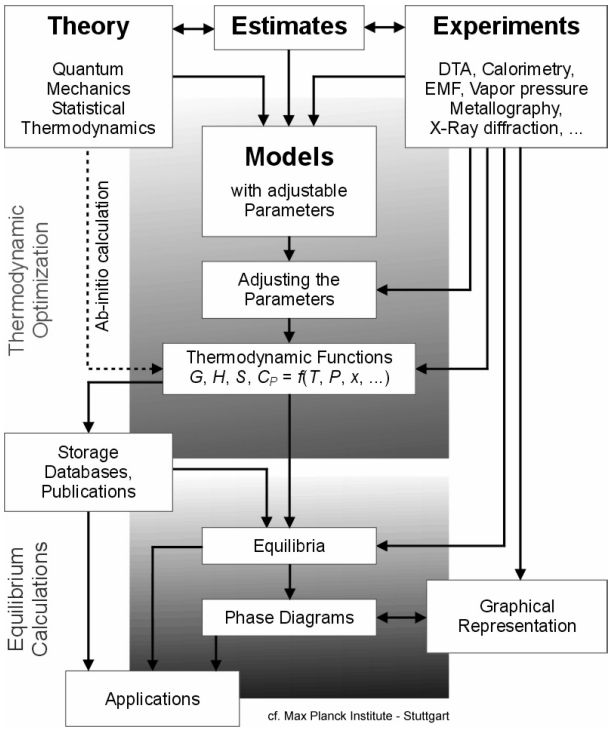

Figure 1 - CALPHAD method.

This method results in an optimized parametric description of the Gibbs energies of the phases of the systems when taking into account the crystallographic structure of the phases and all the experimental thermodynamic and phase boundary data available.

The thermodynamic parameters provide a consistent analytical description of the phase diagrams, chemical potentials, enthalpies of mixing, heat capacities, etc. When a published assessment was available for a particular system, it was analyzed and selected when the available experimental data were well reproduced by the description. Compatibility of the modeling used with respect to assembly of a data set for higher order systems has also been taken into account with in first compatibility with SGTE unary data [1991Dinsdale].

SYSTEMS

The lists of the assessed binary, quasi-binary, ternary and quasi-ternary systems are respectively presented in Table 1, 2, 3 and 4.

For user information, a quality criterion, based on comparison between calculation and available experimental data, has been established for each assessed system.

* **Estimated**
No experimental data available.

** **Perfectible**
Some domains need more experimental information (phase diagram or thermodynamic properties).

*** **Acceptable**
The system is known and satisfactorily modelled.

**** **High quality**
The system is quite well known and modelled.

1	Ba-C	✳	40	Fe-Sr	✳
2	Ba-Cs	✳✳✳	41	Fe-U	✳✳✳
3	Ba-Fe	✳✳	42	Fe-Zr	✳✳✳
4	Ba-La	✳✳	43	La-Mo	✳✳✳✳
5	Ba-Mo	✳✳✳	44	La-O	✳
6	Ba-O	✳✳	45	La-Pu	✳✳
7	Ba-Pu	✳	46	La-Ru	✳✳
8	Ba-Ru	✳	47	La-Si	✳✳
9	Ba-Si	✳✳	48	La-Sr	✳
10	Ba-Sr	✳✳	49	La-U	✳✳✳
11	Ba-U	✳	50	La-Zr	✳
12	Ba-Zr	✳	51	Mo-O	✳✳
13	C-Cs	✳✳	52	Mo-Pu	✳✳
14	C-Fe	✳✳✳	53	Mo-Ru	✳✳✳
15	C-La	✳✳	54	Mo-Si	✳✳✳✳
16	C-Mo	✳✳✳	55	Mo-Sr	✳✳✳
17	C-O	✳	56	Mo-U	✳✳
18	C-Pu	✳✳✳	57	Mo-Zr	✳✳
19	C-Ru	✳✳✳	58	O-Pu	✳✳
20	C-Si	✳✳✳	59	O-Ru	✳
21	C-Sr	✳	60	O-Si	✳✳
22	C-U	✳✳✳✳	61	O-Sr	✳✳
23	C-Zr	✳✳✳	62	O-U	✳✳✳
24	Cs-Fe	✳✳✳	63	O-Zr	✳✳✳
25	Cs-La	✳✳✳	64	Pu-Ru	✳✳
26	Cs-Mo	✳✳✳	65	Pu-Si	✳✳
27	Cs-O	✳✳	66	Pu-Sr	✳
28	Cs-Pu	✳✳✳	67	Pu-U	✳✳
29	Cs-Ru	✳✳✳	68	Pu-Zr	✳✳
30	Cs-Si	✳✳	69	Ru-Si	✳✳
31	Cs-Sr	✳✳✳	70	Ru-Sr	✳
32	Cs-U	✳✳✳	71	Ru-U	✳✳✳
33	Cs-Zr	✳✳✳	72	Ru-Zr	✳✳✳
34	Fe-La	✳✳✳	73	Si-Sr	✳✳✳
35	Fe-Mo	✳✳✳✳	74	Si-U	✳✳
36	Fe-O	✳✳✳	75	Si-Zr	✳✳
37	Fe-Pu	✳✳	76	Sr-U	✳
38	Fe-Ru	✳✳✳	77	Sr-Zr	✳
39	Fe-Si	✳✳✳	78	U-Zr	✳✳✳

Table 1 - Binary systems.

1	$BaO-Fe_2O_3$	✳✳✳	14	$FeO-O_2Zr$	✳✳
2	$BaO-La_2O_3$	✳✳	15	$Fe_2O_3-La_2O_3$	✳✳
3	$BaO-MoO_3$	✳✳	16	Fe_2O_3-OSr	✳✳
4	BaO-OSr	✳✳	17	$Fe_2O_3-O_2Si$	✳
5	$BaO-O_2Si$	✳✳	18	$Fe_2O_3-O_2U$	✳
6	$BaO-O_2U$	✳✳	19	$Fe_2O_3-O_2Zr$	✳
7	$BaO-O_2Zr$	✳✳✳	20	$La_2O_3-O_2Pu$	✳
8	$BaO-O_2Pu$	✳	21	La_2O_3-OSr	✳✳
9	$BaMoO4-Cs_2MoO_4$	✳✳	22	$La_2O_3-O_2Si$	✳✳
10	$Cs_2MoO_4-MoO_3$	✳✳	23	$La_2O_3-O_2U$	✳✳
11	FeO-OSr	✳✳	24	$La_2O_3-O_2Zr$	✳✳✳
12	$FeO-O_2Si$	✳✳	25	MoO_3-ZrO_2	✳✳
13	$FeO-O_2U$	✳✳	26	$OSr-O_2Pu$	✳
27	$OSr-O_2Si$	✳✳	31	O_2Pu-O_2Zr	✳✳
28	$OSr-O_2U$	✳✳	32	O_2Si-O_2U	✳✳✳
29	$OSr-O_2Zr$	✳✳✳	33	O_2Si-O_2Zr	✳✳✳
30	O_2Pu-O_2U	✳✳	34	O_2U-O_2Zr	✳✳✳

Table 2 - Quasi-binary systems.

Only the most important ternary and quasi-ternary systems were critically assessed. For all the other ternary systems including one or more of the elements Ba, La, Ru and Sr, the ternary parameters have been estimated by analogy with other systems of the same type or considered as null.

1	C-Fe-Mo	✳✳	10	Fe-O-U	✳✳✳
2	C-O-U	✳✳	11	Fe-O-Zr	✳✳
3	C-O-Pu	✳✳	12	Fe-Pu-U	✳✳
4	C-O-Zr	✳✳	13	Fe-Pu-Zr	✳✳
5	C-Pu-U	✳✳	14	Fe-U-Zr	✳✳✳
6	C-Si-U	✳✳	15	O-Pu-U	✳
7	C-U-Zr	✳✳	16	O-Pu-Zr	✳
8	Fe-O-Pu	✳	17	O-U-Zr	✳✳✳
9	Fe-O-Si	✳✳✳	18	Pu-U-Zr	✳✳

Table 3 - Ternary systems.

1	$BaMoO_3-BaUO_3-BaZrO_3$	✳	2	$O_2Si-O_2U-O_2Zr$	✳✳

Table 4 - Quasi-ternary systems.

SOLUTION PHASES

1	ALPHA	Pu-Zr
2	BCC	O-Pu
3	BCC_A2	Ba-C-Fe-La-Mo-O-Pu-Ru-Si-Sr-U-Zr
4	BCT	C-O-U
5	BETA	Pu-U-Zr
6	$C_2LA_{(1+x)}$(HT)	C-La
7	$C_3LA_{(2+x)}$	C-La
8	CC	Ba-La-O-Sr-Zr
9	C-FE-MO(KSI)	C-Fe-Mo
10	C-FE-MO(M_3C_1_CEM)	C-Fe-Mo
11	C-FE-MO(M_6C_1)	C-Fe-Mo
12	C-MO(ETA)	C-Mo
13	C-PU-U(M_2C_3)	C-Pu-U
14	CS_2MOO_4(SS)	Ba-Cs-Mo-O
15	DELTA	U-Zr
16	DIA_A4	Ru-Si
17	DZETA	Pu-U-Zr
18	ETA	Pu-U-Zr

19	FCC_A1	Ba-C-Fe-La-Mo-Pu-Ru-Si-Sr-U-Zr
20	FCC_B1	Ba-Fe-O-Sr
21	FCC_B1(4)	C-O-Pu-U-Zr
22	FCC_C1	Ba-Fe-La-O-Pu-Sr-U-Zr
23	FE_1M_6	Fe-Pu-U
24	FE-MO(R)	Fe-Mo
25	FE-MO(SIGMA)	Fe-Mo
26	FE-MO(U)	Fe-Mo
27	GAMMA	Pu-U-Zr
28	HCP_A3	C-Fe-Mo-O-Pu-Ru-U-Zr
29	LAVES	Fe-Pu-U-Zr
30	Liquid	Ba-C-Cs-Fe-La-Mo-O-Pu-Ru-Si-Sr-U-Zr
31	MONOCLINIC	O-Pu-Zr
32	MO-RU(SIGMA1)	Mo-Ru
33	MO-SI(MO_5SI_3)	Mo-Si
34	MO-ZR(C15)	Mo-Zr
35	ORT_A20	Fe-Pu-Si-Zr
36	PEROVSKITE	Ba-Mo-O-Pu-Sr-U-Zr
37	SI_2U_3(SS)	C-Si-U
38	TCHERNOBYLITE	O-Si-U-Zr
39	TET(METAL)	Fe-Mo-Pu-Ru-Si-Zr
40	TET(OXIDE)	Fe-O-Pu-U-Zr
41	TET_A6	Pu-U-Zr
42	TETA	Pu-Zr

COMPOUNDS

1	BA1(SER)	20	BA2MO1O5(S)
2	BA1C1O3(C)	21	BA2O4SI1(S)
3	BA1C2(S)	22	BA2O8SI3(S)
4	BA1CS2MO2O8(S)	23	BA3MO1O6(S)
5	BA1FE12O19(S)	24	BA3O13SI5(S)
6	BA1FE2O4(S)	25	BA5O21SI8(S)
7	BA1H2(C)	26	BA7FE4O13(S)
8	BA1H2O2(C)	27	C0.4PU0.6(S)
9	BA1LA2O4(S)	28	C1(GRA_HEX_A9)
10	BA1MO1O4(S)	29	C1(SER)
11	BA1MO2O7(S)	30	C1CS2O3(S)
12	BA1O2(S)	31	C1FE1O3(S)
13	BA1O3SI1(S)	32	C1H2O2(L)
14	BA1O4U1(S)	33	C1H4(L)
15	BA1O5SI2(S)	34	C1H4O1(L)
16	BA1SI1(S)	35	C1MO1(SHP)
17	BA1SI2(S)	36	C1MO1O6(S)
18	BA2FE2O5(S)	37	C1O3SR1(C)
19	BA2FE6O11(S)	38	C1O5U1(S)
39	C1SI1(S)	87	CS7O1(S)
40	C2H4O2(L)	88	FE1(SER)
41	C2H6(L)	89	FE10O22SR7(S)
42	C2H6O1(L)	90	FE12LA1O19.5(S)
43	C2H6O2(L)	91	FE12O19SR1(S)
44	C2LA1(LT)	92	FE1H1O2(S)
45	C2SI2U3(T1)	93	FE1H2O2(S)
46	C2SR1(S)	94	FE1H3O3(S)
47	C3H6(L)	95	FE1LA1O3(S)
48	C3H6O1(L)	96	FE1MO1O4(S)
49	C3H6O2(L)	97	FE1O1.5(S)
50	C3H8(L)	98	FE1O3SI1(WOLLASTONITE)
51	C3H8O1(L)	99	FE1O4U1(S)
52	C3H8O3(L)	100	FE1SI1(S)
53	C3SI16U20(T2)	101	FE1SI2(S)
54	C5FE1O5(L)	102	FE1U6(S)
55	C6MO1O6(S)	103	FE1ZR2(S)
56	CS1(BCC_A2)	104	FE1ZR3(S)
57	CS1(SER)	105	FE2H2O4(S)
58	CS1H1(S)	106	FE2MO1(LAVES)
59	CS1H1O1(C)	107	FE2O4SI1(FAYALITE)
60	CS1O2(S)	108	FE2O5SR2(S)
61	CS2MO2O7(S)	109	FE2O6SR3(S)
62	CS2MO3O10(S)	110	FE2SI1(S)
63	CS2MO4O13(S)	111	FE333U250ZR417(e)
64	CS2MO5O16(S)	112	FE3O4(S)
65	CS2MO7O22(S)	113	FE3SI7(S)
66	CS2O1(S)	114	FE50U18ZR32(k)
67	CS2O12U4(S)	115	FE5SI3(S)
68	CS2O13U4(S)	116	FE6U71ZR23(l)
69	CS2O16U5(S)	117	FE735ZR265(S)
70	CS2O18U6(S)	118	H2LA1(S)
71	CS2O2(S)	119	H2O1(L)
72	CS2O22U7(S)	120	H2O2SR1(C)
73	CS2O27U9(S)	121	H2O4U1(S)
74	CS2O3.56U1(S)	122	H2PU1(S)
75	CS2O3SI1(C)	123	H2SR1(C)
76	CS2O3ZR1(S)	124	H2ZR1(S)
77	CS2O46U15(S)	125	H3LA1O3(S)
78	CS2O4RU1(S)	126	H3PU1(S)
79	CS2O4U1(S)	127	H3U1(S)
80	CS2O5SI2(C)	128	H4O5U1(S)
81	CS2O7U2(S)	129	H6SI2(S)
82	CS2O9SI4(C)	130	LA1(DHCP)
83	CS4O16ZR7(S)	131	LA1(SER)
84	CS4O17U5(S)	132	LA1RU2(S)
85	CS4O4ZR1(S)	133	LA1SI1(S)
86	CS6O17ZR7(S)	134	LA1SI2(S)

135	LA2MO3O12(S)	178	PU1RU1(S)
136	LA2O5SI1(S)	179	PU1RU2(S)
137	LA2O5ZR1(S)	180	PU1SI1(S)
138	LA2O7SI2(S)	181	PU1SI2(S)
139	LA2O7ZR2(S)	182	PU3RU1(S)
140	LA3RU1(S)	183	PU3SI2(S)
141	LA3SI2(S)	184	PU3SI5(S)
142	LA4O12SI3(S)	185	PU5RU3(S)
143	LA4O7SR1(S)	186	PU5SI3(S)
144	LA4O9SR3(S)	187	RU1(SER)
145	LA5RU2(S)	188	RU1SI1(S)
146	LA5RU3(S)	189	RU1U2(S)
147	LA7RU3(S)	190	RU1ZR1(S)
148	MO0.333SI0.667(C11)	191	RU2SI1(S)
149	MO0.75SI0.25(M1MO3)	192	RU2SI3(S)
150	MO1(SER)	193	RU2ZR1(S)
151	MO1O2(S)	194	RU3U1(S)
152	MO1O2.750(S)	195	RU474U526(S)
153	MO1O2.875(S)	196	RU4SI3(S)
154	MO1O2.889(S)	197	RU4U3(S)
155	MO1O3(S)	198	RU5SI3(S)
156	MO1O4SR1(S)	199	RU5U3(S)
157	MO1U2(S)	200	SI1(SER)
158	MO2O8ZR1(S)	201	SI1.88U1(S)
159	O1(SER)	202	SI1SR1(S)
160	O2RU1(S)	203	SI1SR2(S)
161	O2SI1(CRISTOBALITE)	204	SI1U3(HIGH_T)
162	O2SI1(H_T_QUARTZ)	205	SI1U3(LOW_T)
163	O2SI1(L_T_QUARTZ)	206	SI1ZR1(S)
164	O2SI1(TRIDYMITE)	207	SI1ZR2(S)
165	O2SR1(S)	208	SI1ZR3(S)
166	O3.04PU2(S)	209	SI2SR1(S)
167	O3PU2(HEXAGONAL)	210	SI2ZR1(S)
168	O3SI1SR1(S)	211	SI2ZR3(S)
169	O3U1(S)	212	SI3U1(S)
170	O4SI1SR2(S)	213	SI3ZR5(S)
171	O4SR2ZR1(S)	214	SI4ZR5(S)
172	O5SI1SR3(S)	215	SI511U489(S)
173	O7SR3ZR2(S)	216	SI5U3(S)
174	O8U3(S)	217	SR1(SER)
175	O9U4(S)	218	U1(SER)
176	PU1(SER)	219	ZR1(SER)
177	PU19RU1(S)		

GAS

1	AR1(G)	3	BA1H1(G)
2	BA1(G)	4	BA1H1O1(G)

5	BA1H2O2(G)	53	C3H4(G)2
6	BA1MO1O4(G)	54	C3H4(G)3
7	BA1O1(G)	55	C3H4O1(G)1
8	BA2O1(G)	56	C3H4O1(G)2
9	C1(G)	57	C3H4O1(G)3
10	C1H1(G)	58	C3H4O2(G)1
11	C1H1O1(G)	59	C3H4O2(G)2
12	C1H1O2(G)	60	C3H4O3(G)
13	C1H2(G)	61	C3H6(G)1
14	C1H2O1(G)	62	C3H6(G)2
15	C1H2O2(G)C	63	C3H6O1(G)1
16	C1H2O2(G)T	64	C3H6O1(G)2
17	C1H3(G)	65	C3H6O1(G)3
18	C1H3O1(G)1	66	C3H6O1(G)4
19	C1H3O1(G)2	67	C3H6O1(G)5
20	C1H4(G)	68	C3H6O2(G)
21	C1H4O1(G)	69	C3H6O3(G)
22	C1O1(G)	70	C3H7(G)1
23	C1O2(G)	71	C3H7(G)2
24	C1SI1(G)	72	C3H8(G)
25	C1SI2(G)	73	C3H8O1(G)1
26	C1SI3(G)	74	C3H8O1(G)2
27	C1SI4(G)	75	C3H8O1(G)3
28	C2(G)	76	C3O2(G)
29	C2H1(G)	77	C4(G)
30	C2H2(G)	78	C5(G)
31	C2H2O1(G)	79	C5FE1O5(G)
32	C2H2O2(G)	80	C6MO1O6(G)
33	C2H3(G)	81	CS1(G)
34	C2H4(G)	82	CS1H1(G)
35	C2H4O1(G)1	83	CS1H1O1(G)
36	C2H4O1(G)2	84	CS1O1(G)
37	C2H4O2(G)1	85	CS2(G)
38	C2H4O2(G)2	86	CS2H2O2(G)
39	C2H4O4(G)	87	CS2MO1O4(G)
40	C2H5(G)	88	CS2O1(G)
41	C2H6(G)	89	CS2O2(G)
42	C2H6O1(G)1	90	CS2O4RU1(G)
43	C2H6O1(G)2	91	FE1(G)
44	C2H6O1SI1(G)	92	FE1H2O2(G)
45	C2H6O2(G)	93	FE1O1(G)
46	C2H8SI1(G)	94	FE2(G)
47	C2O1(G)	95	H1(G)
48	C2SI1(G)	96	H1MO1O1(G)
49	C2SI2(G)	97	H1MO3(G)
50	C2SI3(G)	98	H1O1(G)
51	C3(G)	99	H1O1SR1(G)
52	C3H4(G)1	100	H1O2(G)

101	H1SI1(G)	127	O1PU1(G)
102	H1SR1(G)	128	O1SI1(G)
103	H1ZR1(G)	129	O1SR1(G)
104	H2(G)	130	O1U1(G)
105	H2MO1O2(G)	131	O1ZR1(G)
106	H2MO1O4(G)	132	O2(G)
107	H2O1(G)	133	O2PU1(G)
108	H2O2(G)	134	O2SI1(G)
109	H2O2SR1(G)	135	O2SI2(G)
110	H2SI1(G)	136	O2U1(G)
111	H3SI1(G)	137	O2ZR1(G)
112	H4SI1(G)	138	O3(G)
113	H6SI2(G)	139	O3RU1(G)
114	LA1(G)	140	O3U1(G)
115	LA1O1(G)	141	O4RU1(G)
116	LA2O1(G)	142	PU1(G)
117	LA2O2(G)	143	RU1(G)
118	MO1(G)	144	SI1(G)
119	MO1O1(G)	145	SI2(G)
120	MO1O2(G)	146	SI3(G)
121	MO1O3(G)	147	SR1(G)
122	MO2O6(G)	148	SR2(G)
123	MO3O9(G)	149	U1(G)
124	MO4O12(G)	150	ZR1(G)
125	MO5O15(G)	151	ZR2(G)
126	O1(G)		

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