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Thermodata

NUCLEAR THERMODYNAMIC DATABASE

« NUCLEA »

O-U-Zr-Fe-Cr-Ni-Ag-In-B-C-Ba-La-Ru-Sr-Al-Ca-Mg-Si

+

Ar-H

- Version 2007-01 -

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NUCLEA

Nuclear Thermodynamic Database
Version 2007-01

developed by

THERMODATA - INPG - CNRS

&

AEA-Technology

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I. INTRODUCTION

Since 1990 some people were interested in the assessment of thermodynamical data for a number of compounds of reactor materials and fission products based on the recommendations of a specialists meeting held at JRC-Ispra, Italy in 1990 [*]. Critical assessments have been made on a very large number of compounds and systems. NUCLEA is a Thermodynamic Data Base built for collecting all this knowledge.

NUCLEA

is a thermodynamic database for in and ex-vessel applications containing 18 + 2 elements :

O-U-Zr-Ag-In-B-C-Fe-Cr-Ni-Ba-La-Sr-Ru-Al-Ca-Mg-Si + Ar-H

and including the 15 oxide system :

UO_2-ZrO_2-In_2O_3-B_2O_3-FeO-Fe_2O_3-Cr_2O_3-NiO-BaO-La_2O_3-OSr-Al_2O_3-CaO-MgO-SiO_2

This database has to cover the entire field from metal to oxide domains. It allows the user to calculate the thermochemical equilibrium state at any step of a severe accident and to use the results of the thermodynamic approach for improving the predictions of thermo-hydraulic or other accidents codes.

The Gibbs energy of all possible multicomponent condensed or gaseous substances and solution phases are modelled. The binary and ternary Gibbs energy parameters were critically assessed by means of sophisticated optimisation procedures.

Applications of a global thermodynamic approach, i.e. the simultaneous use of a high-quality thermodynamic database and an equilibrium calculation code, are numerous :

- condensed state phase diagrams, transitions, liquidus/solidus, compositions and proportions,
- coupling thermodynamics and thermo-hydraulic, viscosity, segregation, residual power distribution,
- gaseous fission products release in any external conditions …

Such a database in much more than a compilation of thermodynamic data from various sources, its constitution needs a considerable work for self-consistency analysis, to ensure that all the available experimental information is satisfactorily reproduced.

Updating and improving the database has to be a regular task, tightly linked to the needs of end-users.

[*] Fission Product Chemistry in Severe Nuclear Reactor Accidents, Specialist's Meeting at JRC-Ispra, 15-17 January 1990, EUR 12989 EN (1990), A.L. Nichols ed.

2. GENERAL DESCRIPTION

2.1. PURE COMPONENTS.

The NUCLEA Thermodynamic Database for In- and Ex-Vessel Applications contains the 18 + 2 following elements :

O-U-Zr-Fe-Cr-Ni-Ag-In-B-C-Ba-La-Ru-Sr-Al-Ca-Mg-Si + Ar-H.

Ar and H are not taken into account in condensed solution phases.

2.2. CONDENSED SOLUTION PHASES.

The condensed solutions (48 non-stoichiometric phases, based on 281 reference substances) were deduced from the analysis of the assessed sub-systems (binary, ternary, …) ; some of them present possible miscibility gaps.

The list of condensed solutions stored in NUCLEA is presented in table 1.

2.3. CONDENSED SUBSTANCES.

The condensed stoechiometric compounds are presented in table 2.

Hydrogen was added because it is a major component of the system, but the dissolution of hydrogen in condensed solid and liquid solutions is not taken into account at this time.

2.4. GASEOUS SPECIES.

The gaseous species were added as an ideal mixture. The list is presented in table 3.

Table 1 **Condensed solution phases stored in NUCLEA**

N°	NAME	ELEMENTS	TYPE	MG	TMAX
1	LIQUID	Ag, Al, B, Ba, C, Ca, Cr, Fe, In, La, Mg, Ni, O, Ru, Si, Sr, U, Zr	MOC	1	
2	FCC_C1	O, U, Zr, Ba, Ca, In, La, Mg, Sr	O	1	3120
3	TET(OXIDE)	O, U, Zr, In, Mg	O	0	2650
4	PEROVSKIT1	O, Ba, Sr, U, Zr	O	0	3023
5	FCC_B1(4)	C, U, Zr, O	MOC	1	3200
6	BCT	C, O, U	MOC	0	2100
7	B_4C	B, C	C	0	2800
8	BCC_A2(1)	Fe, Cr, Ni, C, Ru, In, U, Zr	MC	0	2180
9	BCC_A2(2)	U, Zr, O, Ag, C, Fe, In, Ru, Cr, Ni	MOC	1	2250
10	FCC_A1(1)	Fe, Cr, Ni, Ru, In, Al, Zr, C	MC	0	1800
11	HCP_A3(1)	Ru, Zr, O, C, Ag, Al, In, Fe, Cr, Mg, Ni, U	MOC	1	2607
12	LAVES	Cr, Fe, U, Zr	M	1	1947
13	FCC_B1(1)	Fe, O, Sr, Ca, Mg, Ni	O	0	1650
14	FCC_B1(2)	Mg, Ni, O, Cr, Fe, Ca	O	0	3100
15	FCC_B1(3)	Ba, Ca, Sr, O, Fe, Mg, Ni	O	1	3172
16	RHO	Al, Cr, Fe, O	O	1	2603
17	SPINEL	Al, Cr, Fe, O, Mg, Ni	O	0	2500
18	CC	La, O, Ba, Ca, Sr, Zr	O	0	2586
19	TCHERNO	O, U, Zr, Si	O	0	1910
20	MULLITE	Al, B, O, Si	O	0	2200
21	M_7C_3	C, Cr, Fe, Ni	MC	0	2100
22	$M_{23}C_6$(1)	C, Cr, Fe, Ni	MC	0	1900
23	M_3C	B, C, Cr, Fe, Ni	MC	0	1600
24	C_2La(H_T)	C, La	MC	0	2800
25	C_3La_2(S)	C, La	MC	0	1700
26	BETA_B	B, Si	M	0	2000
27	DIA_A4	Si, B, Ru	M	0	1687
28	FCC_A1(2)	Ag, Al, In, Mg	M	0	1235
29	HCP_A3(3)	In, Ni	M	0	1210
30	BCC_A2(5)	In, Ni	M	0	1200
31	$M_{23}C_6$(2)	B, C, Fe	MC	0	1200
32	BCC_A2(4)	La, In, Ag, C, Ca, Mg	MC	0	1193
33	FCC_A1(4)	La, In, Ag, Ba, C, Ca, Mg	MC	0	1134
34	BCC_A2(3)	Ba, Ca, Sr	M	0	1115
35	SIGMA	Cr, Fe, Ni	M	0	1088
36	BCC_A2(6)	Ag, Al, In, Mg	M	0	1052
37	TET(METAL)	U, Ru, Zr, Cr, Fe, Al, Si	M	0	1049
38	HCP_A3(2)	Ag, Al, In	M	0	1008
39	ORT_A20	U, Zr, Fe	M	0	942
40	DELTA	U, Zr	M	0	900
41	FCC_A1(3)	Sr, Ba, Ca, La	M	0	820
42	BCC_A12	Al, Mg	M	0	734
43	CUB_A13	Ag, Al	M	0	732
44	FCC_L10	In, Mg	M	0	630
45	FCC_L12	In, Mg	M	0	611
46	TET_A6	In, Mg	M	0	440
47	CW2S_Olivine	Ca, Fe, Si, O	O	0	
48	CWS_Wollastonite	Ca, Fe, Si, O	O	0	

NOTE :

TMAX	maximal stability temperature.	M	metallic.
MG	miscibility gap index.	O	oxide.
		C	carbon.

Table 2 **Condensed stoichiometric compounds stored in NUCLEA.**

Gibbs energy at T = 298.15 K

N°	SUBSTANCES	J / mole	J / g-atom
1	AG1(SER)	0	0
2	AG1BA1(S)	-65411.64	-32705.82
3	AG1CA1(S)	-74932.67	-37466.34
4	AG1CA3(S)	-108103.23	-27025.81
5	AG1IN2(S)	-58960.17	-19653.39
6	AG1LA1(S)	-82861.57	-41430.79
7	AG1MG3(S)	-123785.78	-30946.45
8	AG1SR1(S)	-86085.06	-43042.53
9	AG1ZR1(S)	-34539.29	-17269.64
10	AG1ZR2(S)	-52746.23	-17582.08
11	AG2BA1(S)	-99075.38	-33025.13
12	AG2BA3(S)	-150615.45	-30123.09
13	AG2C1O3(S)	-560775.27	-93462.54
14	AG2CA1(S)	-104725.47	-34908.49
15	AG2CR1O4(S)	-786189.5	-112312.79
16	AG2IN1(S)	-64975.33	-21658.44
17	AG2LA1(S)	-119443.83	-39814.61
18	AG2O1(S)	-66844.27	-22281.42
19	AG2SR1(S)	-122606.57	-40868.86
20	AG2SR3(S)	-205646.79	-41129.36
21	AG3CA5(S)	-266950.98	-33368.87
22	AG3IN1(S)	-82025.94	-20506.48
23	AG3MG1(S)	-95984.28	-23996.07
24	AG46LA14(S)	-2191519.87	-36525.33
25	AG4SR1(S)	-161549.45	-32309.89
26	AG5BA1(S)	-149298.93	-24883.15
27	AG5LA1(S)	-179645.45	-29940.91
28	AG5SR1(S)	-180007.11	-30001.18
29	AG7CA2(S)	-287830.51	-31981.17
30	AG9CA2(S)	-318585.56	-28962.32
31	AL1(SER)	0	0
32	AL11LA1O18(S)	-10292251.95	-343075.07
33	AL11LA3(S)	-681472.96	-48676.64
34	AL12BA1O19(S)	-10946776.01	-342086.75
35	AL12CA1O19(S)	-10824390.41	-338262.2
36	AL12O19SR1(S)	-10867144.19	-339598.26
37	AL13BA7(S)	-667889.54	-33394.48
38	AL13CR2(S)	-310025.98	-20668.4
39	AL13RU4(S)	-832218.53	-48954.03
40	AL14CA12O33(S)	-19722849.59	-334285.59
41	AL1B10(S)	-132380.35	-12034.58
42	AL1B12(S)	-190235.86	-14633.53
43	AL1B2(S)	-55416.53	-18472.18
44	AL1CR2(S)	-58903.03	-19634.34
45	AL1FE1O3(S)	-1264202.16	-252840.43
46	AL1H3(S)	-20238.22	-5059.55

47	AL1H3O3(S)A	-1297326.81	-185332.4
48	AL1LA1(S)	-102389.06	-51194.53
49	AL1LA1O3(S)	-1818974.18	-363794.84
50	AL1LA3(S)	-139527.19	-34881.8
51	AL1NI3(S)	-214739.17	-53684.79
52	AL1RU1(S)	-134994.02	-67497.01
53	AL1SR1(S)	-86239.73	-43119.87
54	AL1ZR1(S)	-109067.05	-54533.52
55	AL1ZR2(S)	-138502.46	-46167.49
56	AL1ZR3(S)	-151961.76	-37990.44
57	AL24LA10(S)	-1775265.06	-52213.68
58	AL2BA1O4(S)	-2385338.43	-340762.63
59	AL2BA3O6(S)	-3583289.8	-325753.62
60	AL2CA1(S)	-122134.47	-40711.49
61	AL2CA1H4O10SI2(S)	-4929367.36	-259440.39
62	AL2CA1O4(S)	-2360141.15	-337163.02
63	AL2CA1O8SI2(ANORTHITE)	-4286579.18	-329736.86
64	AL2CA1SI2(S)	-229256.91	-45851.38
65	AL2CA2O7SI1(MELILITE)	-4048152.09	-337346.01
66	AL2CA3H12O12(S)	-5625109.76	-193969.3
67	AL2CA3O6(S)	-3646856.78	-331532.43
68	AL2CA4H26O20(S)	-8503547.37	-163529.76
69	AL2FE1(S)	-95777.24	-31925.75
70	AL2H2O4(S)B	-2009584.81	-251198.1
71	AL2H2O4(S)D	-2020184.66	-252523.08
72	AL2H4O9SI2(S)D	-4177066.75	-245709.81
73	AL2H4O9SI2(S)H	-4161813.19	-244812.54
74	AL2H4O9SI2(S)K	-4156804.1	-244517.89
75	AL2H6O6(S)	-2628338.7	-187738.48
76	AL2LA1(S)	-157750.02	-52583.34
77	AL2O4SR1(H_T)	-2374296.7	-339185.24
78	AL2O4SR1(L_T)	-2375742.84	-339391.83
79	AL2O6SR3(S)	-3617906.48	-328900.59
80	AL2RU1(S)	-169593.03	-56531.01
81	AL2SR1(S)	-144823.56	-48274.52
82	AL2U1(S)	-125462.65	-41820.88
83	AL2ZR1(S)	-163662.05	-54554.02
84	AL2ZR3(S)	-254369.78	-50873.96
85	AL32O132SR84(S)	-79479655.53	-320482.48
86	AL3FE1(S)	-132431.35	-33107.84
87	AL3FE2(S)	-126493.92	-25298.78
88	AL3LA1(S)	-211212.63	-52803.16
89	AL3NI1(S)	-183167.43	-45791.86
90	AL3NI2(S)	-315869.83	-63173.97
91	AL3RU2(S)	-292431.72	-58486.34
92	AL3U1(S)	-159033.48	-39758.37
93	AL3ZR1(S)	-196422.78	-49105.7
94	AL3ZR2(S)	-280101.93	-56020.39
95	AL3ZR5(S)	-393057.27	-49132.16
96	AL4B2O9(S)	-4689569.94	-312638
97	AL4BA1(S)	-175953.93	-35190.79

98	AL4C3(S)	-246315.48	-35187.93
99	AL4C4SI1(S)	-333137.35	-37015.26
100	AL4CA1(S)	-139548.5	-27909.7
101	AL4CA1O7(S)	-4051114.86	-337592.91
102	AL4CR1(S)	-122910.94	-24582.19
103	AL4MG2O18SI5(S)	-9223667.76	-318057.51
104	AL4O7SR1(S)	-4092161.04	-341013.42
105	AL4SR1(S)	-246166.23	-49233.25
106	AL4U0.9(S)	-162010.38	-33063.34
107	AL4ZR5(S)	-481032.75	-53448.08
108	AL525MG475(S)	-10803297.58	-10803.3
109	AL56MG44(S)	-1062236.3	-10622.36
110	AL5BA4(S)	-284913.42	-31657.05
111	AL5FE2(S)	-228653.05	-32664.72
112	AL6RU1(S)	-243344.11	-34763.44
113	AL8C7SI1(S)	-596661.56	-37291.35
114	AL8CR5(S)	-304868.55	-23451.43
115	AL8MG5(S)	-140899.19	-10838.4
116	AL9CR4(S)	-311799.61	-23984.59
117	B1(SER)	0	0
118	B10H14(C)	-81541.36	-3397.56
119	B12U1(S)	-449523.87	-34578.76
120	B12ZR1(S)	-298738.29	-22979.87
121	B14SI1(S)	-138034.11	-9202.27
122	B1C1U1(S)	-183438.29	-61146.1
123	B1CR1(S)	-83531.44	-41765.72
124	B1CR2(S)	-109036.77	-36345.59
125	B1FE1(S)	-70601.46	-35300.73
126	B1FE1O3(S)	-1073456.08	-214691.22
127	B1FE2(S)	-81124.73	-27041.58
128	B1FE3O6(S)	-1908717.79	-190871.78
129	B1H1O2(C)	-817378.52	-204344.63
130	B1H3O3(S)	-1120457.85	-160065.41
131	B1NI1(S)	-47073.99	-23537
132	B1NI2(S)	-81887.88	-27295.96
133	B1NI3(S)	-94450.22	-23612.56
134	B1O1.5(S)	-644793.39	-257917.36
135	B1RU1(S)	-55899.88	-27949.94
136	B1ZR1(S)	-176509.51	-88254.75
137	B2BA1O4(S)	-2001383.44	-285911.92
138	B2BA3O6(S)	-3156115.24	-286919.57
139	B2C1U1(S)	-230197.37	-57549.34
140	B2C7U5(S)	-780338.33	-55738.45
141	B2CA1O4(S)	-2062745.48	-294677.93
142	B2CA1O8SI2(S)	-3905837.29	-300449.02
143	B2CA2O5(S)	-2778261.49	-308695.72
144	B2CA3O6(S)	-3484066.61	-316733.33
145	B2CA5O10SI1(S)	-5838977.86	-324387.66
146	B2CR1(S)	-129261.02	-43087.01
147	B2FE1O4(S)	-1579891.28	-225698.75
148	B2FE2O5(S)	-1870208.54	-207800.95

149	B2FE3O6(S)	-2160504.75	-196409.52
150	B2FE3U1(S)	-234009.51	-39001.59
151	B2H4O4(S)	-1447850.19	-144785.02
152	B2IN2O6(S)	-2274346.65	-227434.66
153	B2LA2O6(S)	-3200888.71	-320088.87
154	B2LA6O12(S)	-6875312.02	-343765.6
155	B2MG1(S)	-85027.23	-28342.41
156	B2MG2O5(S)	-2586983.82	-287442.65
157	B2MG3O6(S)	-3210718.06	-291883.46
158	B2NI2O5(S)	-1786882.29	-198542.48
159	B2NI3O6(S)	-2684614.08	-244055.83
160	B2O4SR1(S)	-2039632.42	-291376.06
161	B2O5SR2(S)	-2693841.04	-299315.67
162	B2O6SR3(S)	-3345079.69	-304098.15
163	B2RU1(S)	-64529.78	-21509.93
164	B2U1(S)	-180686.63	-60228.88
165	B2ZR1(S)	-332977.04	-110992.35
166	B3CR5(S)	-305745.69	-38218.21
167	B3H3O3(S)	-1312211.18	-145801.24
168	B3NI4(S)	-180515.06	-25787.87
169	B3RU2(S)	-117375.7	-23475.14
170	B3RU7(S)	-248863.36	-24886.34
171	B3SI1(S)	-40318.35	-10079.59
172	B4BA1O7(S)	-3353866.05	-279488.84
173	B4CA1O7(S)	-3401581.06	-283465.09
174	B4CR1(S)	-143702.66	-28740.53
175	B4CR3(S)	-300194.72	-42884.96
176	B4FE1U1(S)	-323844.87	-53974.15
177	B4LA1(S)	-336133.98	-67226.8
178	B4MG1(S)	-109898.64	-21979.73
179	B4MG1O7(S)	-3281304.33	-273442.03
180	B4O7SR1(S)	-3383923.05	-281993.59
181	B4U1(S)	-262832.38	-52566.48
182	B4ZR3(S)	-687794.06	-98256.29
183	B5H9(L)	-12113.99	-865.28
184	B6BA1(S)	-139573.03	-19939
185	B6CA1(S)	-130370.27	-18624.32
186	B6LA1(S)	-495419.13	-70774.16
187	B6LA2O12(S)	-5805804.43	-290290.22
188	B6O10SR1(S)	-4715632.16	-277390.13
189	B6SI1(S)	-68841.13	-9834.45
190	B6SR1(S)	-146468.5	-20924.07
191	B7MG1(S)	-144815.93	-18101.99
192	B8BA1O13(S)	-6022469.4	-273748.61
193	B9LA1(S)	-513384.79	-51338.48
194	BA1(SER)	0	0
195	BA13IN1(S)	-337548.7	-24110.62
196	BA1C1O3(C)	-1244422.84	-248884.57
197	BA1C2(S)	-109126.62	-36375.54
198	BA1CR1O4(S)	-1493281.05	-248880.18
199	BA1CR2O4(S)	-1799480.43	-257068.63

200	BA1FE12O19(S)	-5768158.27	-180254.95
201	BA1FE2O4(S)	-1502694.8	-214670.69
202	BA1H2(C)	-208883.49	-69627.83
203	BA1H2O2(C)	-972184.89	-194436.98
204	BA1IN1(S)	-94163.39	-47081.7
205	BA1IN2(S)	-150651.48	-50217.16
206	BA1IN2O4(S)	-1568262.02	-224037.43
207	BA1IN4(S)	-213763.29	-42752.66
208	BA1LA2O4(S)	-2624374.86	-374910.69
209	BA1MG2(S)	-65742.96	-21914.32
210	BA1NI1O2(S)	-851801.03	-212950.26
211	BA1O2(S)	-666582.79	-222194.26
212	BA1O3SI1(S)	-1653860.2	-330772.04
213	BA1O4U1(S)	-2043006.15	-340501.03
214	BA1O5SI2(S)	-2587876.91	-323484.61
215	BA1SI1(S)	-174914.37	-87457.19
216	BA1SI2(S)	-243646.07	-81215.36
217	BA2FE2O5(S)	-2128609.36	-236512.15
218	BA2FE6O11(S)	-3873018.41	-203843.07
219	BA2IN2O5(S)	-2154375.78	-239375.09
220	BA2MG17(S)	-303668.58	-15982.56
221	BA2O4SI1(S)	-2327410.02	-332487.15
222	BA2O8SI3(S)	-4258753.65	-327596.43
223	BA3CR2O6(S)	-3029858.54	-275441.69
224	BA3IN2O6(S)	-2728999.89	-248090.9
225	BA3NI1O4(S)	-2015105.41	-251888.18
226	BA3O13SI5(S)	-6848913.41	-326138.73
227	BA4IN6O13(S)	-5296598.63	-230286.9
228	BA5IN2(S)	-268810.05	-38401.44
229	BA5IN2O8(S)	-3873125.74	-258208.38
230	BA5IN3(S)	-344383.03	-43047.88
231	BA5O21SI8(S)	-11109843.47	-326760.1
232	BA6MG23(S)	-544661.97	-18781.45
233	BA7FE4O13(S)	-6074799.94	-253116.66
234	C1(GRA_HEX_A9)	-1712.07	-1712.07
235	C1(SER)	0	0
236	C1CA1O3(C)	-1233944.31	-246788.86
237	C1FE1O3(S)	-768261.6	-153652.32
238	C1H2O2(L)	-461252.38	-92250.48
239	C1H4(L)	-117191.52	-23438.3
240	C1H4O1(L)	-276758.56	-46126.43
241	C1MG1O3(C)	-1131323.81	-226264.76
242	C1NI1O3(S)	-705348.18	-141069.64
243	C1O3SR1(C)	-1255980.02	-251196
244	C1O5U1(S)	-1732405.91	-247486.56
245	C1SI1(S)	-75564.13	-37782.07
246	C2CA1(S)	-84419.43	-28139.81
247	C2CA1MG1O6(S)	-2361482.36	-236148.24
248	C2CR3(M3C2)(C-CR-FE-NI)	-85077.34	-17015.47
249	C2H4O2(L)	-527955.84	-65994.48
250	C2H6(L)	-144893.31	-18111.66

251	C2H6O1(L)	-324837.85	-36093.09
252	C2H6O2(L)	-512930.67	-51293.07
253	C2LA1(LT)	-88411.03	-29470.34
254	C2MG1(S)	71647.03	23882.34
255	C2SR1(S)	-105723.58	-35241.19
256	C3H6(L)	34388.3	3820.92
257	C3H6O1(L)	-308062.61	-30806.26
258	C3H6O2(L)	-564656.5	-51332.41
259	C3H8(L)	-180280.25	-16389.11
260	C3H8O1(L)	-360193.89	-30016.16
261	C3H8O3(L)	-723497.9	-51678.42
262	C3MG2(S)	45372.97	9074.59
263	C3U2(S)	-231519	-46303.8
264	C4NI1O4(L)	-727061.22	-80784.58
265	C5FE1O5(L)	-866589.79	-78780.89
266	C6CR1O6(S)	-1171064.1	-90081.85
267	CA1(SER)	0	0
268	CA1CR2O4(S)	-1839001.87	-262714.55
269	CA1FE1O6SI2(hedenbergite)	-2897011.83	-289701.18
270	CA1FE2O4(S)	-1523966.95	-217709.56
271	CA1FE3O5(S)(CWF)	-1799227.2	-199914.13
272	CA1FE4O7(S)	-2318781.61	-193231.8
273	CA1FE5O7(S)(CW3F)	-2332531.66	-179425.51
274	CA1H2(C)	-189343.35	-63114.45
275	CA1H2O2(S)	-1010946.99	-202189.4
276	CA1H4O7SI2(S)	-3189857.9	-227846.99
277	CA1IN1(S)	-108855.4	-54427.7
278	CA1IN2(S)	-151862.11	-50620.7
279	CA1MG1O2(S)	-1262837.85	-315709.46
280	CA1MG1O4SI1(S)	-2293553.05	-327650.44
281	CA1MG1O6SI2(S)	-3242583.18	-324258.32
282	CA1MG2(S)	-67601.02	-22533.67
283	CA1NI2(S)	-82617.09	-27539.03
284	CA1NI3(S)	-99850.58	-24962.64
285	CA1NI5(S)	-123283.62	-20547.27
286	CA1O2(S)	-683929.19	-227976.4
287	CA1O3SI1(PSEUDOWOL)(ASS1)	-1654867.65	-330973.53
288	CA1O3ZR1(S)	-1793173.43	-358634.69
289	CA1O4U1(S)	-2040940.74	-340156.79
290	CA1SI1(S)	-121183.8	-60591.9
291	CA1SI2(S)	-167426.9	-55808.97
292	CA2FE2O5(S)	-2185331.96	-242814.66
293	CA2H2.333O5.166SI1(S)	-2713528.85	-258455.93
294	CA2H2MG5O24SI8(S)	-12509475	-305109.15
295	CA2H5O10.5SI3(S)	-5000088.93	-243906.78
296	CA2MG1O7SI2(S)	-3935082.98	-327923.58
297	CA2NI7(S)	-212712.9	-23634.77
298	CA2O4SI1(ALPHA)(ASS1)	-2341216.25	-334459.46
299	CA2O4SI1(ALPHA2)(ASS1)	-2337492.61	-333927.52
300	CA2O4SI1(LARNITE)(ASS1)	-2344891.27	-334984.47
301	CA2SI1(S)	-145102.2	-48367.4

302	CA3H6O10SI2(S)	-4875790.89	-232180.52
303	CA3IN1(S)	-163480.62	-40870.16
304	CA3MG1O8SI2(S)	-4637291.31	-331235.09
305	CA3O5SI1(HATRURITE)(ASS1)	-2984252.16	-331583.57
306	CA3O7SI2(RANKINITE)(ASS1)	-3997993.42	-333166.12
307	CA4H3O11.5SI3(S)	-6122610.14	-284772.56
308	CA5H11O22.5SI6(S)	-10876620.22	-244418.43
309	CA5H21O27.5SI6(S)	-12420570.82	-208749.09
310	CA5H6O20SI6(S)	-10088745.72	-272668.8
311	CA6H2O19SI6(S)	-10176180.79	-308369.11
312	CR1(SER)	0	0
313	CR1LA1O3(S)	-1568480.14	-313696.03
314	CR1O2(S)	-596795.01	-198931.67
315	CR1O3(C)	-599685.11	-149921.28
316	CR1SI1(S)(2)	-73062.9	-36531.45
317	CR1SI2(S)(2)	-96870.6	-32290.2
318	CR2RU1(S)	-36466.85	-12155.62
319	CR3RU1(S)	-42755.49	-10688.87
320	CR3SI1(S)(2)	-152823.68	-38205.92
321	CR5O12(S)	-3023645.63	-177861.51
322	CR5SI3(S)(2)	-313618.51	-39202.31
323	CR8O21(S)	-4830650.55	-166574.16
324	FE1(SER)	0	0
325	FE10O22SR7(S)	-8939581.75	-229220.04
326	FE12LA1O19.5(S)	-6054445.14	-186290.62
327	FE12O19SR1(S)	-5927749.78	-185242.18
328	FE1H1O2(S)	-576696.07	-144174.02
329	FE1H2O2(S)	-600241.45	-120048.29
330	FE1H3O3(S)	-863802.49	-123400.36
331	FE1LA1O3(S)	-1404196.83	-280839.37
332	FE1O4U1(S)	-1623035.11	-270505.85
333	FE1SI1(S)	-78887.03	-39443.51
334	FE1SI2(S)	-92094.14	-30698.05
335	FE1U6(S)	-139561.05	-19937.29
336	FE1ZR2(S)	-69427.85	-23142.62
337	FE1ZR3(S)	-99821.26	-24955.32
338	FE2H2O4(S)	-1153392.65	-144174.08
339	FE2O5SR2(S)	-2176992.73	-241888.08
340	FE2O6SR3(S)	-2822811.84	-256619.26
341	FE2SI1(S)	-83713.97	-27904.66
342	FE333U250ZR417(e)	-27027.11	-27027.11
343	FE3SI7(S)	-244014.67	-24401.47
344	FE50U18ZR32(k)	-30356.85	-30356.85
345	FE5SI3(S)	-266531.65	-33316.46
346	FE6U71ZR23(l)	-17793.96	-17793.96
347	FE735ZR265(S)	-26835917.79	-26835.92
348	H2LA1(S)	-204522.91	-68174.3
349	H2MG1(S)	-85418.67	-28472.89
350	H2MG1O2(S)	-943519.35	-188703.87
351	H2MG3O12SI4(S)	-5993139.61	-285387.6
352	H2MG7O24SI8(S)	-12243019.3	-298610.23

353	H2O1(L)	-306684.99	-102228.33
354	H2O2SR1(C)	-992218.88	-198443.78
355	H2O4U1(S)	-1574966.17	-224995.17
356	H2SR1(C)	-195503.66	-65167.89
357	H2ZR1(S)	-181153.17	-60384.39
358	H3LA1O3(S)	-1447228.46	-206746.92
359	H3U1(S)	-146154.99	-36538.75
360	H4MG3O9SI2(S)	-4427808.81	-245989.38
361	H4O5U1(S)	-1876492.03	-187649.2
362	H6SI2(S)	-1856.58	-232.07
363	IN1(SER)	0	0
364	IN1LA1(S)	-113481.27	-56740.63
365	IN1LA2(S)	-144762.23	-48254.08
366	IN1LA3(S)	-165393.64	-41348.41
367	IN1MG2(S)	-70328.59	-23442.86
368	IN1MG3(S)	-83590	-20897.5
369	IN1NI1(S)	-67964.87	-33982.43
370	IN1NI2(S)	-82165.11	-27388.37
371	IN1NI3(S)	-93648.86	-23412.21
372	IN1SR1(S)	-80986.76	-40493.38
373	IN1SR3(S)	-118542.62	-29635.66
374	IN1ZR3(S)	-108167.48	-27041.87
375	IN2LA1(S)	-168277.47	-56092.49
376	IN2MG5(S)	-154344.28	-22049.18
377	IN2O3(S)	-953351.67	-190670.33
378	IN2O4SR1(S)	-1602215.86	-228887.98
379	IN2SR1(S)	-131339.35	-43779.78
380	IN2SR3(S)	-181434.37	-36286.87
381	IN3LA1(S)	-208827.36	-52206.84
382	IN3NI2(S)	-167579.58	-33515.92
383	IN3SR1(S)	-154657.23	-38664.31
384	IN3SR2(S)	-214884.35	-42976.87
385	IN3U1(S)	-154535.32	-38633.83
386	IN3ZR1(S)	-171584.73	-42896.18
387	IN42NI58(S)	-3111905.32	-31119.05
388	IN5LA3(S)	-459823.37	-57477.92
389	IN5SR1(S)	-195301.16	-32550.19
390	IN5SR2(S)	-286893.02	-40984.72
391	IN7MG3(S)	-221605.91	-22160.59
392	IN7NI3(S)	-316342.16	-31634.22
393	LA1(DHCP)	-16965.45	-16965.45
394	LA1(SER)	0	0
395	LA1MG1(S)	-39975.49	-19987.75
396	LA1MG12(S)	-163666.79	-12589.75
397	LA1MG2(S)	-55613.79	-18537.93
398	LA1MG3(S)	-72266.96	-18066.74
399	LA1NI1(S)	-83215.34	-41607.67
400	LA1NI3(S)	-159658.92	-39914.73
401	LA1NI5(S)	-208499.96	-34749.99
402	LA1RU2(S)	-174054.54	-58018.18
403	LA1SI1(S)	-162956.09	-81478.05

404	LA1SI2(S)	-205209.61	-68403.2
405	LA2MG17(S)	-257655.85	-13560.83
406	LA2NI3(S)	-211879.53	-42375.91
407	LA2NI7(S)	-346688.07	-38520.9
408	LA2O5SI1(S)	-2852303.74	-356537.97
409	LA2O5ZR1(S)	-2966288.16	-370786.02
410	LA2O7SI2(S)	-3701822.07	-336529.28
411	LA2O7ZR2(S)	-4150169.84	-377288.17
412	LA3NI1(S)	-136079.36	-34019.84
413	LA3RU1(S)	-158894.75	-39723.69
414	LA3SI2(S)	-413874.91	-82774.98
415	LA4O12SI3(S)	-6475491.16	-340815.32
416	LA4O7SR1(S)	-4130654.4	-344221.2
417	LA4O9SR3(S)	-5311300.38	-331956.27
418	LA5RU2(S)	-290549.62	-41507.09
419	LA5RU3(S)	-364435.37	-45554.42
420	LA7NI16(S)	-940192.86	-40877.95
421	LA7NI3(S)	-364718.22	-36471.82
422	LA7RU3(S)	-421715.33	-42171.53
423	MG1(SER)	0	0
424	MG17SR2(S)	-264181.28	-13904.28
425	MG1NI2(S)	-81659.77	-27219.92
426	MG1O3SI1(CLINOENSTATITE)	-1565424.99	-313085
427	MG1O3SI1(ENSTATITE)	-1564852.7	-312970.54
428	MG1O3SI1(PROENSTATITE)	-1556341.36	-311268.27
429	MG1O4U1(S)	-1896226.16	-316037.69
430	MG23SR6(S)	-484397.52	-16703.36
431	MG2NI1(S)	-75027.2	-25009.07
432	MG2O4SI1(FORSTERITE)	-2201234.28	-314462.04
433	MG2SI1(S)	-97942.68	-32647.56
434	MG2SR1(S)	-59205.34	-19735.11
435	MG38SR9(S)	-766325.96	-16304.81
436	NI1(SER)	0	0
437	NI11ZR9(S)	-1181525.32	-59076.27
438	NI1SI1(S)	-79863.4	-39931.7
439	NI1SR1(S)	-27999.23	-13999.61
440	NI1U6(S)	-193014.49	-27573.5
441	NI1ZR1(S)	-118919.31	-59459.66
442	NI1ZR2(S)	-140726.39	-46908.8
443	NI21ZR8(S)	-1570590.04	-54158.28
444	NI29SI9(LOW_T)	-1759481.9	-46302.16
445	NI2O4SI1(S)	-1435629.04	-205089.86
446	NI2SI1(S)	-132192.4	-44064.13
447	NI2U1(S)	-176222.3	-58740.77
448	NI31SI12(S)	-2015064.98	-46861.98
449	NI35SI65(S)	-3229902.04	-32299.02
450	NI3SI1(HIGH_T)	-166182.49	-41545.62
451	NI3SI1(MEDIUM_T)	-181325.53	-45331.38
452	NI3SI2(S)	-215509.64	-43101.93
453	NI3ZR1(S)	-210303.46	-52575.86
454	NI575ZR425(S)	-60481573.4	-60481.57

455	NI5U1(S)	-301273.35	-50212.23
456	NI5ZR1(S)	-249191.04	-41531.84
457	NI769U231(S)	-58767450.18	-58767.45
458	NI778U222(S)	-58338098.71	-58338.1
459	NI7U5(S)	-701163.14	-58430.26
460	NI7ZR2(S)	-455260.68	-50584.52
461	NI9U7(S)	-922100.22	-57631.26
462	O1(SER)	0	0
463	O2RU1(S)	-327959.62	-109319.87
464	O2SI1(CRISTOBALITE)	-920976.83	-306992.28
465	O2SI1(H_T_QUARTZ)	-922066.17	-307355.39
466	O2SI1(L_T_QUARTZ)	-923061.3	-307687.1
467	O2SI1(TRIDYMITE)	-920540.39	-306846.8
468	O2SR1(S)	-651046.78	-217015.59
469	O2ZR1(MONOCLINIC)	-1115579.43	-371859.81
470	O3SI1SR1(S)	-1662133.98	-332426.8
471	O3U1(S)	-1252455.16	-313113.79
472	O4SI1SR2(S)	-2343579.54	-334797.08
473	O4SR2ZR1(S)	-2449213.55	-349887.65
474	O5SI1SR3(S)	-2980874.43	-331208.27
475	O7SR3ZR2(S)	-4233460.37	-352788.36
476	O8U3(S)	-3657757.71	-332523.43
477	O9U4(S)	-4611611.91	-354739.38
478	RU1(SER)	0	0
479	RU1SI1(S)	-130342.45	-65171.22
480	RU1U2(S)	-102970.62	-34323.54
481	RU1ZR1(S)	-153269.53	-76634.77
482	RU2SI1(S)	-104989.5	-34996.5
483	RU2SI3(S)	-303896.05	-60779.21
484	RU2ZR1(S)	-140564.4	-46854.8
485	RU3U1(S)	-167385.3	-41846.33
486	RU474U526(S)	-35067025.96	-35067.03
487	RU4SI3(S)	-421958.8	-60279.83
488	RU4U3(S)	-239055.24	-34150.75
489	RU5SI3(S)	-344813.42	-43101.68
490	RU5U3(S)	-284872.9	-35609.11
491	SI1(SER)	0	0
492	SI1.88U1(S)	-149415.74	-51880.47
493	SI1SR1(S)	-124089.34	-62044.67
494	SI1SR2(S)	-162868.03	-54289.34
495	SI1U3(HIGH_T)	400000	100000
496	SI1U3(LOW_T)	-138370.03	-34592.51
497	SI1ZR1(S)	-163470.17	-81735.09
498	SI1ZR2(S)	-220471.97	-73490.66
499	SI1ZR3(S)	-256466.22	-64116.55
500	SI2SR1(S)	-158317.95	-52772.65
501	SI2U3(S)	-231732.67	-46346.53
502	SI2ZR1(S)	-174982.81	-58327.6
503	SI2ZR3(S)	-402778.02	-80555.6
504	SI3U1(S)	-163923.54	-40980.88
505	SI3ZR5(S)	-609844.7	-76230.59

506	SI4ZR5(S)	-740504.31	-82278.26
507	SI511U489(S)	-51020979.51	-51020.98
508	SI5U3(S)	-419390.36	-52423.8
509	SR1(SER)	0	0
510	U1(SER)	0	0
511	ZR1(SER)	0	0

Table 3 **Gaseous species stored in NUCLEA.**

Gibbs energy at T = 298.15 K

N°	SUBSTANCES	J / mole	J / g-atom
1	AG1(G)	233486.92	233486.92
2	AG1O1(G)	236080.35	118040.18
3	AG2(G)	330017.71	165008.86
4	AL1(G)	264978.9	264978.9
5	AL1B1O2(G)	-621770.95	-155442.74
6	AL1C1(G)	622924.02	311462.01
7	AL1C2(G)	610248.15	203416.05
8	AL1H1(G)	203428.25	101714.13
9	AL1H1O1(G)1	-30727.26	-10242.42
10	AL1H1O1(G)2	-244386.47	-81462.16
11	AL1H1O2(G)	-536048.12	-134012.03
12	AL1H2(G)	183524.24	61174.75
13	AL1H2O2(G)	-727416.65	-145483.33
14	AL1H3(G)	146618.21	36654.55
15	AL1O1(G)	12542.85	6271.42
16	AL1O2(G)	-161240.88	-53746.96
17	AL2(G)	417169.13	208584.57
18	AL2C2(G)	480147.51	120036.88
19	AL2O1(G)	-261749.3	-87249.77
20	AL2O2(G)	-561018.6	-140254.65
21	AL2O3(G)	-643858.28	-128771.66
22	AR1(G)	-46156.01	-46156.01
23	B1(G)	538182.95	538182.95
24	B10H14(G)	-57690.78	-2403.78
25	B1BA1O2(G)	-721293.83	-180323.46
26	B1C1(G)	766281.07	383140.53
27	B1C2(G)	720235.12	240078.37
28	B1H1(G)	391462.73	195731.36
29	B1H1O1(G)1	-258732.23	-86244.08
30	B1H1O1(G)2	-84666.02	-28222.01
31	B1H1O2(G)	-632101.75	-158025.44
32	B1H2(G)	147135.1	49045.03
33	B1H2O1(G)	-138946.62	-34736.66
34	B1H2O2(G)	-549473.36	-109894.67
35	B1H3(G)	50706.01	12676.5
36	B1H3O1(G)	-358422.2	-71684.44
37	B1H3O2(G)	-720786.35	-120131.06
38	B1H3O3(G)	-1072202.07	-153171.72
39	B1O1(G)	-60631.53	-30315.76
40	B1O2(G)	-352997.53	-117665.84
41	B1O2SR1(G)	-716271.78	-179067.94
42	B2(G)	792162.75	396081.38
43	B2C1(G)	712324.94	237441.65
44	B2H4O4(G)	-1388487.46	-138848.75
45	B2H6(G)	-28491.53	-3561.44
46	B2O1(G)	28362.76	9454.25

47	B2O2(G)	-528356.26	-132089.07
48	B2O3(G)	-920534.72	-184106.94
49	B3H3O3(G)	-1304546.82	-144949.65
50	B3H3O6(G)	-2375509.78	-197959.15
51	B5H9(G)	-8866.58	-633.33
52	BA1(G)	147398.23	147398.23
53	BA1H1(G)	138270.27	69135.14
54	BA1H1O1(G)	-342305.72	-114101.91
55	BA1H2O2(G)	-719984.02	-143996.8
56	BA1O1(G)	-197909.36	-98954.68
57	BA2O1(G)	-327217.82	-109072.61
58	C1(G)	669532.48	669532.48
59	C1H1(G)	539587.82	269793.91
60	C1H1O1(G)	-23431.32	-7810.44
61	C1H1O2(G)	-288020.34	-72005.08
62	C1H2(G)	328605.08	109535.03
63	C1H2O1(G)	-181090.29	-45272.57
64	C1H2O2(G)C	-452963.2	-90592.64
65	C1H2O2(G)T	-436592.2	-87318.44
66	C1H3(G)	87828.46	21957.11
67	C1H3O1(G)1	-56395.19	-11279.04
68	C1H3O1(G)2	-93236.36	-18647.27
69	C1H4(G)	-130372.16	-26074.43
70	C1H4O1(G)	-272387.97	-45397.99
71	C1O1(G)	-169430.03	-84715.01
72	C1O2(G)	-457219.64	-152406.55
73	C1SI1(G)	667555.34	333777.67
74	C1SI2(G)	484042.19	161347.4
75	C1SI3(G)	529657.73	132414.43
76	C1SI4(G)	551702.33	110340.47
77	C2(G)	778291.25	389145.63
78	C2H1(G)	415160.63	138386.88
79	C2H2(G)	166847.91	41711.98
80	C2H2O1(G)	-119784.26	-23956.85
81	C2H2O2(G)	-293215.66	-48869.28
82	C2H3(G)	190611.68	38122.34
83	C2H4(G)	-12894.53	-2149.09
84	C2H4O1(G)1	-125057.23	-17865.32
85	C2H4O1(G)2	-244864.61	-34980.66
86	C2H4O2(G)1	-516784.01	-64598
87	C2H4O2(G)2	-439518.14	-54939.77
88	C2H4O4(G)	-920085.32	-92008.53
89	C2H5(G)	34994.68	4999.24
90	C2H6(G)	-153107.32	-19138.41
91	C2H6O1(G)1	-318640.72	-35404.52
92	C2H6O1(G)2	-263775.05	-29308.34
93	C2H6O1SI1(G)	-274911.06	-27491.11
94	C2H6O2(G)	-485787.25	-48578.73
95	C2H8SI1(G)	-161407.65	-14673.42
96	C2O1(G)	217149.19	72383.06
97	C2SI1(G)	562356.42	187452.14

98	C2SI2(G)	565930.03	141482.51
99	C2SI3(G)	472155.08	94431.02
100	C3(G)	749329.1	249776.37
101	C3H4(G)1	204503.03	29214.72
102	C3H4(G)2	118253.14	16893.31
103	C3H4(G)3	110450.99	15778.71
104	C3H4O1(G)1	-84410.12	-10551.27
105	C3H4O1(G)2	-168823.64	-21102.95
106	C3H4O1(G)3	-167782.93	-20972.87
107	C3H4O2(G)1	-415216.78	-46135.2
108	C3H4O2(G)2	-382412.32	-42490.26
109	C3H4O3(G)	-593676.05	-59367.61
110	C3H6(G)1	-17441.99	-1938
111	C3H6(G)2	-59792.92	-6643.66
112	C3H6O1(G)1	-223601.81	-22360.18
113	C3H6O1(G)2	-177491.66	-17749.17
114	C3H6O1(G)3	-305159.22	-30515.92
115	C3H6O1(G)4	-276757.48	-27675.75
116	C3H6O1(G)5	-221370.51	-22137.05
117	C3H6O2(G)	-508581.67	-46234.7
118	C3H6O3(G)	-551960.79	-45996.73
119	C3H7(G)1	-9699.87	-969.99
120	C3H7(G)2	1058.53	105.85
121	C3H8(G)	-184320.5	-16756.41
122	C3H8O1(G)1	-308670.85	-25722.57
123	C3H8O1(G)2	-351344.01	-29278.67
124	C3H8O1(G)3	-364855.88	-30404.66
125	C3O2(G)	-175919.11	-35183.82
126	C4(G)	902613.79	225653.45
127	C4NI1O4(G)	-722670.52	-80296.72
128	C5(G)	906912.04	181382.41
129	C5FE1O5(G)	-858789.13	-78071.74
130	C6CR1O6(G)	-1151001.24	-88538.56
131	CA1(G)	131470.25	131470.25
132	CA1H1(G)	168749.71	84374.85
133	CA1H1O1(G)	-264083.57	-88027.86
134	CA1H2O2(G)	-695884.08	-139176.82
135	CA1O1(G)	-21543.41	-10771.71
136	CA2(G)	260561.61	130280.81
137	CR1(G)	364370.65	364370.65
138	CR1O1(G)	116976.46	58488.23
139	CR1O2(G)	-155552.34	-51850.78
140	CR1O3(G)	-372207.2	-93051.8
141	CR2(G)	558217.14	279108.57
142	FE1(G)	357670.39	357670.39
143	FE1H2O2(G)	-414938.69	-82987.74
144	FE1O1(G)	178944.32	89472.16
145	FE2(G)	469463.25	234731.63
146	H1(G)	183796.42	183796.42
147	H1IN1(G)	152854.46	76427.23
148	H1IN1O1(G)	-177715.11	-59238.37

149	H1MG1(G)	111463.34	55731.67
150	H1MG1O1(G)	-239351.24	-79783.75
151	H1NI1(G)	330523.83	165261.92
152	H1O1(G)	-15399.56	-7699.78
153	H1O1SR1(G)	-264116.81	-88038.94
154	H1O2(G)	-65748.6	-21916.2
155	H1SI1(G)	317547.68	158773.84
156	H1SR1(G)	155860.43	77930.22
157	H1ZR1(G)	451889.28	225944.64
158	H2(G)	-38929.31	-19464.66
159	H2MG1O2(G)	-651873.04	-130374.61
160	H2NI1O2(G)	-342047.19	-68409.44
161	H2O1(G)	-298082.19	-99360.73
162	H2O2(G)	-205539.12	-51384.78
163	H2O2SR1(G)	-673915.64	-134783.13
164	H2SI1(G)	211505.15	70501.72
165	H3SI1(G)	139897.6	34974.4
166	H4SI1(G)	-26675.76	-5335.15
167	H6SI2(G)	-960.95	-120.12
168	IN1(G)	188905.56	188905.56
169	IN1O1(G)	99366.94	49683.47
170	IN2(G)	317670.57	158835.28
171	IN2O1(G)	-132009.52	-44003.17
172	LA1(G)	361792.21	361792.21
173	LA1O1(G)	-192451.31	-96225.65
174	LA2O1(G)	-141915.24	-47305.08
175	LA2O2(G)	-715506.87	-178876.72
176	MG1(G)	99565.8	99565.8
177	MG1O1(G)	-5395.48	-2697.74
178	MG2(G)	203668.81	101834.4
179	NI1(G)	367484.91	367484.91
180	NI1O1(G)	237687.74	118843.87
181	O1(G)	201160.56	201160.56
182	O1SI1(G)	-159349.18	-79674.59
183	O1SR1(G)	-70257.88	-35128.94
184	O1U1(G)	-45138.27	-22569.14
185	O1ZR1(G)	14500.96	7250.48
186	O2(G)	-61164.58	-30582.29
187	O2SI1(G)	-373666.79	-124555.6
188	O2SI2(G)	-490058.61	-122514.65
189	O2U1(G)	-553546.13	-184515.38
190	O2ZR1(G)	-477564.43	-159188.14
191	O3(G)	70540.6	23513.53
192	O3RU1(G)	-160573.12	-40143.28
193	O3U1(G)	-897302.47	-224325.62
194	O4RU1(G)	-269585.7	-53917.14
195	RU1(G)	600987.7	600987.7
196	SI1(G)	400042.8	400042.8
197	SI2(G)	511590.2	255795.1
198	SI3(G)	542661.22	180887.07
199	SR1(G)	111785.53	111785.53

200	SR2(G)	228192.96	114096.48
201	U1(G)	476549.41	476549.41
202	ZR1(G)	535132.84	535132.84
203	ZR2(G)	851510.77	425755.38

3. STATE of VALIDATION

The state of validation of a thermodynamic database is characterised by the good agreement between calculated and available experimental results (phase diagrams and thermodynamic properties) concerning basic sub-systems (binary, ternary, …) or practical global experiments, made in similar conditions and at thermodynamic equilibrium.

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

✳ **Estimated**
No experimental data available.

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

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

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

The complete list of the 153 (18*17/2) metal-metal or metal-oxygen binary systems based on pure elements and 105 (15*14/2) oxide pseudo-binary systems based on pure oxides are presented in tables 5 and 6 respectively.

Due to the very high number of possible ternary (18*17*16/3*2 = 816) and pseudo-ternary (15*14*13/3*2 = 455) systems, it is completely unimaginable to assess all of them in a human delay. For that reason it was decided to assess only the most important ternary systems for practical applications. The list of the selected ternary and pseudo-ternary systems is presented in tables 7 and 8 respectively.

For each system, the order number, source and provisional quality criterion are given. This criterion takes into account both phase diagram and thermodynamic properties, and thus cannot be indicated only on a phase diagram. This point is fundamental for the modelling of multi-component systems.

Moreover, it must be kept in mind that the set of a quality criterion remains somewhere subjective, and the improvement of existing sub-systems with newly available experimental results is a continuous task, which is part of the database management and updating.

3.1. BINARY AND PSEUDO-BINARY SYSTEMS.

Table 4 **Binary systems.**

System	Quality	Date of issue
Ag-Al	✳✳✳	03/2003
Ag-B	✳	01/2006
Ag-Ba	✳✳✳	03/2003
Ag-C	✳✳	01/2006
Ag-Ca	✳✳	03/2003
Ag-Cr	✳	03/2003
Ag-Fe	✳✳✳	03/2003
Ag-In	✳✳✳	03/2003
Ag-La	✳✳✳	03/2003
Ag-Mg	✳✳	03/2003
Ag-Ni	✳✳✳	03/2003
Ag-O	✳✳✳	03/2003
Ag-Ru	✳✳✳	03/2003
Ag-Si	✳✳✳	03/2003
Ag-Sr	✳✳✳	03/2003
Ag-U	✳✳	03/2003
Ag-Zr	✳✳✳	03/2003
Al-B	✳✳	03/2003
Al-Ba	✳✳	03/2003
Al-C	✳✳✳	03/2003
Al-Ca	✳✳✳	03/2007
Al-Cr	✳✳✳	01/2006
Al-Fe	✳✳✳	03/2003
Al-In	✳✳✳	03/2003
Al-La	✳✳	03/2003
Al-Mg	✳✳✳	03/2003
Al-Ni	✳✳	03/2003
Al-O	✳	03/2003
Al-Ru	✳✳	03/2003
Al-Si	✳✳✳	03/2003
Al-Sr	✳✳	03/2003
Al-U	✳✳	03/2003
Al-Zr	✳	03/2003
B-Ba	✳	03/2003
B-C	✳✳	03/2003
B-Ca	✳	03/2003
B-Cr	✳✳	03/2003
B-Fe	✳✳✳	03/2003
B-In	✳	03/2003
B-La	✳✳	03/2007
B-Mg	✳✳✳	03/2003
B-Ni	✳✳✳	03/2003
B-O	✳	03/2003
B-Ru	✳✳	01/2006
B-Si	✳✳	03/2003
B-Sr	✳	03/2003
B-U	✳✳	03/2003
B-Zr	✳✳✳	03/2003
Ba-C	✳	03/2003
Ba-Ca	✳✳✳	03/2003
Ba-Cr	✳	03/2003

System	Quality	Date of issue
Ba-Fe	✳✳	03/2003
Ba-In	✳✳✳	03/2003
Ba-La	✳✳	03/2003
Ba-Mg	✳✳	03/2003
Ba-Ni	✳✳	03/2003
Ba-O	✳✳	03/2003
Ba-Ru	✳	03/2003
Ba-Si	✳✳	03/2003
Ba-Sr	✳✳	03/2003
Ba-U	✳	03/2003
Ba-Zr	✳	03/2003
C-Ca	✳	01/2006
C-Cr	✳✳✳	03/2007
C-Fe	✳✳✳	03/2003
C-In	✳	03/2003
C-La	✳✳	03/2003
C-Mg	✳	01/2006
C-Ni	✳✳✳	03/2007
C-O	✳	03/2003
C-Ru	✳✳✳	03/2003
C-Si	✳✳✳	03/2003
C-Sr	✳	01/2006
C-U	✳✳✳✳	03/2003
C-Zr	✳✳✳	03/2003
Ca-Cr	✳	03/2003
Ca-Fe	✳	03/2003
Ca-In	✳✳	03/2003
Ca-La	✳✳	03/2003
Ca-Mg	✳✳✳	01/2006
Ca-Ni	✳✳	03/2003
Ca-O	✳	03/2003
Ca-Ru	✳	03/2003
Ca-Si	✳✳	03/2003
Ca-Sr	✳✳✳	03/2003
Ca-U	✳	03/2003
Ca-Zr	✳	03/2003
Cr-Fe	✳✳✳✳	03/2003
Cr-In	✳	03/2003
Cr-La	✳✳	03/2003
Cr-Mg	✳	03/2003
Cr-Ni	✳✳✳✳	03/2003
Cr-O	✳✳✳	03/2003
Cr-Ru	✳✳	03/2003
Cr-Si	✳✳✳	03/2003
Cr-Sr	✳	03/2003
Cr-U	✳✳✳	03/2003
Cr-Zr	✳✳	03/2003
Fe-In	✳✳✳	03/2003
Fe-La	✳✳✳	03/2003
Fe-Mg	✳✳	03/2003
Fe-Ni	✳✳✳✳	03/2003

System	Quality	Date of issue
Fe-O	✳✳✳	03/2003
Fe-Ru	✳✳✳	03/2003
Fe-Si	✳✳✳	03/2003
Fe-Sr	✳	03/2003
Fe-U	✳✳✳	01/2005
Fe-Zr	✳✳✳	01/2005
In-La	✳✳✳	03/2003
In-Mg	✳✳✳	03/2003
In-Ni	✳✳✳✳	03/2003
In-O	✳✳	03/2003
In-Ru	✳	03/2003
In-Si	✳✳✳	03/2003
In-Sr	✳✳✳	03/2003
In-U	✳	03/2003
In-Zr	✳	03/2003
La-Mg	✳✳	03/2003
La-Ni	✳✳✳	03/2003
La-O	✳	03/2003
La-Ru	✳✳	01/2006
La-Si	✳✳	03/2003
La-Sr	✳	03/2003
La-U	✳✳✳	03/2003
La-Zr	✳	03/2003
Mg-Ni	✳✳	03/2003
Mg-O	✳	03/2003
Mg-Ru	✳	03/2003
Mg-Si	✳✳✳	03/2003
Mg-Sr	✳✳	03/2003
Mg-U	✳	03/2003
Mg-Zr	✳✳	03/2003
Ni-O	✳✳✳	03/2003
Ni-Ru	✳✳✳	03/2003
Ni-Si	✳✳✳	01/2006
Ni-Sr	✳✳	03/2003
Ni-U	✳✳	03/2003
Ni-Zr	✳✳✳	03/2003
O-Ru	✳	03/2003
O-Si	✳✳	03/2003
O-Sr	✳	03/2003
O-U	✳✳✳	01/2006
O-Zr	✳✳✳	01/2005
Ru-Si	✳✳	03/2003
Ru-Sr	✳	03/2003
Ru-U	✳✳✳	01/2006
Ru-Zr	✳✳✳	03/2003
Si-Sr	✳✳✳	03/2003
Si-U	✳✳	03/2003
Si-Zr	✳✳	03/2003
Sr-U	✳	03/2003
Sr-Zr	✳	03/2003
U-Zr	✳✳✳	01/2005

Table 5 **Pseudo-binary systems.**

System	Quality	Date of issue
Al_2O_3-B_2O_3	✳✳	03/2003
Al_2O_3-BaO	✳✳✳	03/2003
Al_2O_3-CaO	✳✳✳	01/2006
Al_2O_3-Cr_2O_3	✳✳	03/2003
Al_2O_3-FeO	✳✳✳	03/2003
Al_2O_3-Fe_2O_3	✳✳	03/2003
Al_2O_3-In_2O_3	✳	03/2003
Al_2O_3-La_2O_3	✳✳	03/2003
Al_2O_3-MgO	✳✳	03/2003
Al_2O_3-NiO	✳	03/2003
Al_2O_3-OSr	✳✳	03/2003
Al_2O_3-O_2Si	✳✳	03/2003
Al_2O_3-O_2U	✳✳✳	03/2003
Al_2O_3-O_2Zr	✳✳✳	03/2003
B_2O_3-BaO	✳✳	03/2003
B_2O_3-CaO	✳✳	03/2003
B_2O_3-Cr_2O_3	✳✳	03/2003
B_2O_3-FeO	✳✳	03/2003
B_2O_3-Fe_2O_3	✳✳	03/2003
B_2O_3-In_2O_3	✳✳	03/2003
B_2O_3-La_2O_3	✳✳	03/2003
B_2O_3-MgO	✳✳	03/2003
B_2O_3-NiO	✳✳	03/2003
B_2O_3-OSr	✳✳	03/2003
B_2O_3-O_2Si	✳✳	03/2003
B_2O_3-O_2U	✳✳	03/2003
B_2O_3-O_2Zr	✳✳	03/2003
BaO-CaO	✳	03/2003
BaO-Cr_2O_3	✳	03/2003
BaO-FeO		03/2003
BaO-Fe_2O_3	✳✳✳	03/2003
BaO-In_2O_3	✳✳	03/2003
BaO-La_2O_3	✳✳	03/2003
BaO-MgO	✳✳	03/2003
BaO-NiO	✳✳	03/2003
BaO-OSr	✳✳	03/2003
BaO-O_2Si	✳✳	03/2003

System	Quality	Date of issue
BaO-O_2U	✳✳	03/2003
BaO-O_2Zr	✳✳✳	03/2003
CaO-Cr_2O_3	✳✳	03/2003
CaO-FeO	✳	03/2003
CaO-Fe_2O_3	✳✳	03/2003
CaO-In_2O_3	✳	03/2003
CaO-La_2O_3	✳✳✳	03/2003
CaO-MgO	✳✳✳	03/2003
CaO-NiO	✳✳	03/2003
CaO-OSr	✳✳	03/2003
CaO-O_2Si	✳✳✳	03/2003
CaO-O_2U	✳✳	03/2003
CaO-O_2Zr	✳✳✳	03/2003
Cr_2O_3-FeO	✳✳	03/2003
Cr_2O_3-Fe_2O_3	✳✳	12/2004
Cr_2O_3-In_2O_3	✳	03/2003
Cr_2O_3-La_2O_3	✳✳✳	03/2003
Cr_2O_3-MgO	✳✳	03/2003
Cr_2O_3-NiO	✳✳	12/2004
Cr_2O_3-OSr	✳	03/2003
Cr_2O_3-O_2Si	✳	03/2003
Cr_2O_3-O_2U	✳	03/2003
Cr_2O_3-O_2Zr	✳	03/2003
FeO-Fe_2O_3	✳✳✳	03/2003
FeO-In_2O_3	✳	03/2003
FeO-La_2O_3	✳	03/2003
FeO-MgO	✳	03/2003
FeO-NiO	✳✳	03/2003
FeO-OSr	✳✳	03/2003
FeO-O_2Si	✳✳	03/2003
FeO-O_2U	✳✳	03/2003
FeO-O_2Zr	✳✳	03/2003
Fe_2O_3-In_2O_3	✳	03/2003
Fe_2O_3-La_2O_3	✳✳	03/2003
Fe_2O_3-MgO	✳✳	03/2003
Fe_2O_3-NiO	✳✳	03/2003
Fe_2O_3-OSr	✳✳	03/2003

System	Quality	Date of issue
Fe_2O_3-O_2Si	✳	03/2003
Fe_2O_3-O_2U	✳	03/2003
Fe_2O_3-O_2Zr	✳	03/2003
In_2O_3-La_2O_3	✳	03/2003
In_2O_3-MgO	✳	03/2003
In_2O_3-NiO	✳	03/2003
In_2O_3-OSr	✳	03/2003
In_2O_3-O_2Si	✳	03/2003
In_2O_3-O_2U	✳	03/2003
In_2O_3-O_2Zr	✳	03/2003
La_2O_3-MgO	✳✳✳	03/2003
La_2O_3-NiO	✳	03/2003
La_2O_3-OSr	✳✳	03/2003
La_2O_3-O_2Si	✳✳	03/2003
La_2O_3-O_2U	✳✳	03/2003
La_2O_3-O_2Zr	✳✳✳	03/2003
MgO-NiO	✳✳	03/2003
MgO-OSr	✳✳✳	03/2003
MgO-O_2Si	✳✳✳	03/2003
MgO-O_2U	✳✳	03/2003
MgO-O_2Zr	✳✳✳	03/2003
NiO-OSr	✳	03/2003
NiO-O_2Si	✳	03/2003
NiO-O_2U	✳	03/2003
NiO-O_2Zr	✳	03/2003
OSr-O_2Si	✳✳	03/2003
OSr-O_2U	✳✳	03/2003
OSr-O_2Zr	✳✳✳	03/2003
O_2Si-O_2U	✳✳✳	03/2003
O_2Si-O_2Zr	✳✳✳	03/2003
O_2U-O_2Zr	✳✳✳	01/2005

3.2. SELECTED TERNARY AND PSEUDO-TERNARY SYSTEMS.

Table 6 **Ternary systems.**

System	Quality	Date of issue
B-C-Fe	✳✳	03/2003
B-C-U	✳✳	03/2003
B-C-Zr	✳✳	03/2003
B-Fe-U	✳✳	03/2003
B-Fe-Zr	✳	03/2003
C-Cr-Fe	✳✳✳	03/2003
C-Cr-Ni	✳✳✳	03/2003

System	Quality	Date of issue
C-Fe-Ni	✳✳✳✳	03/2003
C-O-U	✳✳	03/2003
C-O-Zr	✳✳	03/2003
C-U-Zr	✳	03/2003
Ca-Fe-O	✳✳✳	01/2006
Cr-Fe-Ni	✳✳	03/2003
Cr-Fe-O	✳✳	03/2003

System	Quality	Date of issue
Cr-Fe-Zr	✳✳	03/2003
Cr-Ni-O	✳✳	03/2003
Fe-Ni-O	✳✳	03/2003
Fe-O-Si	✳✳✳	01/2006
Fe-O-U	✳✳✳	01/2005
Fe-O-Zr	✳✳	01/2005
Fe-U-Zr	✳✳✳	01/2005
O-U-Zr	✳✳✳	01/2006

Table 7 **Pseudo-ternary systems.**

System	Quality	Date of issue
Al_2O_3-B_2O_3-CaO	✳✳	03/2003
Al_2O_3-B_2O_3-O_2Si	✳✳	03/2003
Al_2O_3-B_2O_3-MgO	✳✳	03/2003
Al_2O_3-CaO-O_2Si	✳✳✳	03/2003
Al_2O_3-O_2Si-O_2U	✳✳	03/2003
Al_2O_3-O_2Si-O_2Zr	✳✳	03/2003

System	Quality	Date of issue
Al_2O_3-O_2U-O_2Zr	✳✳	03/2003
B_2O_3-CaO-MgO	✳✳	03/2003
B_2O_3-CaO-O_2Si	✳✳	03/2003
B_2O_3-FeO-Fe_2O_3	✳✳	03/2003
B_2O_3-MgO-O_2Si	✳✳	03/2003
O_2Si-O_2U-O_2Zr	✳✳	03/2003

3.3. DOMAIN OF APPLICATION AND LIMITATIONS.

In this version of NUCLEA most of the binary and pseudo-binary systems have been analysed and critically assessed either by THERMODATA or AEA-T.

Only a limited number of binary systems (mainly based on the C-Cr-Fe-Ni quaternary system) were taken in open literature.

However, some of them are still insufficiently known, and further experimental work is needed for the ones interesting the nuclear field.

In a very high-number component system such as the one covered by NUCLEA, the number of possible ternaries and pseudo-ternaries is equal to 1271, while the time cost to assess only one is about one-man year. Few experimental data are available in open literature for ternaries of high interest for nuclear safety. Consequently, the complete assessment of all ternaries is not achievable in a human delay and only some selected ternary systems of main importance for nuclear safety applications were assessed at this time.

Moreover, a simple overlook of the stars attributed to all sub-systems is not the best approach to estimate the global quality of the database. In fact, only some sub-systems are especially relevant in the nuclear domain. The quality of these specific sub-systems, designated by principal users, is much more important for NUCLEA dedicated to severe accident applications. Thus, further work will still have to be done for the selected sub-systems with less than three stars.

In any case, well-selected global experiments will always have to be done to validate definitively the thermodynamic approach on the final user point of view.

Simultaneously, fulfilling and improving the sub-systems in the NUCLEA is a continuous task, the assessment work being based on the CALPHAD method, and ideally never completely realised.

In summary, the Nuclear Thermodynamic Database could be considered as well validated if sufficient predicting power was reached for practical applications, both in the In- and Ex-Vessel fields.

3.4. FUTURE.

In the future, specific actions will have to be foreseen to improve the state of validation of NUCLEA, both for In- and Ex- Vessel applications.

- ➔ On the one hand, such a database must be continuously updated for all binary or pseudo-binary, and selected ternary sub-systems, by taking into account the newly available experimental results in the optimisation process based on the CALPHAD method.

- ➔ On the other hand, the database must also be compared to available experimental results in higher-order systems, in order to validate the global thermodynamic approach or eventually to identify remaining uncertainties or insufficient knowledge.

This task involves two different aspects :

- ➔ Obviously a **very high quality scientific work** for obtaining reliable thermodynamic data, by using adapted thermodynamic models and sophisticated optimisation codes.

- ➔ But also a **considerable technical work**, which is the database management, in order to maintain an updated experimental database (phase diagram and thermodynamic properties), and to be able to re-assess binary or ternary sub-systems if necessary, when new experiments becomes available.

4. ASSESSMENT of FE-O-U-ZR

An important experimental and modelisation work was done in the last 10 years by many people in the world to obtain now a rather good knowledge and representation of that main quaternary system.

In the present version of the database all the available information (equilibrium points of phase diagrams, activities measurements, vapour pressures etc…), up to the year 2004, was taken into account in the optimisation procedure.

To allow the user to have an idea of the validity of the obtained results the calculated phase diagrams are compared, in the following pages, with some experimental points. But if anybody is interested more in detail by the experiments or by critical assessment and optimisation work he has to look at the numerous scientific papers published in the recent years.

4.1. BINARY SYSTEMS.

Fe-O, Fe-U, Fe-Zr, O-U, O-Zr, U,Zr.

4.2. PSEUDO-BINARY SYSTEMS.

O_2U-O_2Zr.

IMPORTANT NOTE :

It must be underlined that pseudo-binary systems including iron oxides are not real quasi-binary phase diagrams. These ones are only used for evaluation of the interaction parameters, but they have to be further controlled by calculating them as valid sections of the ternary systems Fe-O-U or Fe-O-Zr.

4.3. TERNARY SYSTEMS.

Fe-O-U, Fe-O-Zr, Fe-U-Zr, O-U-Zr.

FE-O

The phase diagram of the Fe-O binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a miscibility gap between an Fe rich liquid (L_1) and an FeO/Fe_2O_3 rich liquid (L_2) ;
- the intermediate solid oxides, Fe_3O_4(S) or magnetite, Fe_2O_3(S) or hematite, corundum ;
- the oxide solid solution, FeO_{1+x}, or wustite, with the face-centred cubic structure, of NaCl type, noted fcc_B1 ;
- pure solid iron, with a negligible solubility of oxygen, and different allotropic structures, cubic face centred (fcc_A1) and body cubic centred (bcc_A2) ;
- the gas phase, which shows an extended solubility of iron in oxygen above 2800 K.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of the stoichiometric compounds $Fe_{0.947}O_1$(fcc_B1), Fe_3O_4(S), Fe_2O_3(S) have been assessed separately in consistency with the available experimental data. The liquid phase has been described by a non-ideal associate model, with the formula (Fe_1, Fe_1O_1, $Fe_1O_{1.5}$,O_1)(L), and the solid solution FeO_{1+x} by a simple one lattice model, with the formula (Fe_1O_1, $Fe_1O_{1.5}$)(fcc_B1). The gas phase has been described by an ideal mixture of gaseous species, with the formula (Fe_1, Fe_1O_1, $Fe_1O_{1.5}$, O_1, O_2, O_3)$_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the activity of iron and oxygen are in satisfactory agreement with the experimental ones in the solid state and are strongly constrained by the assessed thermodynamic properties of stoichiometric compounds ;
- the wustite phase limits are very well reproduced ;
- the liquidus in the iron rich region is in satisfactory agreement with the experimental one up to 2200 K, as well as the melting point of Fe_3O_4(S) and all the invariant reactions ;
- the miscibility gap in the liquid state was assumed to be closed around 3000 K, in agreement with only one series of experimental points, which should be validated again.

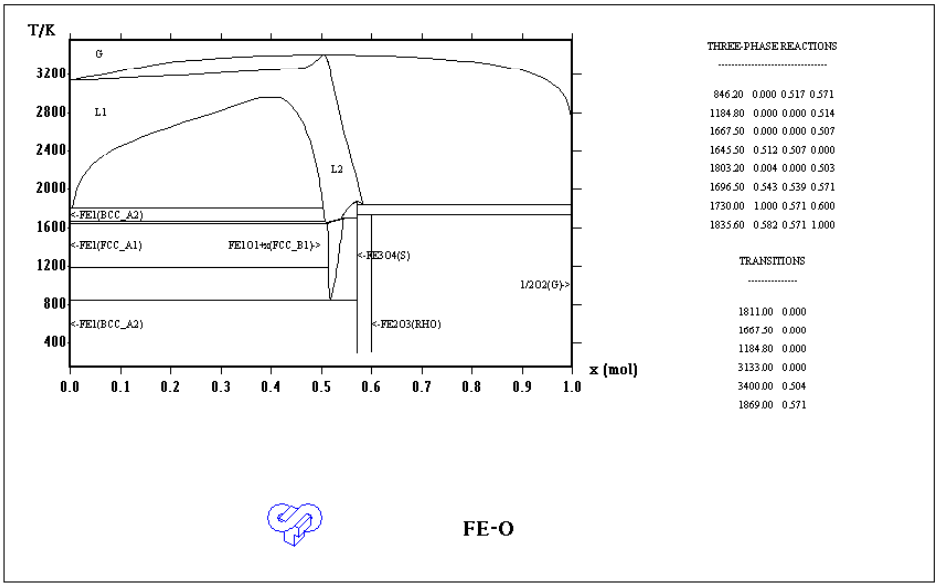

Figure 1 **Calculated Fe-O phase diagram with special points and invariant reactions.**

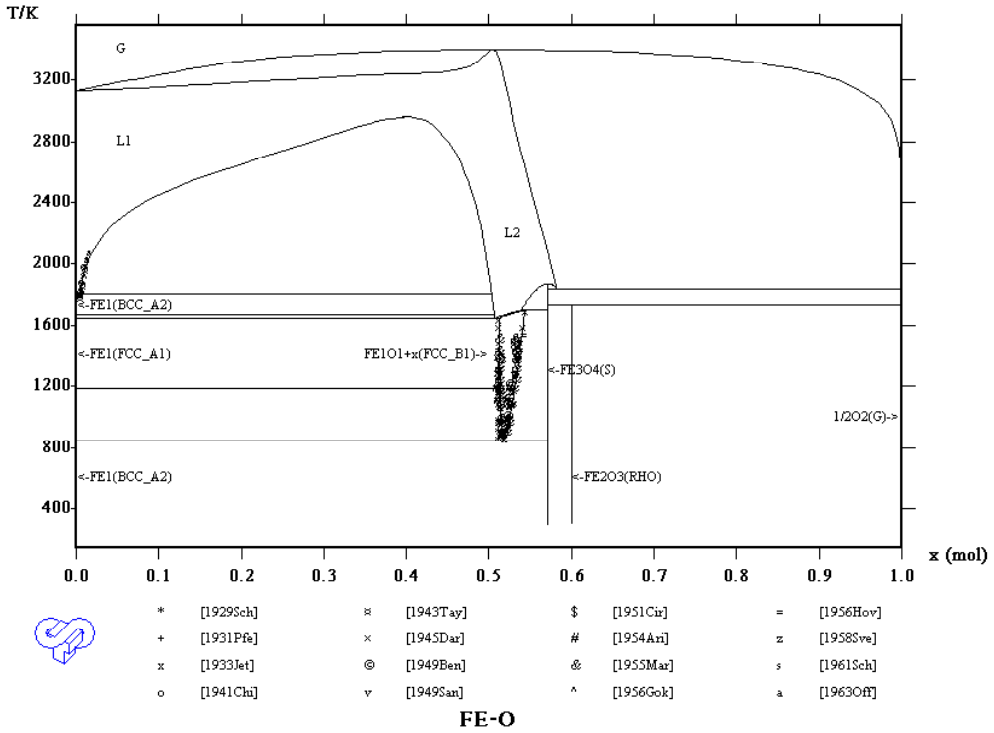

Figure 2 **Calculated Fe-O phase diagram compared with selected experimental data.**

[1929Sch] "Equilibrium investigations on the reduction, oxidation and carburization processes in iron. VIII"
R. Schenck, T. Dingmann, P.H. Kirscht and H. Wesselkock,
Z. Anorg. Allg. Chem., 182, 97-117 (1929).

[1931Pfe] "The constitution of scale"
L.B. Pfeil,
J. Iron Steel Inst., 123, 237-255 (1931).

[1933Jet] "A study of the homogeneity limits of wüstite (FeO) by X-Ray methods"
E.R. Jette and F. Foote,
Trans. AIME, 105, 276-284 (1933).

[1941Chi] " "
J. Chipman and K.L. Fetters,
Trans. ASM, 29, 953-967 (1941).

[1943Tay] " "
C.R. Taylor and J. Chipman,
Trans. AIME, 154, 228-245 (1943).

[1945Dar] "The system iron-oxygen. I. The wüstite field and related equilibria"
L.S. Darken and R.W. Gurry,
J. Am. Chem. Soc., 67, 1398-1412 (1945).

[1949Ben] "Research on variations in composition of wüstite"
J. Benard,
Bull. Soc. Chim. Fr. (Ser.5), 16, D109-D119 (1949).

[1949San] "Reduction equilibria of iron oxides. I. Measurement of the equilibrium of reaction Fe_3O_4 (in wüstite) + CO = 3 FeO (in wüstite) + CO_2"
K. Sanbongi,
Sci. Rep. Res. Inst. Tohoku Univ., 1 , 213-222 (1949).

[1951Cir] "The limits of composition of wüstite"
V. Cirilli and C. Brisi,
Ann. Chimica, 41, 508-514 (1951).

[1954Ari] "Thermodynamics of oxide phases with variable compositions. I. Thermodynamics of iron protoxide"
S.M. Ariya, M.P. Mororozova and L.A. Shneider,
Zh. Obshch. Khim., 24, 41-47 (1954).

[1955Mar] "Contribution to the study of iron protoxide"
F. Marion,
Doc. Metall., (Soc. Ind. Miner. St Etienne), Paris, 24, 87-136, (1955).

[1956Gok] "Equilibria in reaction of hydrogen, and carbon monoxide with dissolved oxygen in liquid iron ; equilibrium in reduction of ferrous oxide with hydrogen, and solubility of oxygen in liquid iron"
N.A. Gokcen,
Trans. AIME, 206, 1558-1567 (1956).

[1956Hov] "The oxygen content of wüstite in equilibrium with different gases"
N.A. Hovgard and P.N. Jensfelt,
Jernkontorets Ann., 140, 467-493 (1956).

[1958Sve] " "
V.N. Svechnikov, V.M. Pan and A.K. Shurin,
Fiz. Metal. i Metalloved, 6, 662-664 (1958) ; Phys. Metals Metallog. (USSR), 6, 4, 80-82 (1958).

[1961Sch] " "
H.Schenck und W.Pfaff,
Archiv fuer Eisenhuttenwesen, Vol. 32, 741-751, (1961).

[1963Off] "Contribution to the study of iron protoxide. I. Limits of the iron protoxide phase"
C. Offroy and J. Aubry,
Mem. Sci. Rev. Metall., 60, 6, 476-480 (1963).

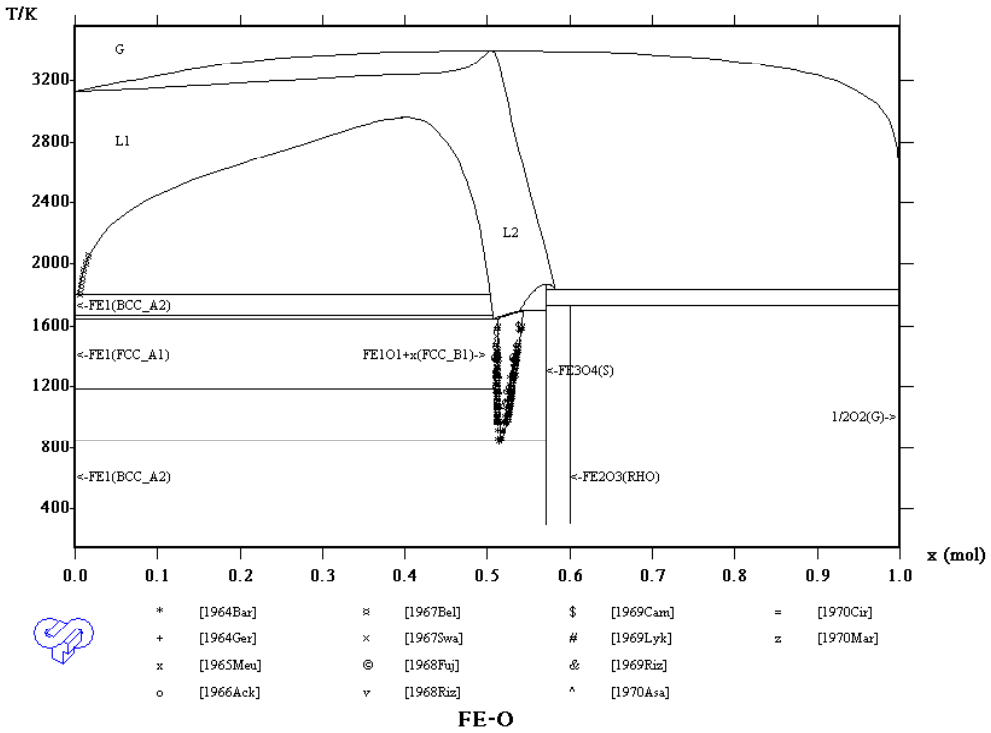

Figure 3 **Calculated Fe-O phase diagram compared with selected experimental data.**

[1964Bar] "The stability of wüstite by electromotive force measurements on all-solid electrolytic cells"
G.B. Barbi,
J. Phys. Chem., 68, 10, 2912-2916 (1964).

[1964Ger] "Utilization of the thermobalance in experiments on transfer of oxygen between oxides"
P. Gerdanian and M. Dode,
C.R. Acad. Sci. (Paris), 258, 892-895 (1964).

[1965Meu] "Studies of high-temperature materials (properties of FeO)"
R.A. Meussner, L.E. Richards and C.T. Fujii,
Rep. NRL Prog. Naval Res. Lab. Washington, DC, 26-28 (1965). Cited by [1968Riz2].

[1966Ack] "A thermodynamic study of the wüstite phase"
R.J. Ackermann and R.W. Sandford Jr.,
USAEC, Argonne Nat. Lab., Rep. ANL-7250 (1966).

[1967Bel] "Determination of the solubility of oxygen in molten iron, cobalt and nickel"
B.F. Belov, I.A. Novokhatskiy and Yu.A. Lobanov,
Izv. Akad. Nauk SSSR, Met., 3, 53-62 (1967) ; Russ. Metall., 3, 19-23, (1967).

[1967Swa] "On the vacancy concentration of wüstite (FeO_x) near the p to n transition"
B. Swaroop and J.B. Wagner, Jr.,
Trans. Metall. Soc. AIME, 239, 1215-1218 (1967).

[1968Fuj] "Chromium solubility in wüstite at 1000°C : changes in oxygen activity and lattice parameter"
C.T. Fujii and R.A. Meussner,
Trans. Metall. Soc. AIME, 242, 1259-1265 (1968).

[1968Riz] "Coulometric titration of wüstite"
F.E. Rizzo and J.V. Smith,
J. Phys. Chem., 72, 2, 485-488 (1968).

[1969Cam] "Determination of the boundaries of the iron protoxyde domain at high temperature"
J. Campserveux, G. Boureau, C. Picard and P. Gerdanian,
Rev. Int. Hautes Temp. Refract., 6, 165-174 (1969).

[1969Lyk] "Thermodynamics of wüstite"
A.A. Lykasov, Yu.S. Kuznetsov, E.I. Pil'Ko, V.I. Shishkov and V.A. Kozheurov,
Zh. Fiz. Khim., 43, 12, 3124-3125 (1969).

[1969Riz] "The determination of phase boundaries and thermodynamic functions in the iron-oxygen system by EMF measurements"
H.F. Rizzo, R.S. Gordon and I.B. Cutler,
J. Electochem. Soc., 116, 2, 266-274 (1969).

[1970Asa] "Thermodynamic properties of wüstite($FeO_{(1+y)}$)"
H. Asao, K. Ono, A. Yamaguchi and J. Moriyama,
Mem. Fac. Eng., Kyoto Univ., 33, 66-77 (1970).

[1970Cir] "Limits of composition of wüstite and solid solutions among wüstite, calcium oxide, and magnesium oxide"
V. Cirilli, A. Burdese and C. Brisi,
Ann. Chim. (Paris), 5, 4, 283-286 (1970).

[1970Mar] "Determination of partial molar magnitudes of mixing of oxygen in iron protoxide at 1075°C. II. Measurements of s(O_2)M"
J.F. Marucco, C. Picard, P. Gerdanian and D. Dode,
J. Chim. Phys. Phys.-Chim. Biol., 67, 914-916 (1970).

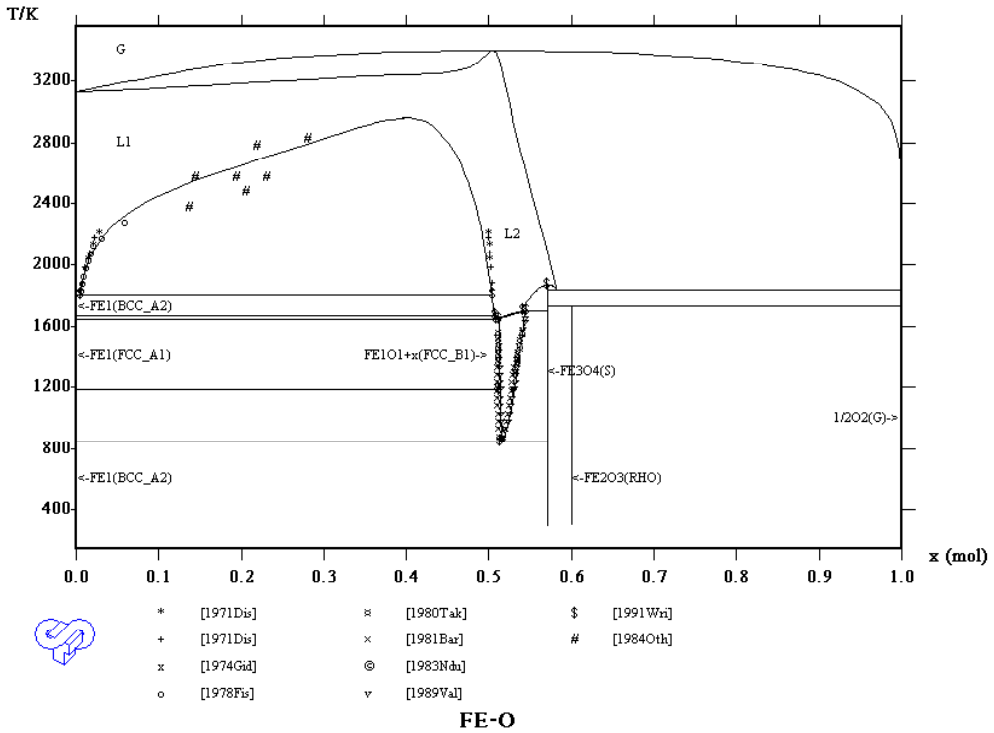

Figure 4 **Calculated Fe-O phase diagram compared with selected experimental data.**

[1971Dis] "Solubility of oxygen in liquid iron from 1785 to 1960°C. A new technique for the study of slag metal equilibria"
P.A. Distin, S.G. Whiteway and C.R. Mason,
Can. Metall. Q., 10, 1, 13-18 (1971).

[1974Gid] "Solid-state coulometric titration: critical analysis and application to wustite"
R.A. Giddings and R.S. Gordon,
J. Electrochem. Soc., 121, 6, 793-800 (1974).

[1978Fis] "The solubility of oxygen in pure iron from the melting point to 2046°C, determined with the levitation melting method"
W.A. Fischer and J.F. Schumacher,
Arch. Eisenhüttenwes., 49, 9, 431-435 (1978).

[1980Tak] "Thermodynamic properties and subphases of wustite field determined by means of thermogravimetric method in the temperature range of 1100-1300°C"
E. Takayama and N. Kimizukaon,
J. Electrochem. Soc., 127, 4, 970-976 (1980).

[1981Bar] "The lower temperature range of the wustite stability field"
J.A. Barbero, M.A. Blesa and J.G. Moroto,
Z. Phys. Chem. Neue Folge, 124, 139-147 (1981).

[1983Ndu] "The solubility of liquid oxysulfide phase in liquid Fe-O-S alloys"
M. Nduaguba and J.F. Elliott,
Metall. Trans. B, 14, 679-683 (1983).

[1989Val] "The Fe-O (Iron-Oxygen) phase diagram in the range of the non-stoichiometric monoxide and magnetite at the Fe-rich limit : reduction diagrams"
P. Vallet,
Bull. Alloy Phase Diagrams, 10, 3, 209-218 (1989).

[1991Wri] "The Fe-O (Iron-Oxygen) system"
H.A. Wriedt,
J. Phase Equilibria, 12, 2, 170-200 (1991).

[1984Oth] "Composition of the core : I. solubility of oxygen in molten iron at high temperatures"
E. Ohtani and A.E. Ringwood,
Earth Plan. Sci. Lett., 71, 85-93 (1984).

FE-U

The phase diagram of the Fe-U binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a complete miscibility from iron to uranium ;
- the intermetallic compounds, $Fe_2U_1(S)$ with the Laves structure, and $Fe_1U_6(S)$;
- pure solid iron, with a negligible solubility of uranium, with two allotropic structures, Fe_1(bcc_A2) and Fe_1(fcc_A1) ;
- the uranium rich terminal solid solutions, tetragonal (tet) and body cubic centred, bcc_A2, with a small solubility of iron.
- pure orthorhombic uranium U_1(ort_A20), with a negligible solubility of iron.

The heat capacity (Cp) of the stoichiometric compounds $Fe_2U_1(S)$ and $Fe_1U_6(S)$ have been assessed separately in consistency with the available experimental data. The fundamental properties at room temperatures (ΔH_{298}, S_{298}) have been assessed in consistency with all other data. The liquid, bcc_A2 and tet phases (ϕ) have been described by a simple substitutional model, with the formula (Fe_1, U_1)(ϕ). A realistic extrapolation of the excess Gibbs energy of the liquid phase at high temperature is proposed. The gas phase has been described by an ideal mixture of gaseous species, with the formula (Fe_1, U_1)$_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the activity of iron and uranium are in satisfactory agreement with the experimental ones in the liquid state ;
- the calculated and experimental phase diagrams are in very satisfactory agreement.

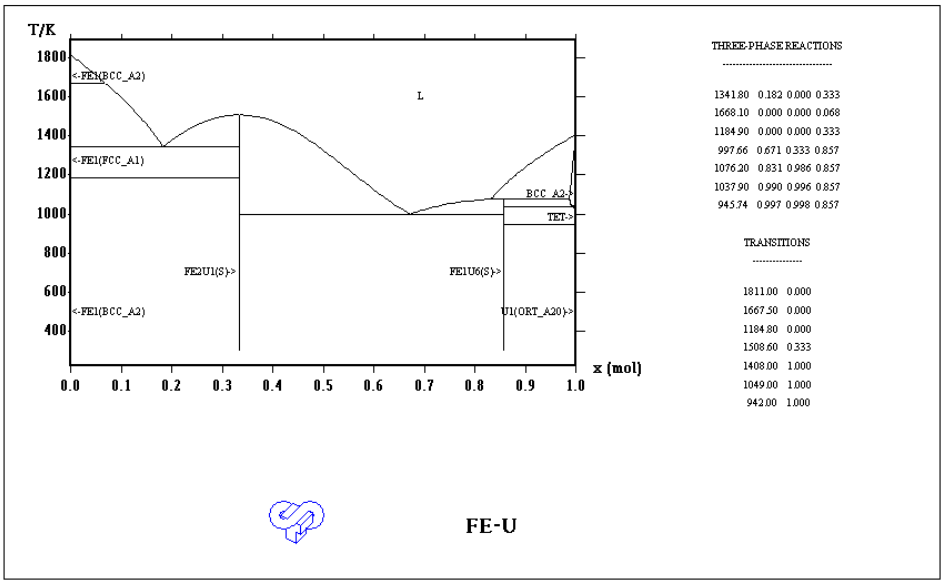

Figure 1 **Calculated Fe-U phase diagram with special points and invariant reactions.**

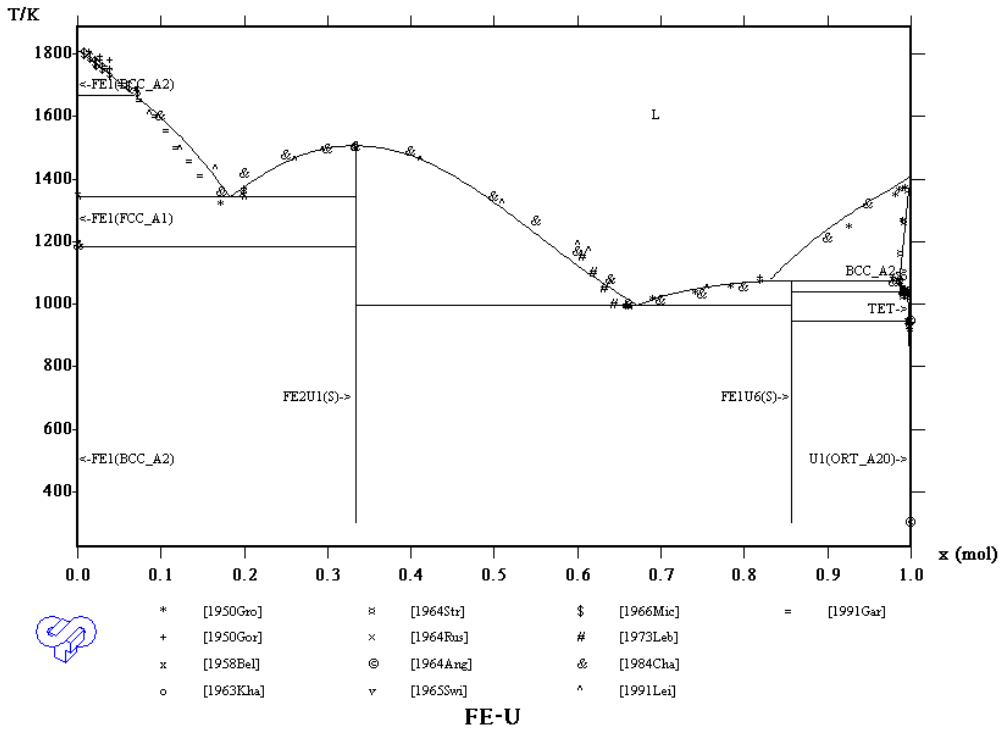

Figure 2 **Calculated Fe-U phase diagram compared with selected experimental data.**

[1950Gro] "The uranium-iron system"
J.D.Grogan,C.J. Birkett Clews,
Journal of the Institute of Metals, Vol.77, pp.571-580, (1950).

[1950Gor] " "
P.Gordon, A.R.Kaufmann,
Transactions of the AIME, Vol.188, pp.182-194, (1950).

[1958Bel] " "
J.Bellot, A.Blanchon, R.Chazot, P.Dosiere, J.M.Henry, M.Colas,
Comptes Rendus, Vol.246, pp. 3063-3065, (1958).

[1963Kha] " "
D.K.Khakimova, Yu.S.Virgilev, O.S.Ivanov,
in O.S. Ivanov (ed.), "Stroenie i Svoistva Splavov Urana, Toriya i Tsirkoniya", 5-8, Gosatomizdat, Moiscow, (1963).

[1964Str] " ",
J.A.Straatmann, N.F.Neumann,
U.S. At. Energy Comm. MCW-1487, 23p (1964).

[1964Rus] " "
R.B.Russel,
U.S. At. Energy Comm. NMI-2813, 44p (1964).

[1964Ang] " "
C.L.Angerman,
U.S. At. Energy Comm. DPST-64-219 (1964).

[1965Swi] "The solubility of iron in solid uranium between 0.003 wt % and 0.3 wt % iron"
N.Swindells,
Journal of Nuclear Materials, Vol.18, pp.261-271, (1966).

[1966Mic] " "
G.G.Michaud,
Canadian Metallurgical Quarterly, Vol.5, p.355, (1966).

[1973Leb] "Thermodynamic properties of U-Fe alloys"
V.A.Lebedev, N.V.Nazarov, V.I.Pyatkov, I.F.Nichkov, S.P.Raspopin,
Izvestia Akademii Nauk SSSR, Metally, Vol.2, pp.212-216, (1973).

[1984Cha] "Revision of the uranium-iron phase diagram"
L.R.Chapman, C.E.Holcombe, Jr.,
Journal of Nuclear Materials, Vol.126, pp.323-326, (1984).

[1991Lei] "Thermodynamics and phase equilibria of the iron-uranium system"
L.Leibowitz, R.A.Blomquist,
Journal of Nuclear Materials, Vol.184, pp.47-52, (1991).

[1991Gar] "Thermodynamique des alliages (U,Fe) et (U,Ga) en spectrométrie de masse à haute température"
P.Gardie, J.J.Poupeau, G.Bordier, J.Le Ny,
Calorim. Anal. Therm., Vol.22, pp.69-76, (1991).

FE-ZR

The phase diagram of the Fe-Zr binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a complete miscibility from iron to zirconium ;
- the intermetallic compounds, $Fe_{765}Zr_{265}$(S), Fe_1Zr_2(S), Fe_1Zr_3(S) ;
- the intermediate non-stoichiometric Laves phase, Fe_2Zr_1(Laves) ;
- the terminal iron-rich solid solutions, bcc_A2 and fcc_A1, with a small solubility of zirconium ;
- the terminal zirconium rich solution, bcc_A2, with a limited solubility of iron ;
- the terminal zirconium rich solution, with the hexagonal closed packed structure, hcp_A3, and a very small solubility of iron.

The heat capacity (Cp) of the stoichiometric compounds Fe_2Zr_1(Laves), Fe_1Zr_2(S), Fe_1Zr_3(S) have been estimated from the Neuman-Kopp rule. The fundamental properties at room temperatures (ΔH_{298}, S_{298}) have been assessed in consistency with all other data. The liquid, bcc_A2 and fcc_A1 phases (ϕ) have been described by a simple substitutional model, with the formula $(Fe_1,Zr_1)(\phi)$. The Laves phase has been described with a two sublattice model, with the formula $(Fe_1, Zr_1)_2(Fe_1, Zr_1)_1$. A realistic extrapolation of the excess Gibbs energy of the liquid phase at high temperature is proposed. The gas phase has been described by an ideal mixture of gaseous species, with the formula $(Fe_1, Zr_1, Zr_2)_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the activity of iron and zirconium are in satisfactory agreement with the experimental ones in the liquid state ;
- the selected enthalpy of mixing of the liquid phase is incompatible with the liquidus shape in the zirconium rich region ;
- the calculated and experimental phase diagrams are in satisfactory agreement : the non-stoichiometry.. range of the Laves phase and the temperatures of the invariant reactions are perfectly reproduced ; the liquidus shape in the zirconium rich region should be improved.

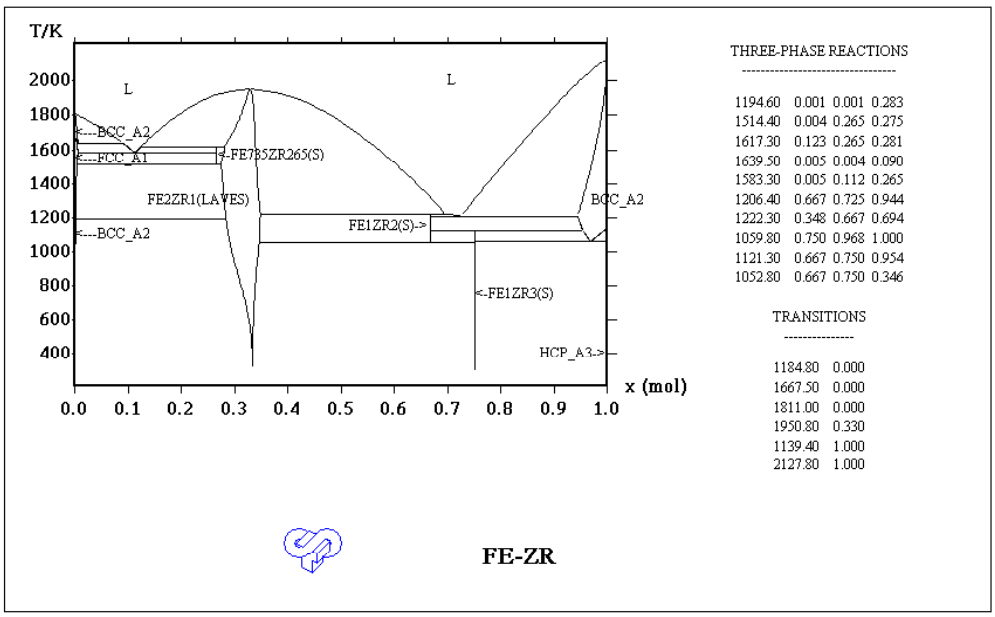

Figure 1 **Calculated Fe-Zr phase diagram with special points and invariant reactions.**

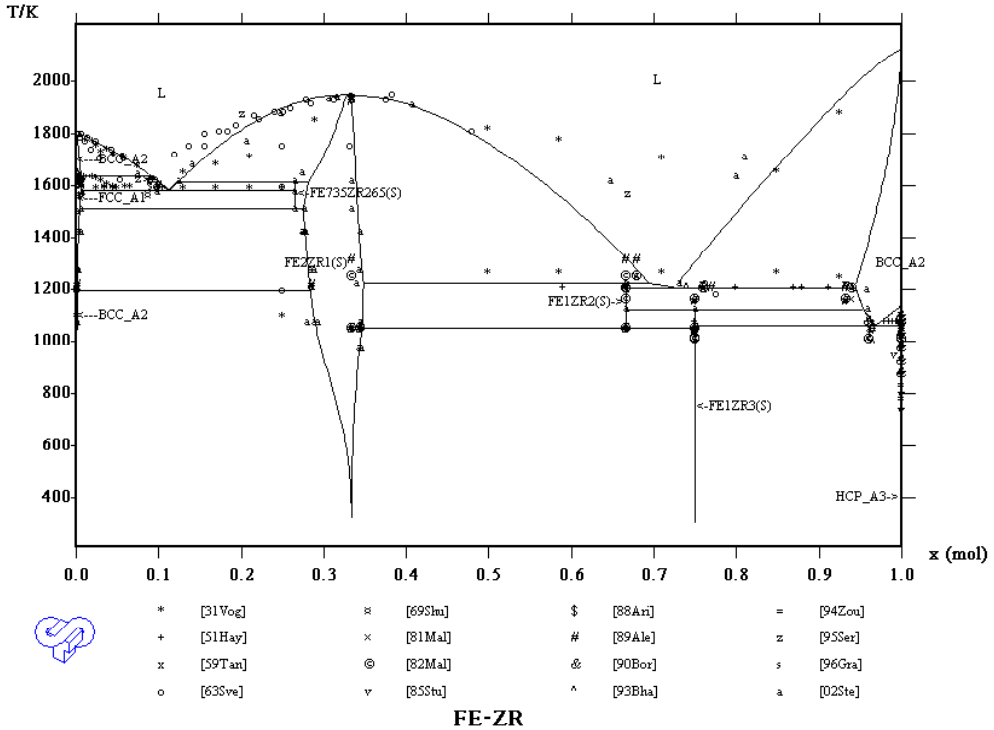

Figure 2 **Calculated Fe-Zr phase diagram compared with selected experimental data.**

[1931Vog] "The Fe-Zr system"
R.Vogel, W.Tonn,
Archiv fuer EisenHuttenwesen, Vol.5, pp.387-389, (1931-1932).

[1951Hay] "Constitution and mechanical properties of zirconium iron alloys"
E.T.Hayes, A.H.Robertson, W.L.O'Brien,
Transactions of the ASM, Vol.43, pp.888-897, (1951).

[1959Tan] "Observations on the system zirconium-iron"
L.E.Tanner, D.W.Levinson,
Transactions of the Metallurgical Society of AIME, Vol.215, pp.1066-1067, (december 1959).

[1963Sve] "Intermediate phases in the iron-zirconium system"
V.N.Svechnikov, V.M.Pan, A.Ts.Spektor,
Russian Journal of Inorganic Chemistry, Vol.8, N.9, pp.1106-1109, (September 1963).

[1969Shu] "Constitution of binary alloys, second supplement"
F.A.Shunk,
MacGraw-Hill Book Company, New-York, St Louis, San Francisco, London, Sydney, Toronto, Mexico, Panama, 1969.

[1981Mal] "The Zr-Fe phase diagram in the range 20-40 at% Fe and the crystalline structure of the intermetallic compound Zr_3Fe"
T.O.Malakhova, Z.M.Alekseyeva,
J. Less Com. Met., vol.81, pp.293-300 (1981).

[1982Mal] "The Zr-Fe phase diagram (0-66.6 at% Fe)"
T.O.Malakhova, A.N. Kobylin,
Russian Metallurgy, vol.2, pp.205-209 (1982).

[1985Stu] "Determination of Fe solubility in alpha-Zr by Mossbauer spectroscopy"
M.M.Stupel, M.Bamberger, B.Z.Weiss,
Scripta Metallurgica, Vol.19, pp.739-740, (1985).

[1988Ari] "The Fe-Zr (Iron-Zirconium) system"
D.Arias, J.P.Abriata,
Bulletin of Alloy Phase Diagrams, Vol.9, N.5, pp.597-604, (1988).

[1989Ale] "The Zr-Fe phase diagram"
Z.M. Alekseeva, N.V. Korotkova,
Izvestiya Akademii Nauk SSSR. Metally, vol.4, pp.202-208 (1989).

[1990Bor] "Study of the solubility of iron in zirconium by thermo-electric power measurements"
R.Borrelly, P.Merle, L.Adamy,
Journal of Nuclear Materials, Vol.170, pp.147-156, (1990).

[1993Bha] "Modification of zirconium-iron phase diagram"
K.Bhanumurthy, G.B.Kale,
Scripta Metallurgica et Materialia, Vol.28, pp.753-756, (1993).

[1994Zou] "The solid solubility of Fe in alpha-Zr : a secondary ion mass spectrometry study"
H.Zou, G.M.Hood, J.A.Roy, R.J.Schultz and J.A.Jackman,
Journal of Nuclear Materials, Vol.210, pp.239-243, (1994).

[1995Ser] Experimental and thermodynamic assessment of the Fe-Zr system.
C. Servant, C. Guéneau, I. Ansara,
J. Alloys and Compounds, vol.220, N°1-2, pp. 19-26 (1995).

[1996Gra] "Intermetallic phases in the iron-rich region of the Zr-Fe phase diagram"
M.S.Granovsky, D.Arias,
Journal of Nuclear Materials, Vol.229, pp.29-35, (1996).

[2002Ste] "Experimental determination of intermetallic phases, phase equilibria, and invariant reaction temperatures in the Fe-Zr system",
F. Stein, G. Sauthoff, M. Palm,
J. Phase Equilibria, Vol. 23, N°6, pp. 480-494 (2002).

O-U

The phase diagram of the O-U binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a miscibility gap between an UO_2 rich liquid (L_1) and an uranium rich liquid (L_2) ;
- the intermediate solid oxides, O_3U_1(S) or UO_3, O_8U_3(S) or U_3O_{8-z}, O_9U_4(S) or U_4O_{9-y} ; the compounds U_5O_{13+x}, U_8O_{21}, $UO_{2.61}$, have also been cited ;
- the oxide solid solution, UO_{2+x}, with the face-centred cubic structure, of CaF_2 (fluorite) type, Fm_3m, cF_{12}, noted fcc_C1 ;
- pure solid uranium, with a negligible solubility of oxygen, and different allotropic structures, orthorhombic, U_1(ort_A20), tetragonal, U_1(tet), and body cubic centred, U_1(bcc_A2) ;
- the gas phase, which shows an extended solubility of uranium above 2000 K.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of the stoichiometric compounds O_3U_1(S), O_8U_3(S), O_9U_4(S) and O_2U_1(S) have been assessed separately in consistency with the available experimental data. The liquid phase has been described by a non-ideal associate model, with the formula (O_1, O_2U_1, U_1)(L), and the solid solution UO_{2+x} by a three sublattice model, with the formula $(U_1)_1(O_1, \square)_2(O_1, \square)_1$(fcc_C1). In order to be compatible with the whole thermodynamic database and to allow the introduction of iron, the model has been simplified in a simple one lattice model, with the formula $(O_1, O_2U_1, U_1)_1$(fcc_C1). The gas phase has been described by an ideal mixture of gaseous species, with the formula (O_1, O_1U_1, O_2U_1, O_2, O_3, O_3U_1, U_1)$_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the oxygen potential experimental database is perfectly reproduced in the UO_{2+x} region, while the calculated curvature is stronger than the experimental one in the UO_{2-x} region, especially with the simplified model. However, the values in the diphasic domains are in good agreement ;
- the phase equilibria (solid UO_{2+x} region, liquidus, miscibility gap tie line) are well represented, but the UO_{2+x} region at high temperature has to be experimentally validated. The non-stoichiometry range of U_3O_{8-z} and U_4O_{9-y} have not been taken into account. The hypothesis of a small solubility of oxygen in liquid uranium has been retained.

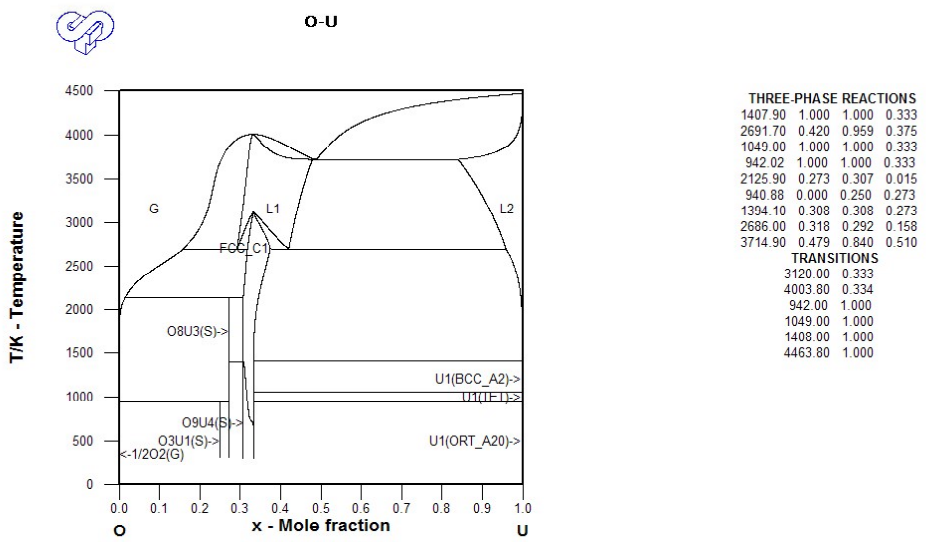

Figure 1 **Calculated O-U phase diagram with special points and invariant reactions.**

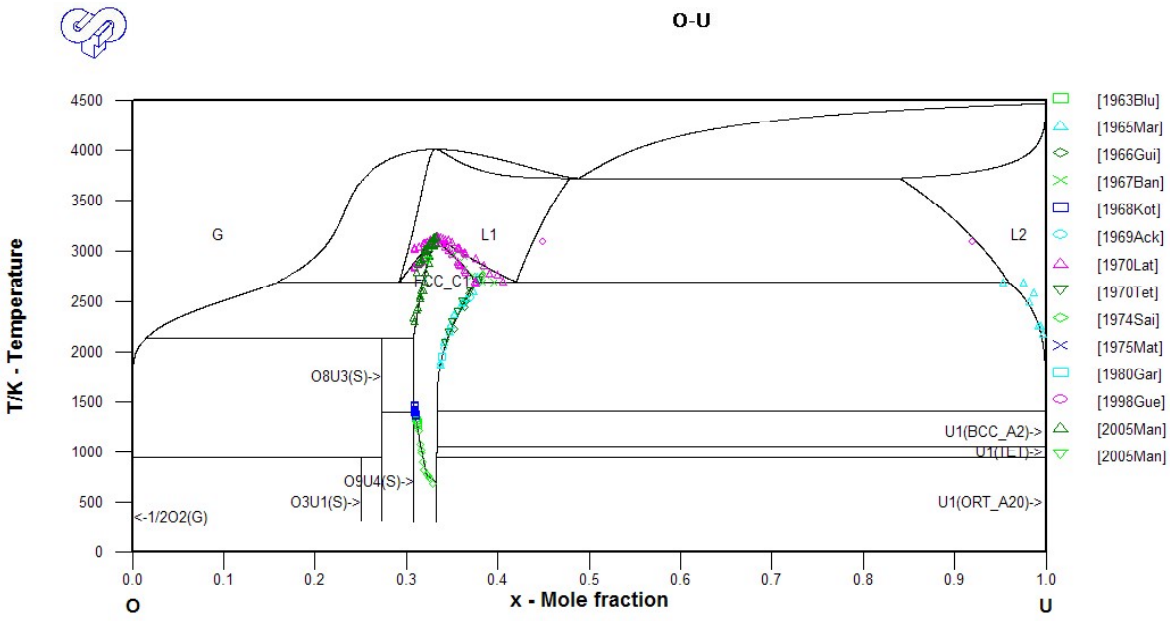

Figure 2 **Calculated O-U phase diagram compared with selected experimental data.**

[1963Blu] "Sur le système binaire uranium-dioxyde d'uranium"
P.L. Blum, P. Guinet et H. Vaugoyeau,
C.R. Acad. Sciences, T. 257, No. 22, pp. 3401-3403 (1963).

[1965Mar] " "
A.E. Martin and R.K. Edwards,
J. Phys. Chem., 69, 5 (1965) 1788 ; R. K. Edwards and A.E. Martin, p. 423 in Thermodynamics of Nuclear Materials", Vol. II, IAEA, Vienna, 1966.

[1966Gui] "Le système binaire uranium-dioxyde d'uranium au-dessus de 1130°C"
P. Guinet, H. Vaugoyeau et P.L. Blum,
C.R. Acad. Sciences, T. 263, Série C, pp. 17-20 (1966).

[1967Ban] "Melting Temperatures in the System Uranium-Uranium dioxide"
M.J. Bannister,
Journal of Nuclear Materials, 24 (1967) 340-342.

[1968Kot] "Détermination des limites de phases du système U-O par transfert d'oxygène. Diagramme de phases pour la région 2.19<O/U<2.653 et 1080°C<T<1200°C.
A. Kotlar, P. Gerdanian et M. Dode,
J. Chem. Phys., 65, 687-691 (1968).

[1969Ack] "A Thermodynamic Study of the Urania-Uranium System"
R.J. Ackermann, E.G. Rauh and M.S. Chandrasekharaiah,
The Journal of Physical Chemistry, 73, 4 (1969) 762-769.

[1970Lat] "Détermination of Solidus-Liquidus Temperatures in the $UO_{(2+x)}$ System (- 0.50 < x < 0.20)"
R.E. Latta and R.E. Fryxell,
Journal of Nuclear Materials, 35 (1970) 195-210.

[1970Tet] "Total pressure of uranium-bearing species over oxygen-deficient urania"
M. Tetenbaum and P.D. Hunt,
Journal of Nuclear Materials, 34 (1970) 86-91.

[1974Sai] "Non-stoichiometry in uranium dioxide"
Y. Saito,
Journal of Nuclear Materials, 51 (1974) 112-125.

[1975Mat] "Phase relation and defect structures of nonstoichiometric U_4O_{9+-y} and UO_{2+x} at high temperatures"
T. Matsui and K. Naito,
Journal of Nuclear Materials, 56 (1975) 327-335.

[1980Gar] "Solubility of Oxygen in Liquid Uranium and the Composition of the Lower Phase Boundary of Uranium Dioxide at 1950 K"
S.P.Garg and R.J.Ackermann,
Journal of Nuclear Materials, Vol. 88, pp. 309-311 (1980).

[1998Gue] "Liquid immiscibility in a (O,U,Zr) model corium"
C. Gueneau, V. Dauvois, P. Perodeaud, C. Gonella, O. Dugne,
Journal of Nuclear Materials, 254 (1998) 158-174.

[2005Man] "Melting of stoichiometric and hyperstoichiometric uranium dioxide"
D. Manara, C. Ronchi, M. Sheindlin,
Journal of Nuclear Materials, 342 (2005) 148-163.

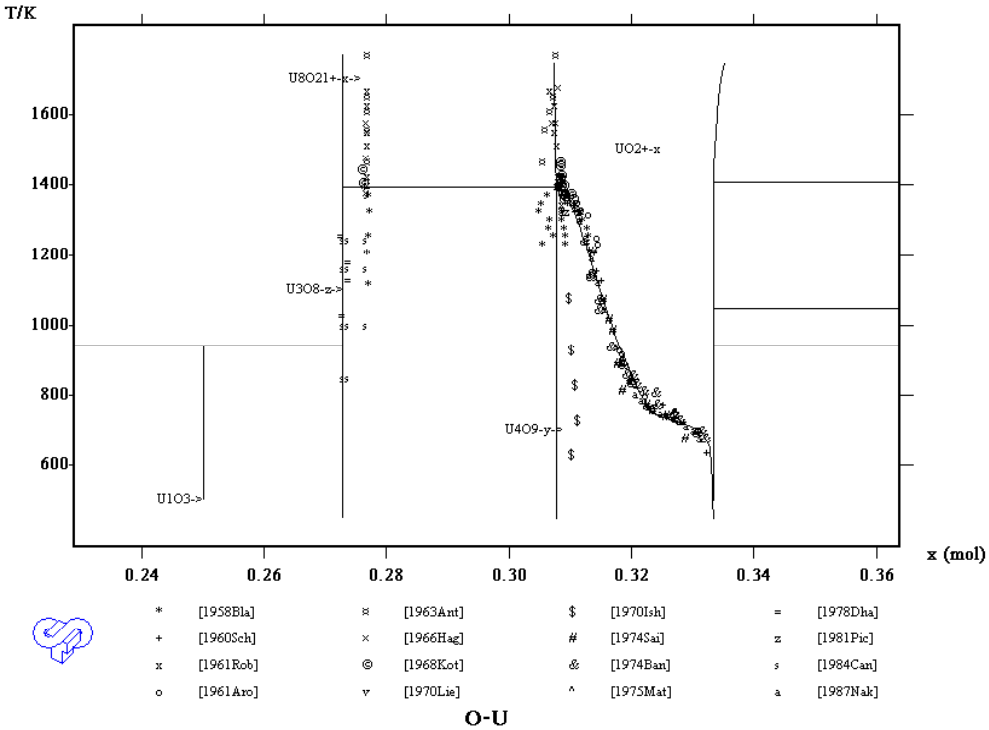

Figure 3 **Calculated UO_{2+x} solid region compared with selected experimental data.**

[1958Bla] " "
P.E. Blackburn,
J. Phys. Chem., 62, 8 (1958) 897-902.

[1960Sch] " "
B.E. Schaner,
J. Nucl. Mater., 2,2 (1960) 110-120.

[1961Rob] " "
L.E. Roberts and A.J. Walter,
J. Inorg. Nucl. Chem., 22 (1961) 213-229.

[1961Aro] " "
S. Aronson, J.E. Rulli and B.E. Schaner,
J. Chem. Phys. 35, 4 (1961) 1382-1388

[1963Ant] " "
A.M. Anthony, R. Kiyoura and T. Sata,
J. Nucl. Mater. 10, 1(1963) 8-14.

[1966Hag] "Equilibrium oxygen pressures Over the non-stoichiometric uranium oxides UO_{2+x} and U_3O_{8-z} at higher temperatures"
K. Hagemark and M. Broli,
J. Inorg. Nucl. Chem., 28 (1966) 2837-2850.

[1968Kot] "Détermination des limites de phases du système U-O par transfert d'oxygène. Diagramme de phases pour la région 2.19<O/U<2.653 et 1080°C<T<1200°C.
A. Kotlar, P. Gerdanian et M. Dod,,
J. Chem. Phys., 65, 687-691 (1968).

[1970Lie] " "
W.V. Lierde, J. Pelsmaekers and A. Lecoq-Robert,
J. Nucl. Mater. 37 (1970) 276-285.

[1970Ish] " "
T. Ishii, K. Naito and K. Oshima,
Solid State Communications 8 (1970) 677-683.

1974Sai] "Non-stoichiometry in uranium dioxide"
Y. Saito,
Journal of Nuclear Materials, 51 (1974) 112-125.

[1974Ban] "A dilatometric study of U_4O_9 in UO_2"
M.J. Bannister and W.J. Buykx,
Journal of Nuclear Materials, 55 (1974) 345-351.
[1975Mat] " "
T. Matsui and K. Naito,
Journal of Nuclear Materials, 56 (1975) 327-335.
[1978Dha] " "
S.R. Dharwadkar, M.S. Chandrasekharaiah and M.D. Karkhanavaia,
Journal of Nuclear Materials, 71 (1978) 268-276.
[1981Pic] " "
C. Picard and P. Gerdanian,
Journal of Nuclear Materials, 99 (1981) 184-189.
[1984Can] " "
A. Caneiro and J.P. Abriata,
Journal of Nuclear Materials, 126 (1984) 255-267.
[1987Nak] "Thermodynamic study of UO_{2+x} by solid state emf technique"
A. Nakamura and T. Fujino,
Journal of Nuclear Materials, 149 (1987) 80-100.

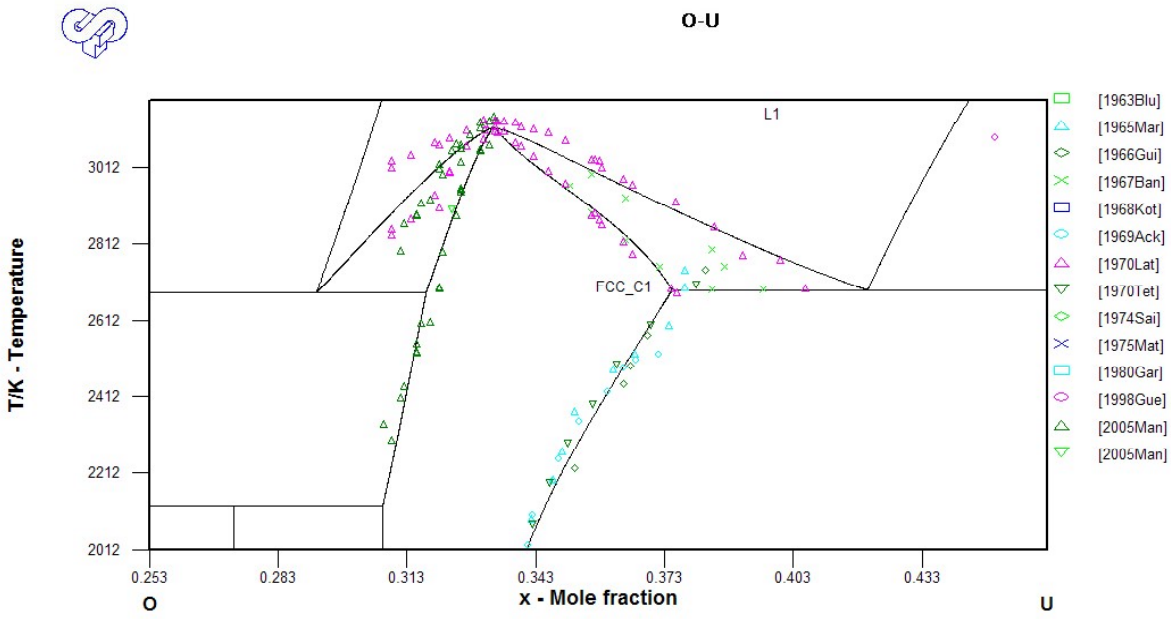

Figure 4 **Calculated UO_{2+x} region compared with selected experimental data.**

[1963Blu] "Sur le système binaire uranium-dioxyde d'uranium"
P.L. Blum, P. Guinet et H. Vaugoyeau,
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[1965Mar] " "
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[1967Ban] "Melting Temperatures in the System Uranium-Uranium dioxide"
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[1968Kot] "Détermination des limites de phases du système U-O par transfert d'oxygène. Diagramme de phases pour la région 2.19<O/U<2.653 et 1080°C<T<1200°C.
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[1970Lat] "Determination of Solidus-Liquidus Temperatures in the $UO_{(2+x)}$ System (-0.50<x<0.20)"
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1974Sai] "Non-stoichiometry in uranium dioxide"
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Journal of Nuclear Materials, 254 (1998) 158-174.

[2005Man] "Melting of stoichiometric and hyperstoichiometric uranium dioxide"
D. Manara, C. Ronchi, M. Sheindlin,
Journal of Nuclear Materials, 342 (2005) 148-163.

O-ZR

The phase diagram of the O-Zr binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a complete miscibility from O_2Zr_1 oxide to Zr metal ;
- the pure solid oxides, with the allotropic forms monoclinic O_2Zr_1(mon) and tetragonal O_2Zr_1(tet) ;
- the oxide solid solution, ZrO_{2-x}, with the face-centred cubic structure, of CaF_2 (fluorite) type, Fm_3m, cF_{12}, noted fcc_C1 ;
- the terminal zirconium rich solid solutions, body cubic centred (bcc_A2), and hexagonal closed packed (hcp_A3) pure solid uranium, with a solubility of oxygen limited to about 10 at% and 30 at% respectively ;
- the gas phase, which shows an extended solubility of zirconium above 3000 K.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of the stoichiometric compound O_2Zr_1(mon, tet, fcc_C1) have been assessed separately in consistency with the available experimental data. The liquid phase has been described by a non ideal associate model, with the formula $(O_1, O_2Zr_1, Zr_1)_1$(L), and the solid solution ZrO_{2-x}, bcc_A2 and hcp_A3 by three and two sublattice models, with the respective formula $(Zr_1)_1(O_1, \square)_2((O_1, \square)_1$(fcc_C1), $(Zr_1)_1(O_1, \square)_3$(bcc_A2), and $(Zr_1)_1(O_1, \square)_{0.5}$(hcp_A3). In order to be compatible with the whole thermodynamic database and to allow the introduction of iron, the model of the fcc_C1 solid solution has been simplified in a simple one lattice model, with the formula $(O_1, O_2Zr_1, Zr_1)_1$(fcc_C1). The gas phase has been described by an ideal mixture of gaseous species, with the formula $(O_1, O_1Zr_1, O_2, O_2Zr_1, O_3, Zr_1, Zr_2)_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the oxygen potential experimental database is correctly reproduced in the monophasic regions ZrO_{2-x}, fcc_C1 and hcp_A3, while some disagreements have been observed in the diphasic region fcc_C1+hcp_A3 ;
- the phase equilibria (solid ZrO_{2-x} region, diphasic regions O_2Zr_1(mon, tet) + hcp_A3, fcc_C1 + hcp_A3, hcp_A3 + bcc_A2) are well represented, but the liquidus L + ZrO_{2-x} should be validated ;
- several stoichiometric oxides observed in the zirconium rich domain at low temperature (T < 750 K) could be included.

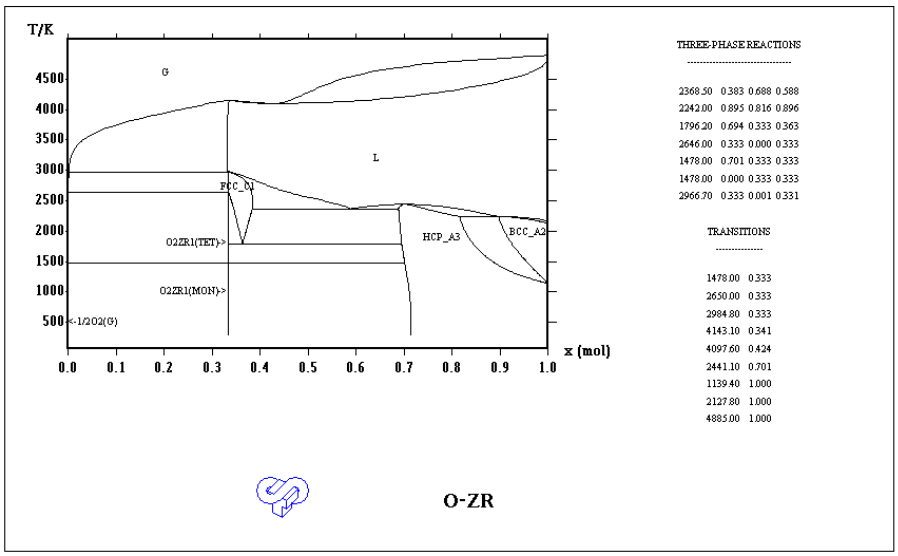

Figure 1 **Calculated O-Zr phase diagram with special points and invariant reactions.**

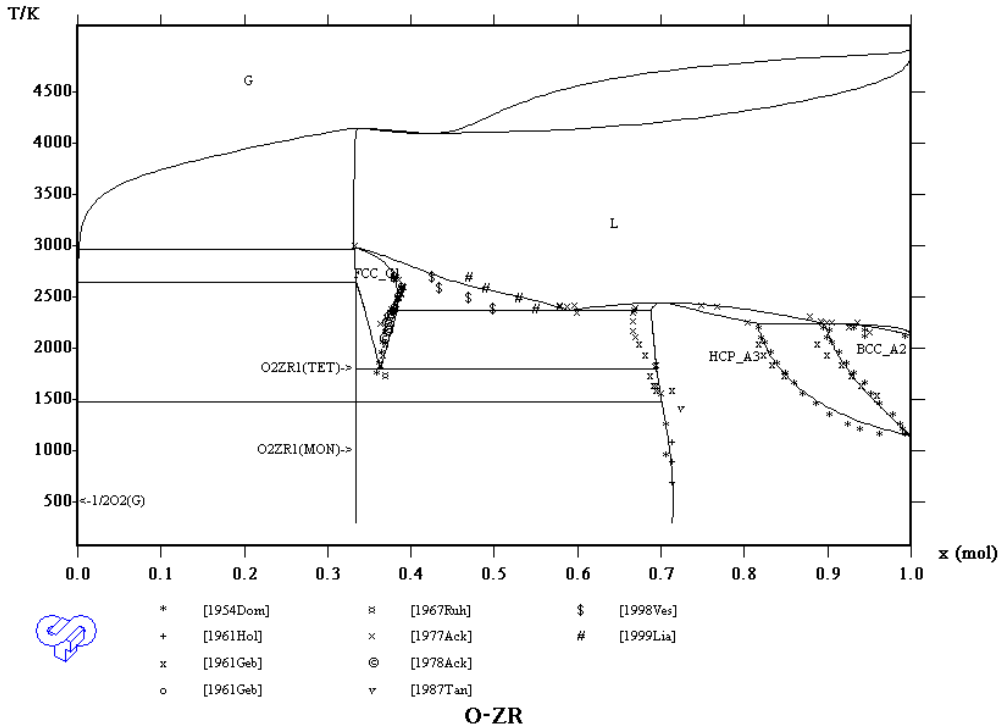

Figure 2 **Calculated O-Zr phase diagram compared with selected experimental data.**

[1954Dom] "System zirconium-oxygen"
R.F.Domagala and D.J.McPherson
Journal of Metals, Transactions of the AIME, 238-246, February 1954.

[1961Hol] "X-Ray studies on solid solutions of oxygen in alpha-zirconium"
Bo Holmberg and Tore Dagerhamn
Acta Chemica Scandinavica, Vol.15, N.4, 919-925, (1961).

[1961Geb] “Research on the system zirconium-oxygen”
E.Gebhardt, H.D.Seghezzi and W.Duerrschnabel
Journal of Nuclear Materials, Vol.4, N.3, 255-268, (1961).

[1967Ruh] "Non-stoichiometry of ZrO_2 and its relation to tetragonal-cubic inversion in ZrO_2"
R.Ruh and H.J.Garrett,
Journal of the American Ceramic Society, Vol.50, N.5, 257-261, (1967)

[1977Ack] "High-temperature phase diagram for the system Zr-O"
R.J.Ackermann, S.P.Garg, E.G.Rauh
Journal of The American Ceramic Society, Vol.60, N°.7-8, 341-345, (1977).

[1978Ack] "The lower phase boundary of ZrO_{2-x}"
R.J.Ackermann, S.P.Garg, E.G.Rauh
Journal of The American Ceramic Society, Vol.61, N.5-6, 275-276, (1978).

[1987Tan] "AES and XPS studies of oxygen stabilized alpha zirconium"
T.Tanabe, M.Tanaka and S.Imoto
Surface Science, Vol.187, 499-510, (1987).

[1998Ves] "Analysis of the FZK previous tests and pre-test calculations of the FZK new tests on ZrO_2 dissolution by molten zircaloy"
M.Veshunov
In vessel cluster INV-CIT(98)-M006, IPSN/DRS/SEMAR 98/36, Minutes of the 4th CIT project meeting, Pisa (10th and 11th June 1998) ; M.Barrachin and B.Adroguer.

[1999Lia] "Thermodynamic assessment of the O-Zr system"
P. Liang, H. Seifert, H.L. Lukas, S. Fries, N. Dupin, I. Ansara and F. Aldinger,
Calphad XXVII.

U-ZR

The phase diagram of the U-Zr binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a complete miscibility from uranium to zirconium ;
- the body cubic centred solid solution, bcc_A2, with also a complete miscibility at high temperature and a small miscibility gap deported on the uranium side between 950 K and 1000 K ;
- the terminal solid solutions, uranium rich orthorhombic and tetragonal, ort_A20 and tet, with a small solubility of zirconium, and zirconium rich hexagonal closed packed, hcp_A3, with a small solubility of uranium ;
- the intermetallic solid solution, δ, which extents from 64 to 78 at% Zr.

The liquid, bcc_A2, ort_A20, tet and hcp_A3 phases (ϕ) have been described by a simple substitutional model, with the formula $(U_1, Zr_1)(\phi)$, and the δ intermetallic solid solution by a two sublattice model, with the formula $(U_1, Zr_1)_2(Zr_1)(\delta)$. The gas phase has been described by an ideal mixture of gaseous species, with the formula $(U_1, Zr_1)_1(G)$. The excess Gibbs energy of the liquid and bcc_A2 solid solution has been assessed more physically than in other assessments found in open literature.

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- some experimental activities were found to be too negative and discarded for experimental reasons (interaction with crucible, impurities) ;
- the calculated phase diagram is in satisfactory agreement with the experimental one ;
- thermodynamic properties in the liquid phase should be determined at high temperature.

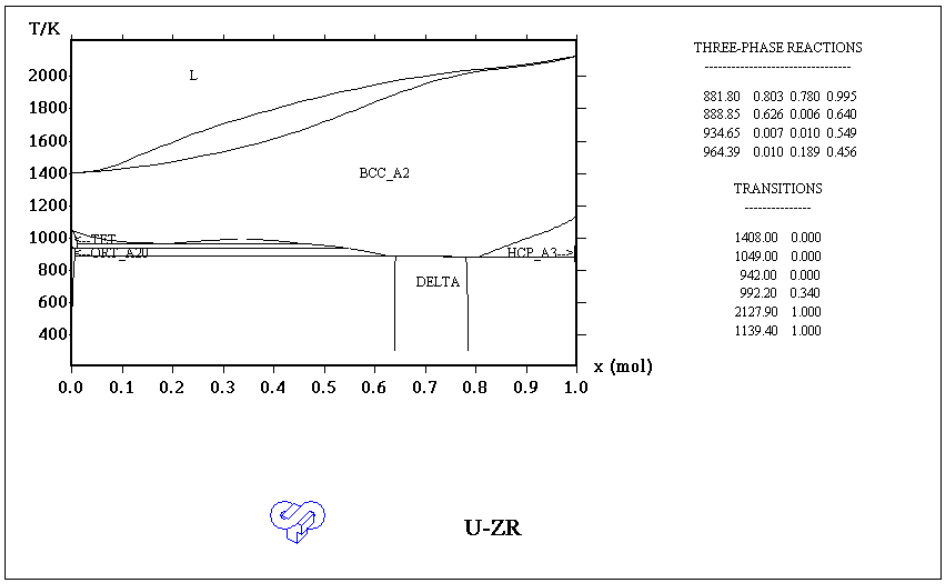

Figure 1 **Calculated U-Zr phase diagram with special points and invariant reactions.**

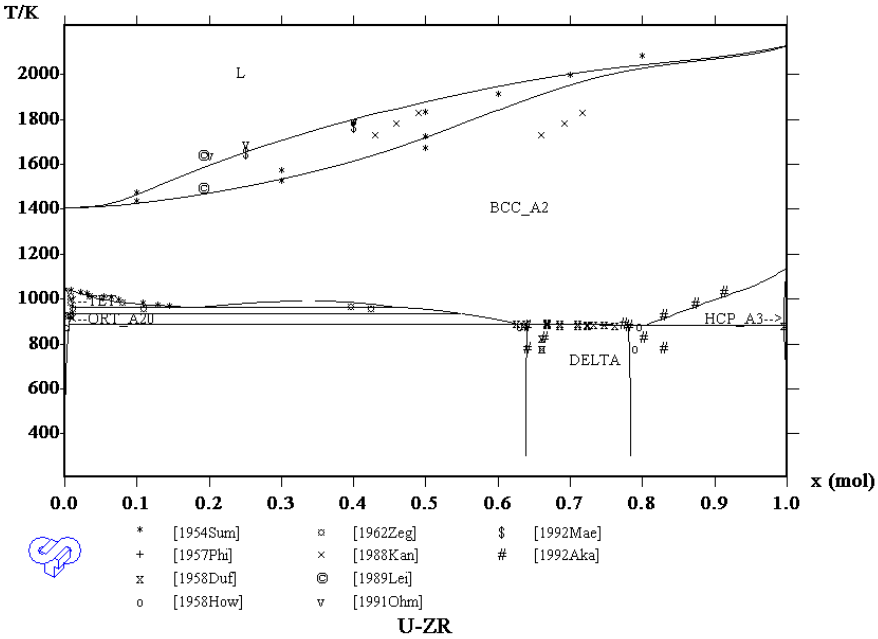

Figure 2 **Calculated U-Zr phase diagram compared with selected experimental data.**

[1954Sum] "The Constitution of Uranium-Zirconium Alloys"
D.Summers-Smith,
Journal of the Institute of Metals, Vol.83, pp.277-282, (1954-55).

[1957Phi] "Etablissement des diagrammes d'équilibre des alliages binaires par des expériences de diffusion intermétalliques. Application au système uranium-zirconium"
J.Philibert, Y.Adda,
Comptes Rendus de l'Académie des Sciences, pp.2507-2510, (23 décembre 1957).

[1958Duf] "Delta phase field of the U-Zr equilibrium diagram"
J.F.Duffey, C.A.Bruch,
Transactions of the Metallurgical Society of AIME, 17-19, (Février 1958).

[1958How] " "
B.W.Howlett, A.G.Knapton,
2nd UN Internatinal Conference on Peaceful Use of Atomic Energy, Geneva, Vol.6, p.104, (1958).

[1962Zeg] "The uranium-rich end of the uranium-zirconium system"
S.T.Zegler,
USAEC Rep.ANL-6055 (1962).

[1988Kan] "Thermodynamic activity measurements of U-Zr alloys by Knudsen effusion mass spectrometry"
M.Kanno, M.Yamawaki, T.Koyama, N.Morioka,
Journal of Nuclear Materials, Vol. 154, pp.154-160, (1988).

[1989Lei] "Thermodynamics of the uranium-zirconium system"
L.Leibowitz, R. A.Blomquist, A.D.Pelton,
Journal of Nuclear Materials, Vol. 167, pp.76-81, (1989).

[1991Ohm] " "
T.Ohmichi,
private communication, reported by T. Ogawa, T. Iwai, Journal of the Less-Common Metals, vol.170, pp.101-108 (1991).

[1992Mae] " "
A.Maeda, Y.Suzuki,T.Ohmichi,
Journal of Alloys and Compounds, Vol. 179, L21-24, (1992).

[1992Aka] "Stability and structure of the delta phase of the U-Zr alloys"
M.Akabori, A.Itoh, T.Ogawa, F.Kobayashi, Y.Suzuki,
Journal of Nuclear Materials, Vol. 188, pp .249-254, (1992).

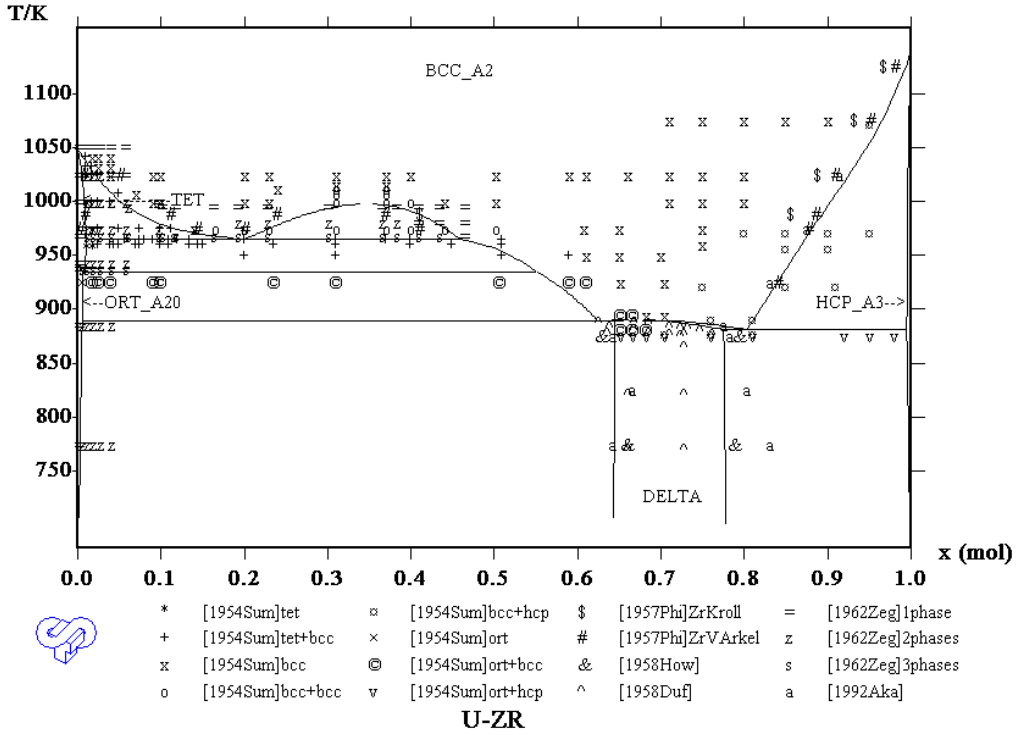

Figure 3 **Partial calculated U-Zr phase diagram compared with selected experimental data.**

[1954Sum] "The constitution of uranium-zirconium alloys"
D.Summers-Smith,
Journal of the Institute of Metals, Vol. 83, pp.277-282, (1954-55).

[1957Phi] "Etablissement des diagrammes d'équilibre des alliages binaires par des expériences de diffusion intermétalliques. Application au système uranium-zirconium"
J.Philibert, Y.Adda,
Comptes Rendus de l'Académie des Sciences, pp.2507-2510, (23 décembre 1957).

[1958How] " "
B.W.Howlett, A.G.Knapton,
2nd UN International Conference on Peaceful Use of Atomic Energy, Geneva, Vol. 6, p.104, (1958).

[1958Duf] "Delta phase field of the U-Zr equilibrium diagram"
J.F.Duffey, C.A.Bruch,
Transactions of the Metallurgical Society of AIME, 17-19, (Février 1958).

[1962Zeg] "The Uranium-rich end of the uranium-zirconium system"
S.T.Zegler,
USAEC Rep.ANL-6055 (1962).

[1992Aka] "Stability and structure of the delta phase of the U-Zr alloys"
M.Akabori, A.Itoh, T.Ogawa, F.Kobayashi, Y.Suzuki,
Journal of Nuclear Materials, Vol. 188, pp. 249-254, (1992).

O_2U_1-O_2ZR_1

The phase diagram of the O_2U_1-O_2Zr_1 pseudo-binary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a complete miscibility from O_2U_1 oxide to O_2Zr_1 oxide ;
- the pure solid oxide, with the allotropic form monoclinic, O_2Zr_1(mon) ;
- the oxide solid solution, (U, Zr)O_2, with the face-centred cubic structure, of CaF_2 (fluorite) type, Fm_3m, cF_{12}, noted fcc_C1 ;
- the terminal O_2Zr_1 rich solid solutions, tetragonal (tet_oxide), with a solubility of O_2U_1 limited to about 23 mol%.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of the stoichiometric compounds O_2U_1(fcc_C1) and O_2Zr_1(mon, tet, fcc_C1) have been assessed separately in consistency with the available experimental data. The liquid, fcc_C1 and tetragonal phases (ϕ) have been described by a simple substitutional model, with the formula (O_2U_1, $O_2Zr_1)_1(\phi)$, which is compatible with the two sublattice model (U_1, $Zr_1)O_2(\phi)$.

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the experimental activity of O_2U_1 and O_2Zr_1 in the fcc_C1 and tetragonal solid solutions are satisfactorily reproduced ;
- the calculated phase diagram is in good agreement with the experimental data.

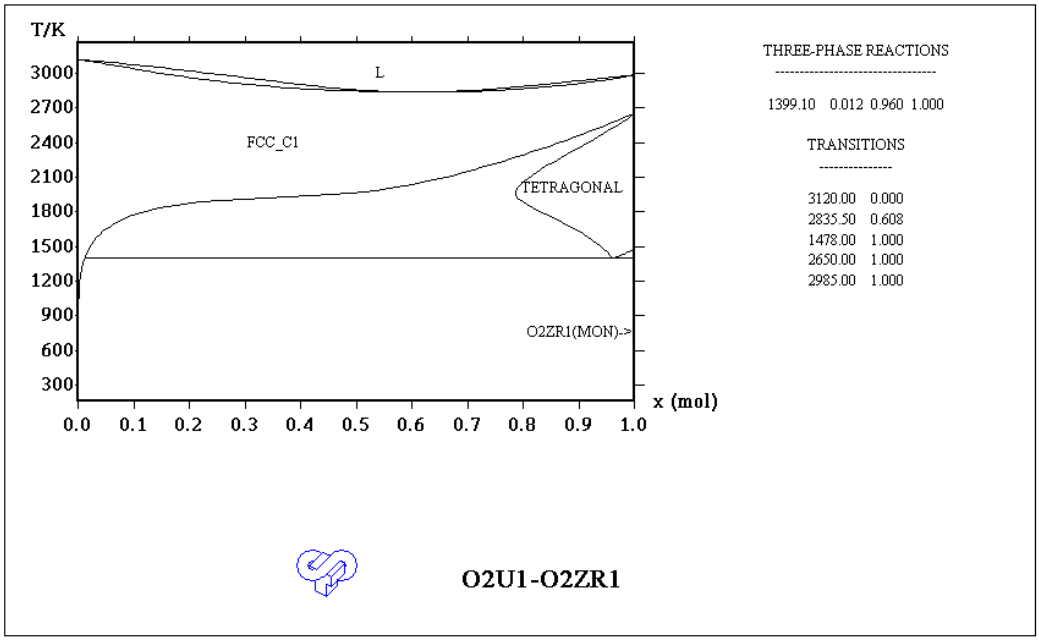

Figure 1 **Calculated O_2U_1-O_2Zr_1 pseudo-binary phase diagram with special points and invariant reactions.**

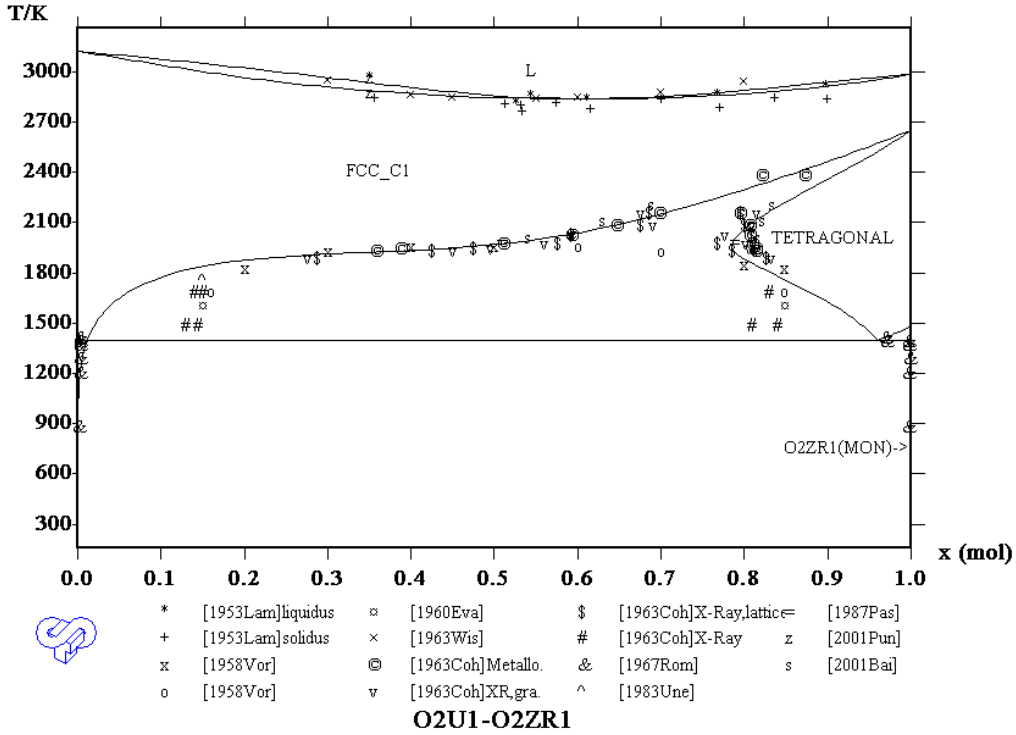

Figure 2 **Calculated O_2U_1-O_2Zr_1 pseudo-binary phase diagram compared with selected experimental data.**

[1953Lam] "Uranium oxide phase equilibrium systems"
W.A. Lambertson, M.H. Muller,
J. Am. Cer. Soc., vol.36, N°11, p.365 (1953).

[1958Vor] "Phase equilibrium diagrams of the UO_2-ZrO_2 and ThO_2-ZrO_2 Systems"
N. M. Voronov, E.A. Voitekhova and A.S. Danilin,
Proc. 2nd Genova Conf., Vol. 6, pp.221-225, (1958).

[1960Eva] "The system UO_2-ZrO_2"
P.E. Evans,
J. Am. Ceram. Soc, 43, vol.9, pp.443-447 (1960).

[1963Wis] " "
L. G. Wisnyi and S. W. Pijanowsko,
Knolls Atomic Power Laboratory (U.S.A.) Report, KAPL-1702 (1957).

[1963Coh] "A metallographic and x-ray study of the UO_2-ZrO_2 system"
I. Cohen, B.E. Schaner,
J. Nucl. Mat., Vol.9, N°1, pp.18-52 (1963).

[1967Rom] "Phase equilibrium studies in the UO_2-ZrO_2 system"
K.A. Romberger, C.F. Baes and H.H. Stone,
J. Inorg. Nucl. Chem., Vol. 29, pp.1619-1630 (1967).

[1983Une] "Oxygen potential of $U_{0.85}Zr_{0.15}O_{2+x}$ solid solutions at 1500C"
K. Une, M. Oguma,
J. Amer. Ceram. Soc., Vol. 66, pp.179-180 (1983).

[1987Pas] "Phase equilibria in the BaO-UO_2-ZrO_2-MoO_2 system"
J.O.A. Pashoal, H. Kleykamp and F. Thümmler,
J. Nucl. Mat., Vol.151, pp.10-21 (1987).

[2001Pun] "Determination of the solidus and liquidus temperatures of uranium-zirconium oxides"
J.S. Punni, M.A. Mlignanelli,
ENTHALPY Project, SAM-ENTHA(01)-D004, August 2001.

[2001Bai] "Mass spectrometric study of UO_2-ZrO_2 pseudo-binary system"
M. Baichi, C. Chatillon, C. Guéneau, S. Chatain,
Journal of Nuclear Materials, Vol. 294, pp. 84-87 (2001).

FE-O-U

The phase diagram of the Fe-O-U ternary system presents the following solutions and substances, with the symbols used in this work :

- the liquid phase, L, which shows a miscibility gap between an Fe-U-O rich metal-oxygen liquid (L_1) and a FeO-Fe_2O_3-UO_2 rich oxide liquid (L_2) ; it extends from the Fe-O side to the O-U side it could present a miscibility gap between a Fe_2O_3/Fe_3O_4 rich phase (L_2) and a UO_2 rich liquid (L_3) ;
- the oxide solid solution, $(U,Fe)O_{2+x}$, with the face-centred cubic structure, of CaF_2 (fluorite) type, Fm_3m, cF_{12}, noted fcc_C1, and which can dissolves until 15 mol% FeO in UO_2 ;
- the oxide solid solution, FeO_{1+x}, or wustite, with the face-centred cubic structure, of NaCl type, noted fcc_B1 ; no solubility of urania in wustite is reported ;
- the uranium rich terminal solid solutions, tetragonal, tet_metal, and body cubic centred, bcc_A2, with a small solubility of iron.
- the pure solid oxides, Fe_3O_4(S) or magnetite, Fe_2O_3(S) or hematite, corundum, O_3U_1(S), O_8U_3(S), O_9U_4(S) ;
- the inter-metallic compounds, Fe_2U_1(S) with the Laves structure, and Fe_1U_6(S) ;
- the ternary solid oxide, $Fe_1O_4U_1$(S) ;
- pure solid iron, with a negligible solubility of oxygen and uranium, and two allotropic structures, body cubic centred, Fe_1(bcc_A2), and cubic face centred, Fe_1(fcc_A1) ;
- pure orthorhombic uranium U_1(ort_A20), with a negligible solubility of iron and oxygen ;
- the gas phase (G), which shows an extended solubility in oxygen of iron above 2800 K and of uranium above 2000 K.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of the stoichiometric compounds $Fe_{0.947}O_1$(fcc_B1), Fe_3O_4(S), Fe_2O_3(S), O_3U_1(S), O_8U_3(S), O_9U_4(S), O_2U_1(fcc_C1) have been assessed in the individual sub-systems, as well as the thermodynamic modelling of all binary or pseudo-binary phases. The ternary liquid phase has been described by a non- ideal associate model, with the formula (Fe_1, Fe_1O_1, $Fe_1O_{1.5}$, O_1, O_2U_1, $U_1)_1$(L). The fcc_C1 and fcc_B1 solid solutions have been described will a one lattice model, with the formula $(Fe_1O_1,O_2U_1)_1$(fcc_C1) and $(Fe_1O_1, Fe_1O_{1.5})_1$(fcc_B1) respectively. The Gibbs energy of the ternary solid oxide $Fe_1O_4U_1$(S) has been assessed from the experimental information (thermodynamics and phase diagram). The gas phase has been described by an ideal mixture of gaseous species, with the formula (Fe_1, Fe_1O_1, $Fe_1O_{1.5}$, O_1, O_1U_1, O_2, O_2U_1, O_3, O_3U_1, $U_1)_1$ (G).

In the metal-oxygen field, the only used experimental information [1997Kle] on phase diagram is located on the line Fe-UO_2 and indicate a very low solubility of UO_2 in liquid iron at very high temperature (2873 K).

In the ternary oxide field, the $Fe_1O_4U_1$(S) was found to be decomposed at 1310 K.

Most of the more recent experimental informations are located in the pseudo-binary vertical sections, FeO-UO_2 ([1998Hel], [2003Pet], [2004Cor]) and Fe_2O_3/Fe_3O_4-UO_2 ([1969Ril], [2005Kis]), and come from the CORPHAD and SARNET international projects.

The main features of the FeO-UO_2 isopleth to section [2004Cor] are a complete solubility between FeO and UO_2 in the oxide liquid (L_2), and a non negligible solubility of iron oxide in the UO_2 rich fcc_C1 solid solution. The eutectic point was experimentally assessed as T = 1615 K (1342°C) and 4 mol% UO_2 (13.6 wt%). The solubility of iron oxide in fcc_C1 at the eutectic temperature was assessed as 17 mol% FeO (5 wt%).

The Fe_2O_3/Fe_3O_4-UO_{2+x} isopleth section has been experimentally studied in air [1969Ril], and its edges vary with composition from UO_{2+x}, U_3O_8 or U_4O_8 below 2126 K and 1394 K, and from Fe_2O_3 to Fe_3O_4 (melting point, 1869 K) above 1730 K ; according to Riley [1969Ril], the eutectic reaction L ⇔ U_3O_8 + Fe_2O_3 is located at 1513 K (1240 °C) and 30 wt% Fe_2O_3, 70 wt% UO_2, corresponding to

59.2 mol% $Fe_1O_{1.5}$, 40.8 mol% UO_2. Whatever, this diagram is still imprecise and presumption of a liquid miscibility gas was recently put in evidence by Kiselova and Petrov [2005Kis]. According to these authors, the eutectic L ⇔ UO_2 + $FeO_{1.33}$ was located at 1621 K (1348 °C) and 68.5 wt% UO_2, 31.5 wt% Fe_3O_4, and a miscibility gap was found between 1673 K (1400 °C) and 1973 K (1700 °C) on the iron oxide rich side.

In a first approximation, the excess interaction parameters between Fe_1O_1 and O_2U_1 on the one hand and $Fe_1O_{1.5}$ and O_2U_1 on the other hand have been estimated by assuming the pseudo-binary sections as quasi-binary ones.

The real isothermal or isopleth sections may be then calculated from the complete thermodynamic modelling. The main features of the FeO-UO_2 pseudo-binary system are qualitatively well reproduced, but the residual uncertainty on the Fe_2O_3/Fe_3O_4-UO_2 pseudo-binary system leads to quantitative differences between re-calculated liquidus and experimental one, due to the presence of $Fe_1O_{1.5}$ species in the liquid phase.

The Fe_2O_3/Fe_3O_4-UO_2 pseudo-binary system has been considered without the new assumption of a liquid miscibility gap and the corrected eutectic temperature [2005Kis].

Finally, the refinement of the liquid interaction parameters between Fe_1O_1 and O_2U_1 and $Fe_1O_{1.5}$ and O_2U_1 will be mainly linked to the improvement of the description of the Fe_2O_3/Fe_3O_4-UO_2 pseudo-binary system.

At high temperatures (T > 2273 K), the ternary phase diagram is characterised by the following phase equilibria : L_1 + fcc_C1, L_1 + L_2 + fcc_C1, L_2 + fcc_C1, L_2 + G, L_2 + G + fcc_C1, L_1 + L_2.

[1969Ril] Fe_2O_3-O_2U_1 "The UO_2-Fe_2O_3 and PuO_2-Fe_2O_3 Systems in Air"
B.Riley
Transactions of the American Nuclear Society, Vol.12, pp.543-544, (1969).

[1997Kle] H. Kleykamp, "Phase equilibria in the UO_2-austenitic steel system up to 3000 °C"
Journal of Nuclear Materials, 247, (1997), 103-107.

[1998Hel] Fe_1O_1-O_2U_1 "The FeO-UO_2 System"
S.Helmann, M.Nie,
In vessel cluster INV-CIT(98)-M006, IPSN/DRS/SEMAR 98/36, Minutes of the 4th CIT Project Meeting, Pisa, (10th and 11th June 1998).

[2003Pet] Fe_1O_1-O_2U_1"Study of UO_2-FeO system at induction melting in inert atmosphere"
Y. Petrov,
A.P. Alexandrov Research Institute, second CORPHAD Meeting, St Petersburg, September 17, 2003.

[2004COR,VPA/IMCC]
Fe_1O_1-O_2U_1 "System UO -FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.

[2004COR,Galakhov]
Fe_1O_1-O_2U_1 "System UO -FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.

[2004COR,Galakhov,discarded]
Fe_1O_1-O_2U_1 "System UO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.

[2004COR,IMCC/EDX]
Fe_1O_1-O_2U_1 "System UO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.

[2005Kis] M. Kiselova, Y.B. Petrov, "New crystallization studies of UO_2-ZrO_2-Fe_3O_4 system and the presumed melting diagram",
SARNET meeting, Köln, February 2005.

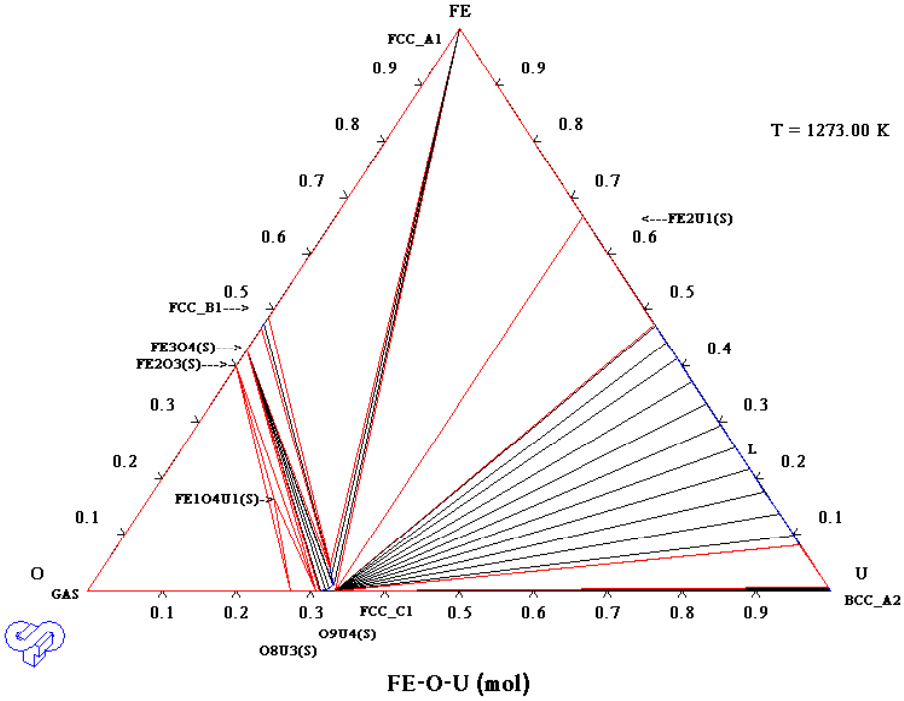

Figure 1 Calculated Fe-O-U isothermal section at 1273 K.

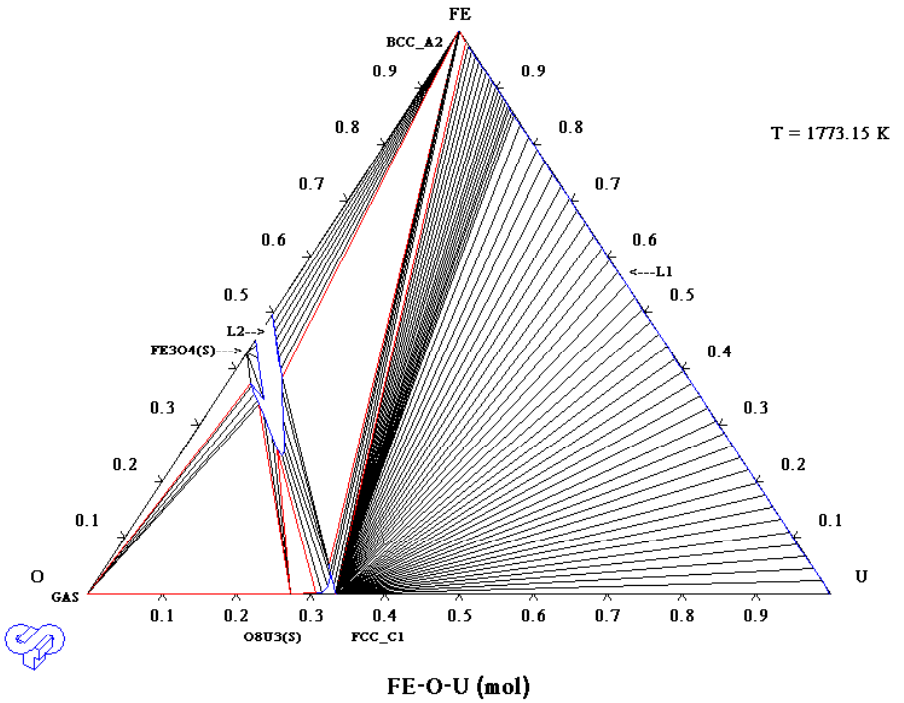

Figure 2 Calculated Fe-O-U isothermal section at 1773.15 K.

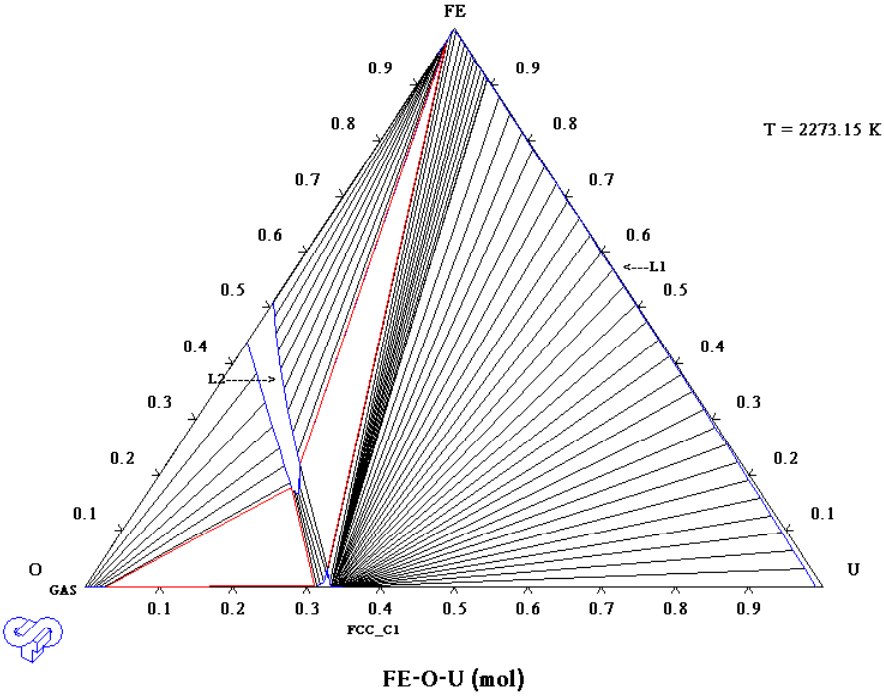

Figure 3 Calculated Fe-O-U isothermal section at 2273.15 K.

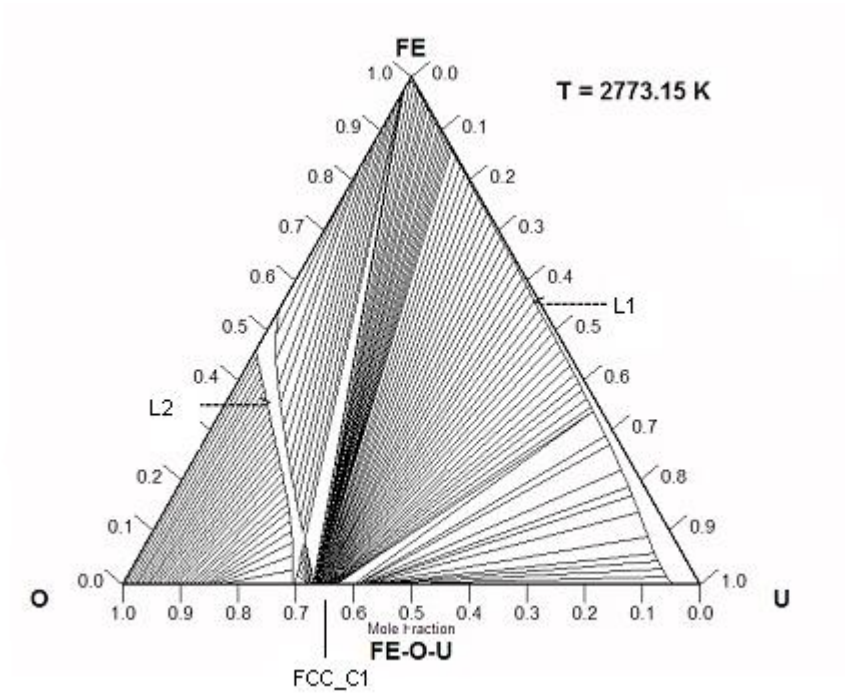

Figure 4 Calculated Fe-O-U isothermal section at 2273.15 K.

FE-O-ZR

The phase diagram of the Fe-O-Zr ternary system presents the following solutions and substances, with the symbols used in this work :

- the liquid phase, L, which shows a miscibility gap between an Fe-Zr rich metallic liquid (L_1) and an FeO/Fe_2O_3-ZrO_2 rich oxide liquid (L_2) ; it extends from the Fe-O side and closes at zirconium rich content ; it may also exist a liquid miscibility gap in the oxide field, observed in the Fe_2O_3/Fe_3O_4-ZrO_2 system between 2100 K and 2600 K, while there is a complete liquid miscibility in the FeO-ZrO_2 system.
- the ZrO_2 rich oxide solid solution, with the face-centred cubic structure, of CaF_2 (fluorite) type, Fm_3m, cF_{12}, noted fcc_C1, and which can dissolves until 18 mol% FeO in ZrO_2 ;
- the ZrO_2 rich oxide solid solution, with the tetragonal structure, noted tet_oxide, and which can dissolve until 7 mol% $Fe_1O_{1.5}$ in ZrO_2 ;
- the oxide solid solution, FeO_{1+x}, or wustite, with the face-centred cubic structure, of NaCl type, noted fcc_B1 ; no solubility of zirconia in wustite is reported ;
- the terminal zirconium rich solid solution, body cubic centred (bcc_A2), with a solubility of oxygen limited to about 10 at% and a solubility of iron limited to 5 at% ;
- the terminal zirconium rich solid solution, hexagonal closed packed (hcp_A3) with a solubility of oxygen limited to about 30 at% and a very small solubility of iron ;
- the terminal iron-rich solid solutions, bcc_A2 and fcc_A1, with a small solubility of zirconium and a negligible solubility of oxygen ;
- the intermediate non-stoichiometric Laves phase, Fe_2Zr_1(Laves) ;
- the pure solid oxides, Fe_3O_4(S) or magnetite, Fe_2O_3(S) or hematite, corundum, O_3U_1(S), O_8U_3(S), O_9U_4(S) ;
- the intermetallic compounds, $Fe_{765}Zr_{265}$(S), Fe_1Zr_2(S), Fe_1Zr_3(S) ;
- the pure solid zirconium oxide, with the allotropic form monoclinic O_2Zr_1(mon) ;
- the gas phase (G), which shows an extended solubility in oxygen of iron above 2800 K and of zirconium above 3000 K.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of the stoichiometric compounds $Fe_{0.947}O_1$(fcc_B1), $Fe_1O_{1.5}$(S), Fe_3O_4(S), Fe_2O_3(S), O_2Zr_1(fcc_C1, tet, mon), Fe_2Zr_1(Laves), $Fe_{765}Zr_{265}$(S), Fe_1Zr_2(S), Fe_1Zr_3(S) have been assessed in the individual sub-systems, as well as the thermodynamic modelling of all binary or pseudo-binary phases. The ternary liquid phase has been described by a non ideal associate model, with the formula $(Fe_1,Fe_1O_1,Fe_1O_{1.5},O_1,O_2Zr_1,Zr_1)_1$(L). The fcc_C1, tet_oxide and fcc_B1 solid solutions have been described with a one lattice model, whith the formula $(Fe_1O_1,O_2Zr_1)_1$(fcc_C1), $(Fe_1O_1,Fe_1O_{1.5},O_2Zr_1)_1$(tet_oxide) and $(Fe_1O_1,Fe_1O_{1.5})$(fcc_B1) respectively. The terminal iron-zirconium rich solid solutions, bcc_A2 and hcp_A3, have been described by a two-sublattice model, with the respective formula $(Fe_1,Zr_1)_1(O_1,\square)_3$(bcc_A2), and $(Fe_1,Zr_1)_1(O_1,\square)_{0.5}$(hcp_A3). The gas phase has been described by an ideal mixture of gaseous species, with the formula $(Fe_1, Fe_1O_1, Fe_1O_{1.5}, O_1, O_1Zr_1, O_2, O_2Zr_1, O_3, Zr_1, Zr_2)_1$ (G).

In the metal-oxygen field, the only used experimental information on phase diagram is located on the line Fe-ZrO_2 and gives the solubility of oxygen in iron rich-zirconium liquid alloys. (1873 K - 2073 K).

Most of the more recent experimental informations are located in the pseudo-binary vertical sections, FeO-ZrO_2 ([1997Fis], [1998Hel], [1999Bec], [2003Gus], [2004Cor]) coming from the CORPHAD international project, and Fe_2O_3/Fe_3O_4-ZrO_2 ([2003Pil], [2004Pet]) coming from the ECOSTAR international project.

The main features of the FeO-ZrO_2 isopleth section [2004Cor] are a complete solubility between FeO and ZrO_2 in the oxide liquid (L_2), and a non negligible solubility of iron oxide in the ZrO_2 rich fcc_C1 and tet_oxide solid solutions.

The eutectic temperature was located in the temperature range 1588 – 1603 K (1315 – 1330 °C) and the corresponding composition 10.26 mol% ZrO_2 (16.4 wt%). The solubility of iron oxide in

tetragonal ZrO_2, tet_oxide, is about 2.2 mol% FeO (1.3 wt%) at the eutectic temperature. The solubility of iron oxide in cubic ZrO_2, fcc_C1, is about 8-12 mol% FeO (5-7 wt%) in the temperature range 2073-2373 K (1800 – 2100 °C).

The Fe_2O_3/Fe_3O_4-ZrO_2 isopleth section has been experimentally studied in the ECOSTAR project ([2003Pil], [2004Pet]). It shows a miscibility gap in the liquid state, located between the monotectic temperature 2143 K (1870 °C) and the critical point 2483 K (2210 °C), and an eutectic temperature at 1798 K (1525 °C). There is a non negligible solubility of $FeO_{1.333}$ in tetragonal ZrO_2, tet_oxide, the maximal one being about 6.6 wt% Fe_3O_4 at the monotectic temperature. The solid solubility of Fe_3O_4 in cubic ZrO_2, fcc_C1, and of ZrO_2 in Fe_3O_4 are less than 2.5 wt%.

In a first approximation, the excess interaction parameters between Fe_1O_1 and O_2Zr_1 on the one hand and $Fe_1O_{1.5}$ and O_2Zr_2 on the other hand have been estimated by assuming the pseudo-binary sections as quasi-binary ones. The real isothermal or isopleth sections may be than calculated from the complete thermodynamic modelling. The main features of the FeO-ZrO_2 pseudo-binary system are qualitatively and quantitatively well represented. The Fe_2O_3/Fe_3O_4-ZrO_2 calculated isopleth differs from the experimental one due to the presence of the Fe_1O_1 species in the liquid, and the excess interaction parameter between $Fe_1O_{1.5}$ and O_2Zr_1 should be refined to represent the experimental liquid miscibility gap.

At high temperatures (T > 2273 K), the ternary phase diagram is characterised by the following phase equilibria : L_1 + fcc_C1, L_1 + L_2 + fcc_C1, L_2 + fcc_C1, L_2 + G, L_2 + G + fcc_C1, L_1 + L_2 .

[1957Fis] Fe_1O_1-O_2Zr_1 "Gleichgewichtsuntersuchungen im System Eisen(II)-oxyd-Zirkonoxyd"
Von W.A. Fischer, A. Hoffmann,
Archiv Eisenh□tten, Vol.28, N°11, pp.739-743 (1957).

[1998Hel]crust
Fe_1O_1-O_2Zr_1 "The FeO-ZrO_2 System"
S. Helmann, M. Nie,
In vessel cluster INV-CIT(98)-M006, IPSN/DRS/SEMAR 98/36, Minutes of the 4th CIT Project Meeting, Pisa (10th and 11th June 1998).

[1998Hel]thermocouple
Fe_1O_1-O_2Zr_1 "The FeO-ZrO_2 System"
S. Helmann, M. Nie,
In vessel cluster INV-CIT(98)-M006, IPSN/DRS/SEMAR 98/36, Minutes of the 4th CIT Project Meeting, Pisa (10th and 11th June 1998).

[1999Bec] Fe_1O_1-O_2Zr_1 "The FeO-ZrO_2 System"
S. Bechta,
Private communication

[2003Gus] Fe_1O_1-O_2Zr_1 "Phase diagram of the ZrO_2-FeO system"
V. Gusarov,
Alexandrov Research Institute of Technology NITI, second CORPHAD Meeting, St Petersburg, September 17, 2003.

[2003Pil] $Fe_1O_{1.5}$-O_2Zr_1 "The Fe_3O_4-ZrO_2 pseudo-binary system"
P. Piluso,
Note Technique DTP/STH/LMA-03/001

[2004COR]Figure
Fe_1O_1-O_2Zr_1 "FeO-ZrO_2 Phase diagram (CORPHAD measurements)"
M. Barrachin,
Private communication, october 2004.

[2004COR]VPA/IMCC
Fe_1O_1-O_2Zr_1 "System ZrO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.

[2004COR]VPA/Galakhov
Fe_1O_1-O_2Zr_1 "System ZrO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.

[2004COR]DTA
Fe_1O_1-O_2Zr_1 "System ZrO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.
[2004COR]DSC
Fe_1O_1-O_2Zr_1 "System ZrO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.
[2004COR]IMCC/EDX
Fe_1O_1-O_2Zr_1 "System ZrO_2-FeO"
V.B. Khabensky et al.,
ISTC Project-1950.2 CORPHAD, NITI Progress report, October 2004.
[2004Pet] $Fe_1O_{1.5}$-O_2Zr_1 "New miscibility gap for ex-vessel corium oxide compositions"
Y. Petrov, Y. Udalov, K. Jurek, P. Sazavski, M. Kiselova, P. Selucky, C. Journeau, P. Piluso,
Proceeding of ICAPP'04, Pittsburgh, PA USA, June 13-17, 2004, Paper 4077.
[2004Pet]1Liquid
$Fe_1O_{1.5}$-O_2Zr_1 "New miscibility gap for ex-vessel corium oxide compositions"
Y. Petrov, Y. Udalov, K. Jurek, P. Sazavski, M. Kiselova, P. Selucky, C. Journeau, P. Piluso,
Proceeding of ICAPP'04, Pittsburgh, PA USA, June 13-17, 2004, Paper 4077.
[2004Pet]estimated
$Fe_1O_{1.5}$-O_2Zr_1 "New miscibility gap for ex-vessel corium oxide compositions"
Y. Petrov, Y. Udalov, K. Jurek, P. Sazavski, M. Kiselova, P. Selucky, C. Journeau, P. Piluso,
Proceeding of ICAPP'04, Pittsburgh, PA USA, June 13-17, 2004, Paper 4077.

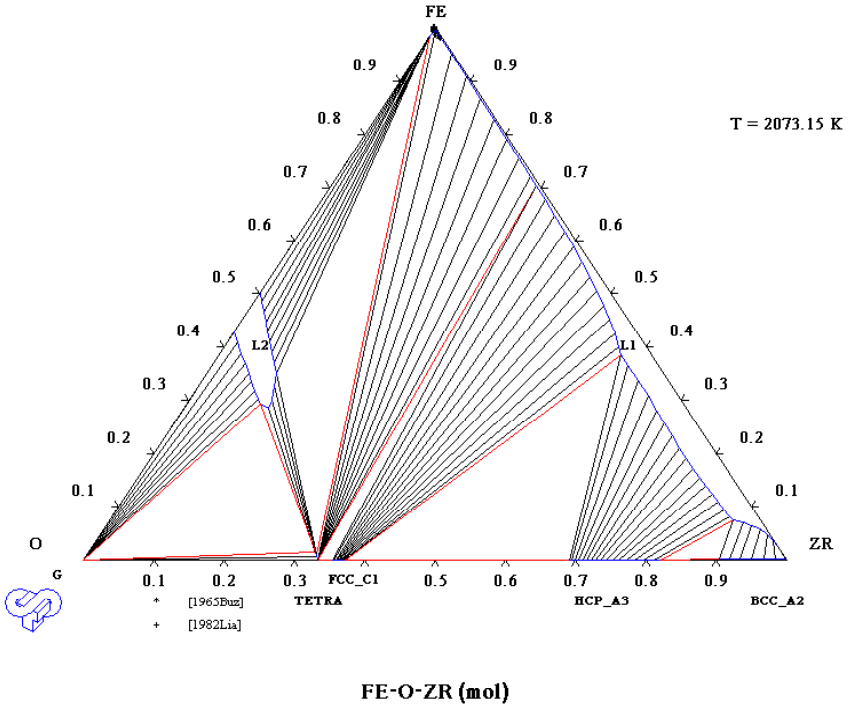

Figure 1 **Calculated Fe-O-Zr isothermal section at 2073.15 K.**

[1965Buz] Fe-O-Zr " "
Z. Buzek,A. Hutla,
Sbornik VSB Ostrave, (Hutuicka), 11, 383 (1965).
[1982Lia] Fe-O-Zr "Solubility of Oxides in Liquid Alloys Containing Titanium and Zirconium",
W.W. Liang,W. Schuster,
Transactions of the Japan Institute of Metals, 23(7), 368-377 (1982).

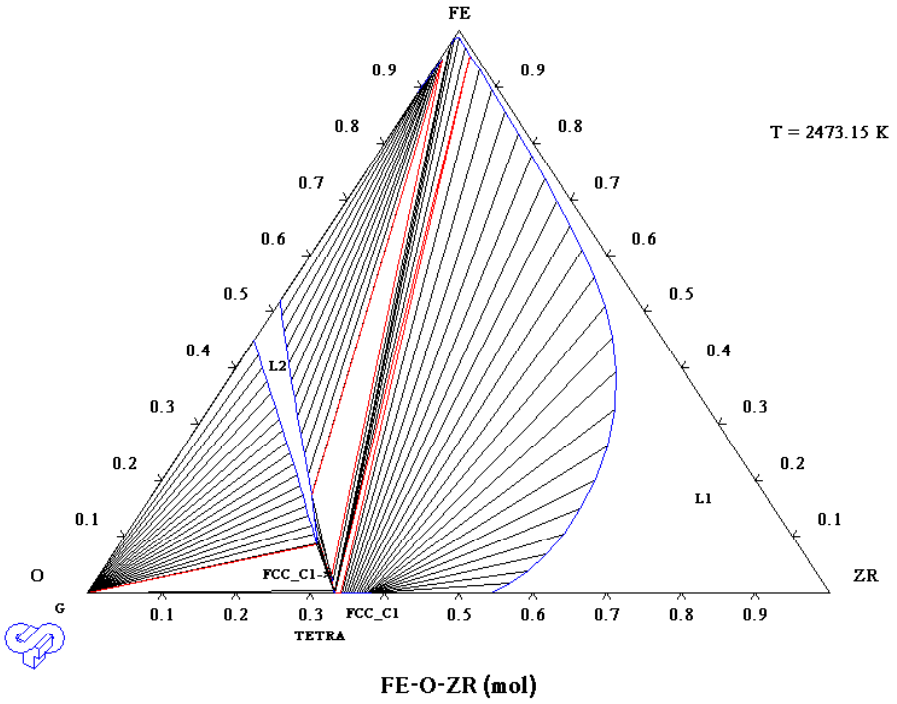

Figure 2 Calculated Fe-O-Zr isothermal section at 2473.15 K.

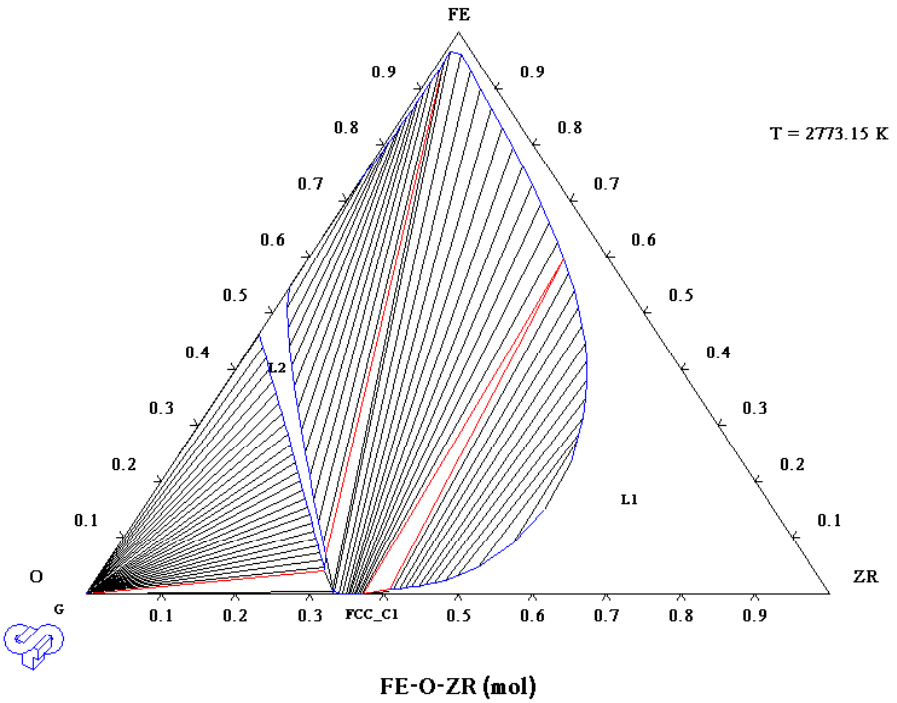

Figure 3 Calculated Fe-O-Zr isothermal section at 2773.15 K.

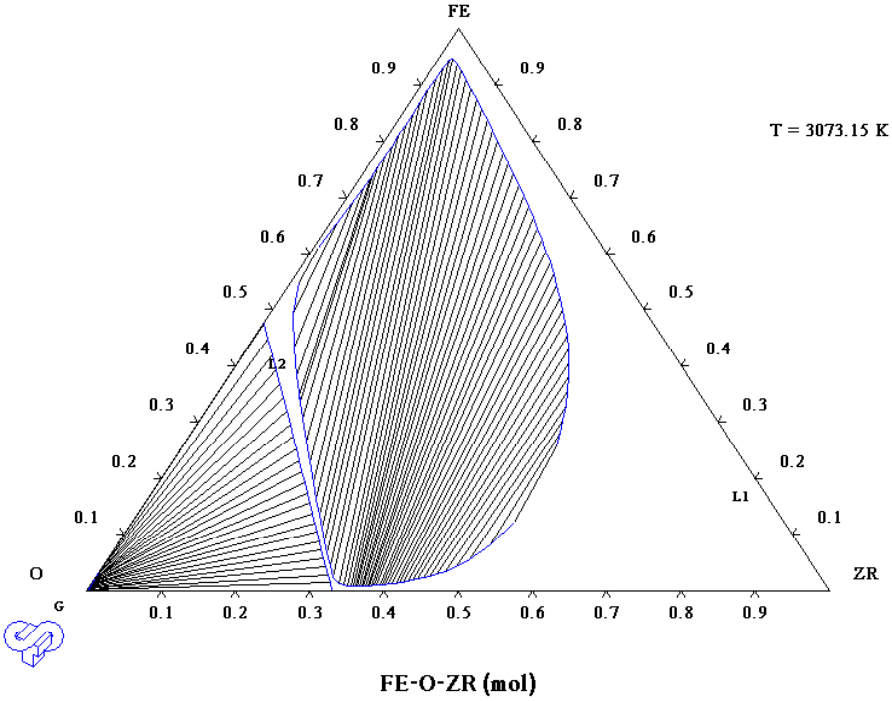

Figure 4 Calculated Fe-O-Zr isothermal section at 3073.15 K.

FE-U-ZR

The phase diagram of the Fe-U-Zr ternary system presents the following condensed solutions and substances, with the symbols used in this work or found in open literature :

- the liquid phase, L, which shows a complete miscibility between all elements ;
- the intermetallic Laves phase, Fe_2(U, Zr)(Laves), which shows a miscibility gap at low temperature between a Fe_2U_1 rich Laves phase and a Fe_2Zr_1 rich Laves phase ;
- the terminal iron rich solid solutions, body cubic centred, bcc_A2, and face cubic centred, fcc_A1, with a negligible solubility of uranium and a small solubility of zirconium ;
- the terminal uranium-zirconium solid solution, body cubic centred, bcc_A2, with a limited solubility of iron ;
- the terminal uranium rich solid solution, tetragonal (tet_metal), with a very small solubility of iron and zirconium ;
- the terminal uranium rich orthorhombic solid solution, ort_A20, with a negligible solubility of iron and a very small solubility of zirconium ;
- the terminal zirconium rich solution, with the hexagonal closed packed structure, hcp_A3, and a very small solubility of iron and uranium ;
- the intermetallic solid solution, δ, which extents from 64 to 78 at % Zr ;
- the binary intermetallic compounds, Fe_1U_6(S), $Fe_{765}Zr_{265}$(S), Fe_1Zr_2(S) and Fe_1Zr_3(S) ;
- the ternary intermetallic compounds, $Fe_{0.333}U_{0.25}Zr_{0.417}(\varepsilon)$, $Fe_{0.06}U_{0.71}Zr_{0.23}(\lambda)$, $Fe_{0.50}U_{0.18}Zr_{0.32}(\chi)$.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of substances, Fe_2U_1(Laves), Fe_1U_6(S), Fe_2Zr_1(Laves), $Fe_{765}Zr_{265}$(S), Fe_1Zr_2(S) and Fe_1Zr_3(S) have been assessed in the individual sub-systems, as well as the thermodynamic modelling of all binary phases. The liquid, bcc_A2, fcc_A1, hcp_A3 phases (ϕ) have been described by a non ideal substitutional model, with the formula $(Fe_1,U_1,Zr_1)(\phi)$. The intermetallic Laves phase, Fe_2(U,Zr)(Laves), has been described by a two-sublattice model, with the formula $(Fe_1, U_1, Zr_1)_2(Fe_1, U_1, Zr_1)_1$. In order to reproduce the non-stoichiometric field in the Fe-Zr binary system. The thermodynamic properties of the three ternary intermetallic compounds, $Fe_{0.333}U_{0.25}Zr_{0.417}(\varepsilon)$, $Fe_{0.06}U_{0.71}Zr_{0.23}(\lambda)$, $Fe_{0.50}U_{0.18}Zr_{0.32}(\chi)$ have been estimated from the phase diagram information. The gas phase has been described by an ideal mixture of gaseous species, with the formula $(Fe_1, U_1, Zr_1, Zr_2)_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- the ternary intermetallic compounds are reproduced in accordance with experimental phase diagram at temperatures below 1000 K ;
- the miscibility gap in the ternary Laves phase is present up to 1373 K ;
- above 1573 K, the only solid phases are the Fe_2Zr_1 rich Laves phase, the iron rich (fcc_A1, bcc_A2) and uranium-zirconium rich (bcc_A2) solution phases. Then, the liquid domain is more and more extended, pure iron melts at 1811 K, pure Fe_2Zr_1 at 1950 K, and pure zirconium at 2128 K. There is no available experimental information at high temperature (T > 1500 K).

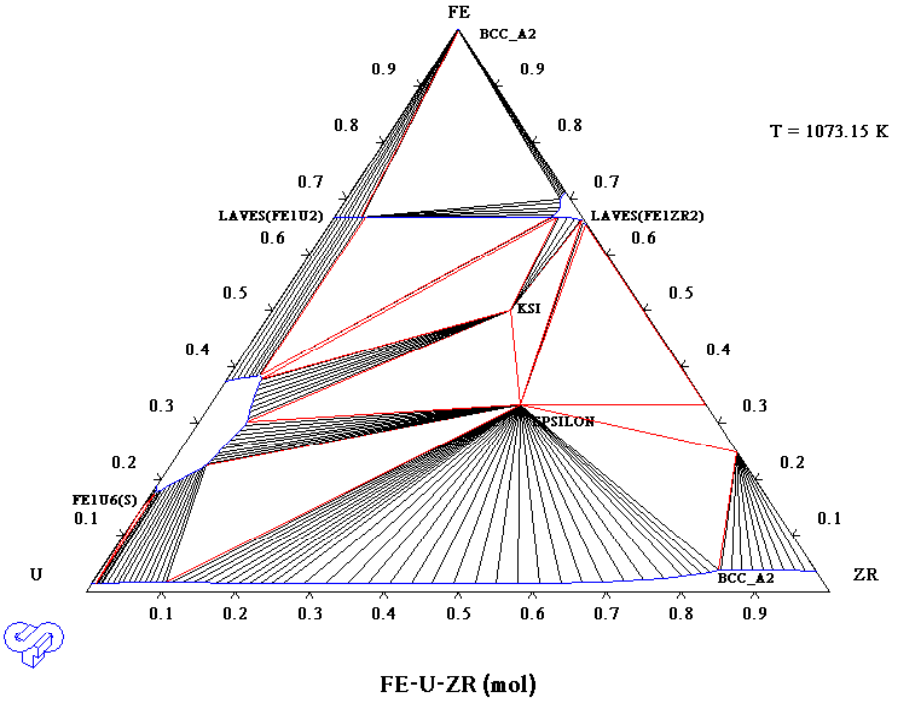

Figure 1 Calculated Fe-U-Zr isothermal section at 1073.15 K.

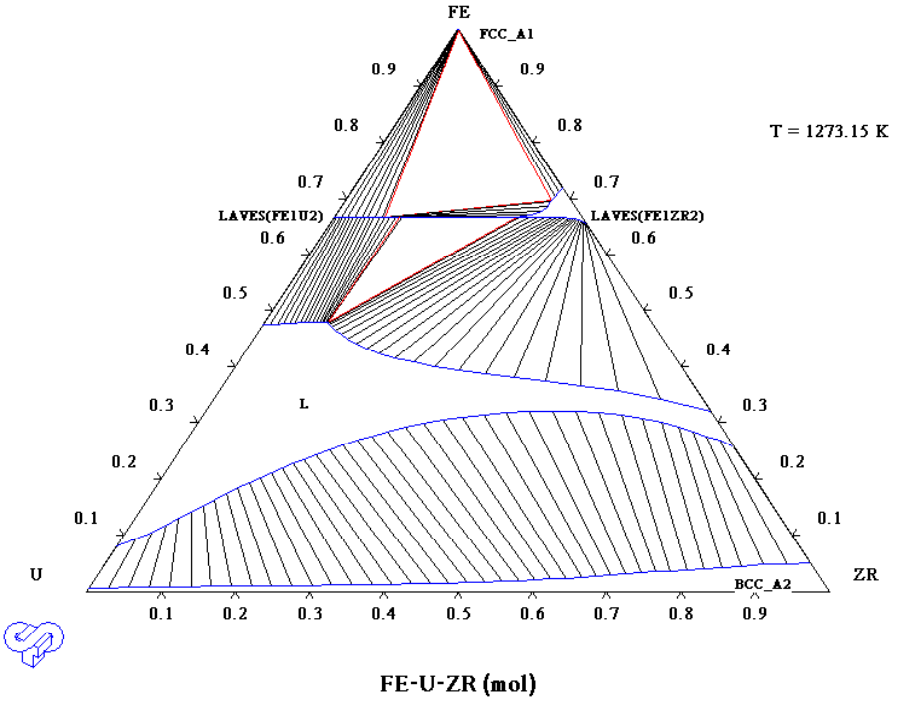

Figure 2 Calculated Fe-U-Zr isothermal section at 1273.15 K.

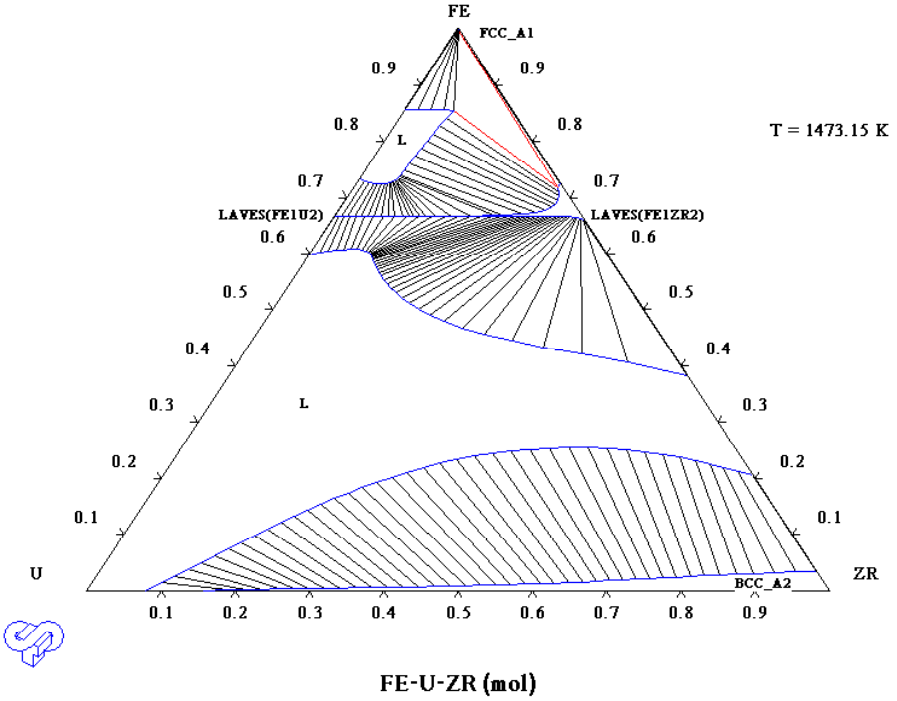

Figure 3 Calculated Fe-U-Zr isothermal section at 1473.15 K.

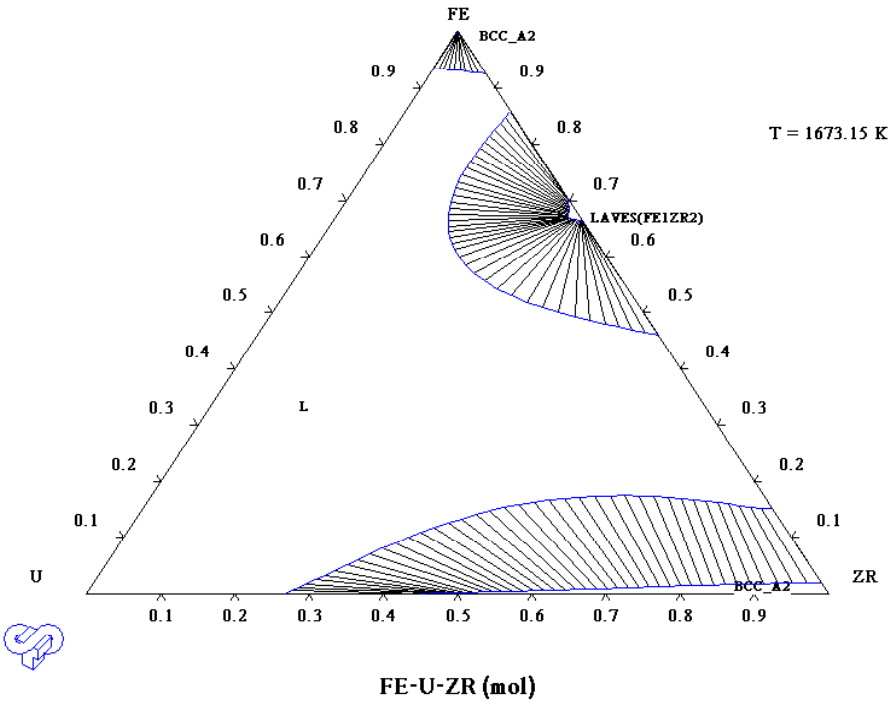

Figure 4 Calculated Fe-U-Zr isothermal section at 1673.15 K.

O-U-ZR

The phase diagram of the O-U-Zr ternary system presents the following solutions and substances, with the symbols used in this work :

- the liquid phase, L, which shows a miscibility gap between an uranium-zirconium rich metallic liquid (L_1) and a UO_2-ZrO_2 rich oxide liquid (L_2) ; the miscibility gap is closed at high zirconium content ;
- the oxide solid solution, $(U,Zr)O_{2+x}$, with the face-centred cubic structure, of CaF_2 (fluorite) type, Fm_3m, cF_{12}, noted fcc_C1 ;
- the terminal zirconia rich solid solution, $(U,Zr)O_2$, tetragonal, tet_oxide, with a solubility of O_2U_1 limited to about 23 mol% ;
- the terminal uranium-zirconium rich solid solution, body cubic centred, bcc_A2, with a limited solubility of oxygen on the O-Zr side, showing a complete miscibility at high temperature and a small miscibility gap deported on the uranium side between 950 K and 1000 K in the U-Zr system ;
- the terminal zirconium rich hexagonal closed packed solid solution, hcp_A3, with a solubility of oxygen limited to about 10 at% and 30 at% respectively, and a small solubility of uranium (< 3 at%) ;
- the intermediate solid oxides, O_3U_1(S), O_8U_3(S), O_9U_4(S) ;
- the pure solid oxide, with the allotropic form monoclinic, O_2Zr_1(mon) ;
- pure solid uranium, with a negligible solubility of oxygen, and different allotropic structures, orthorhombic, U_1(ort_A20), tetragonal, U_1(tet) ;
- the terminal uranium rich solid solutions, orthorhombic, ort_A20, and tetragonal, tet_metal, with a small solubility of zirconium ;
- the intermetallic solid solution, δ, which extents from 64 to 78 at% Zr ;
- the gas phase, which shows an extended solubility of uranium above 2000 K and zirconium above 3000 K.

The fundamental thermodynamic properties (Cp, ΔH_{298}, S_{298}) of substances, O_3U_1(S), O_8U_3(S), O_9U_4(S), O_2U_1(fcc_C1), O_2Zr_1(fcc_C1, tet, mon), have been assessed in the individual sub-systems, as well as the thermodynamic modelling of all binary or pseudo-binary phases. The liquid phase has been described by a non ideal associate model, with the formula (O_1, O_2U_1, O_2Zr_1, U_1,Zr_1)(L). The solid solution $(U,Zr)O_{2+x}$ has been described by a three sublattice model, with the formula $(U_1, Zr_1)_1(O_1, \square)_2(O_1, \square)_1$(fcc_C1), and simplified in a simple one lattice model, with the formula (O_1, O_2U_1, O_2Zr_1, U_1, $Zr_1)_1$(fcc_C1), in order to be compatible with the whole thermodynamic database and to allow the introduction of iron and selected fission products, Ba, La and Sr. The terminal uranium-zirconium rich solid solutions, bcc_A2 and hcp_A3, have been described by a two sublattice model, with the respective formula $(U_1, Zr_1)_1(O_1, \square)_3$(bcc_A2), and $(U_1, Zr_1)_1(O_1, \square)_{0.5}$(hcp_A3). The gas phase has been described by an ideal mixture of gaseous species, with the formula (O_1, O_1U_1, O_1Zr_1, O_2U_1, O_2Zr_1, O_2, O_3, O_3U_1, U_1, Zr_1, $Zr_2)_1$(G).

The comparison of the calculated thermodynamic properties and phase diagram with the experimental information leads to the following conclusions :

- on a qualitative point of view, the overall topology of the O-U-Zr ternary phase diagram is in agreement with the experimental data between 1273 K and 3173 K ;
- on a quantitative point of view, the solubility of oxygen in uranium-zirconium liquid alloys, the liquid miscibility gap and the liquidus temperatures are in agreement with the selected experimental data ;
- the remaining uncertainties are the accurate shape of the diphasic domain L_1 + fcc_C1 between 2000 K and 2500 K, the liquidus temperatures in the zirconium rich domain, the solidus temperatures, and the presence of an hyper-stoichiometric liquid at low temperatures, resulting from necessary improvement of the hyper-stoichiometric O-U region.

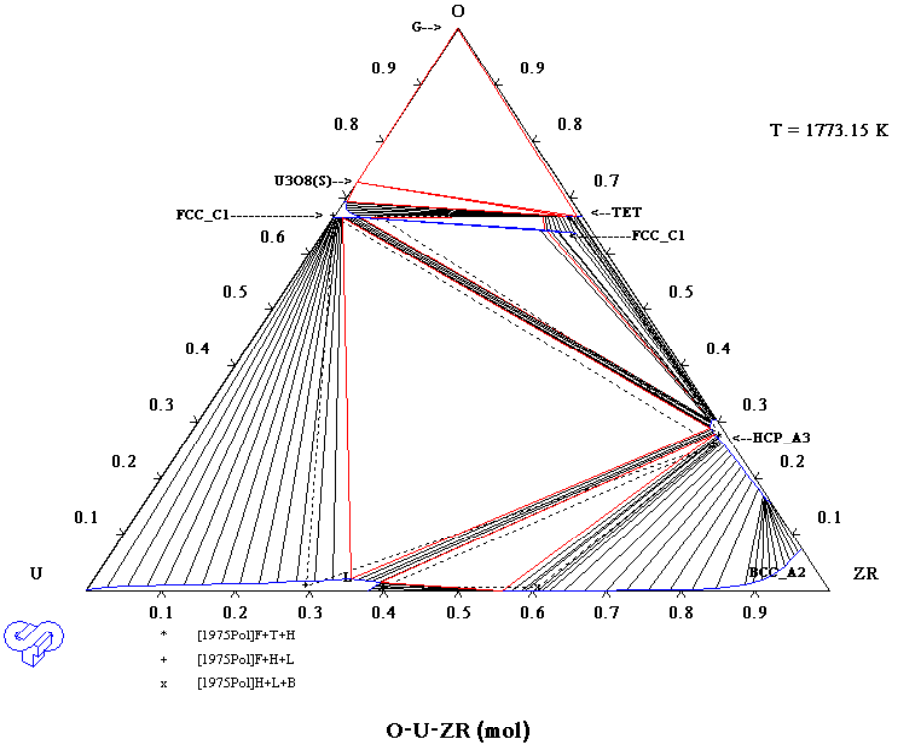

Figure 1 **Calculated O-U-Zr isothermal section at 1773.15 K.**

[1975Pol]F+T+H
[1975Pol]F+H+L
[1975Pol]H+L+B

"Untersuchungen in dreistoffsystem uran-zirkon-sauerstoff"
C. Politis
Kernforschungszentrum Karlsruhe, KFK 2167, 1-53 (1975).

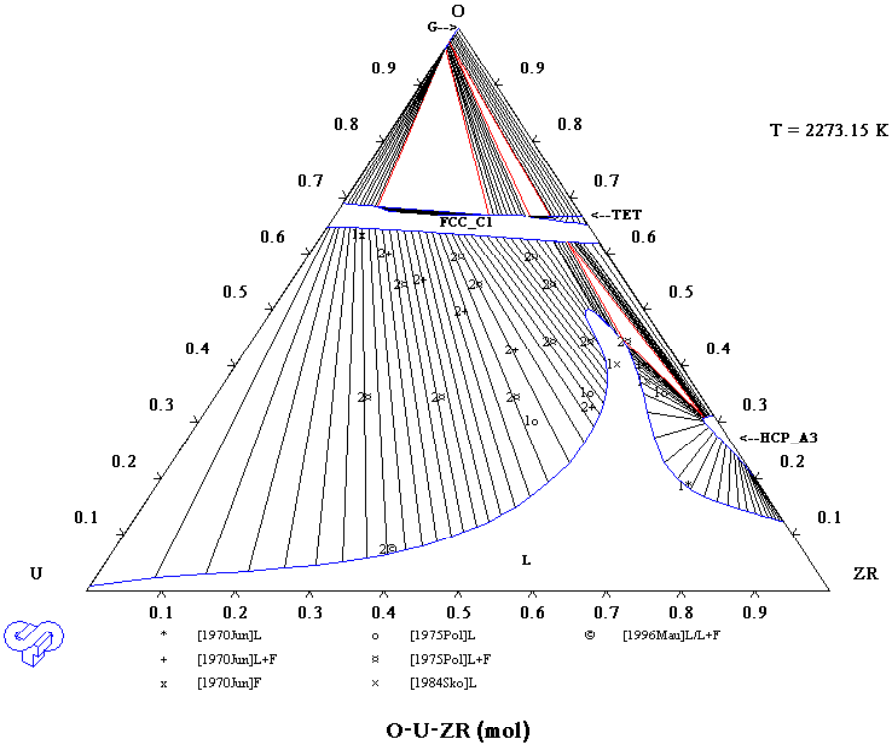

Figure 2 **Calculated O-U-Zr isothermal section at 2773.15 K.**

[1970Jun]L
[1970Jun]L+F
[1970Jun]F
"Untersuchungen in dreistoffsystem uran-zirkon-sauerstoff"
E.F. Junke and J.F. White
GEMP-731 (1970).

[1975Pol]L
[1975Pol]L+F
"Untersuchungen in dreistoffsystem uran-zirkon-sauerstoff"
C. Politis
Kernforschungszentrum Karlsruhe, KFK 2167, 1-53 (1975).

[1984Sko]L
"On the reaction between UO_2 and Zr"
A. Skokan
5th Int. Meeting "Thermonuclear reactor safety", Karlsruhe (september 9-13 1984).

[1996Mau]L/L+F
"Experimental determination of the liquidus L/(U,Zr)O_{2-x} in the (U,Zr,O) system at 2273K"
A Maurisi, C. Gueneau, P. Perodeaud, B. Schneider, O. Dugne, F. Valin and G. Bordier, Euromat (October 1996)

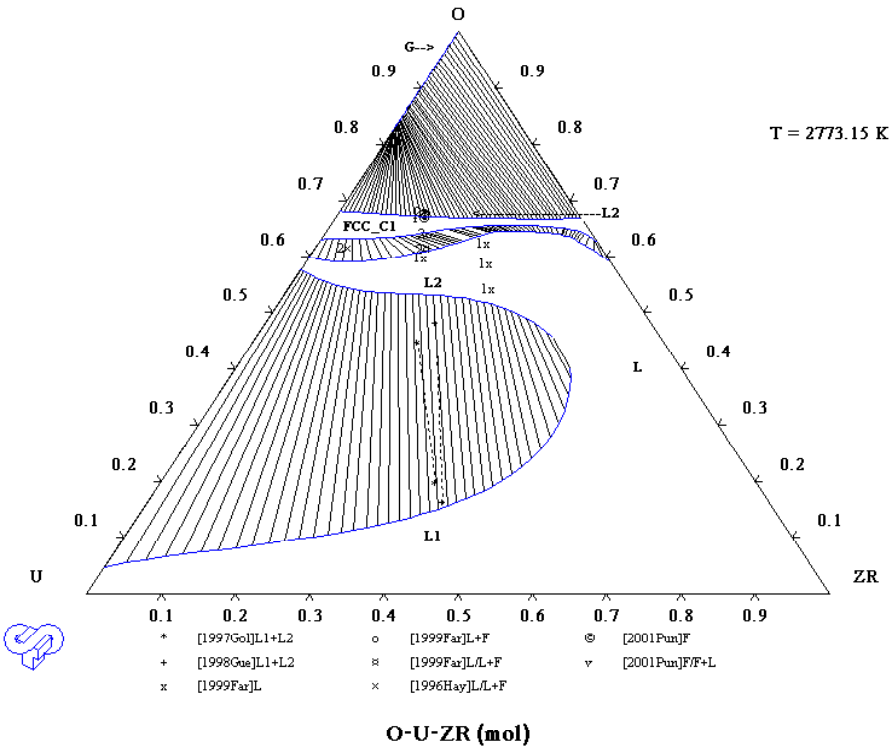

Figure 3 **Calculated O-U-Zr isothermal section at 2773.15 K.**

[1997Gol]L1+L2
"DPEA/SPEA Experiments"
S. Golstein et al.
Private communication, 1997

[1998Gue]L1+L2
"DPEA/SPEA Experiments"
C. Gueneau, V. Dauvois, P. Pérodeaud, C. Gonella, O. Dugne,
Journal of Nuclear Materials, 254 (1998) 158.

[1999Far]L
[1999Far]L+F
[1999Far]L/L+F
"Final report on severe accident material property measurements,"
M.T. Farmer, L.M. McUmber, R.W. Aeschlimann and B.W. Spencer,
ANL-NT TECHNICAL MEMORUNDUM N° 88, October 1998.

[1996Hay]L/L+F
"Dissolution of UO_2 in molten zircalloy-4 :
Part3 : solubility from 2000 to 2500°C.
Part 4 : phase evolution during dissolution and cooling of 2000 to 2500°C specimens"
P.J. Hayward and I.M. George
Journal of Nuclear Materials, 232, 1, 1-22 (1996)

[2001Pun]F
[2001Pun]F/F+L
"AEAT"
AEA,
ENTHALPY Private communication

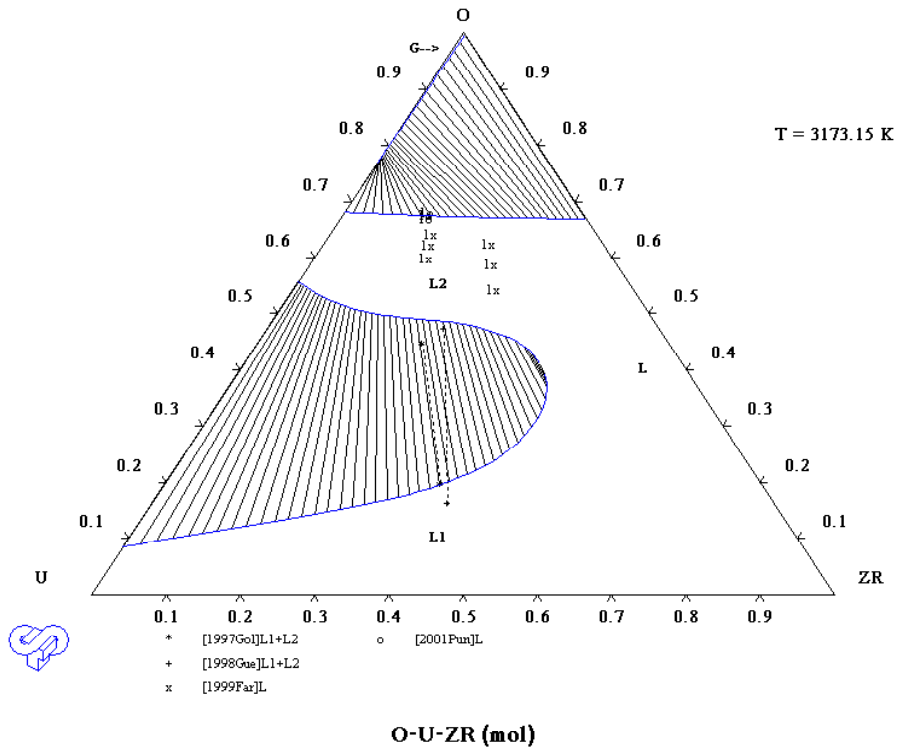

Figure 4 **Calculated O-U-Zr isothermal section at 3173.15 K.**

[1997Gol]L1+L2
"DPEA/SPEA Experiments"
S. Golstein et al.,
Private communication, 1997

[1998Gue]L1+L2
"DPEA/SPEA Experiments"
C. Gueneau, V. Dauvois, P. Pérodeaud, C. Gonella, O. Dugne,
Journal of Nuclear Materials, 254 (1998) 158.

[1999Far]L
"Final report on severe accident material property measurements,"
M.T. Farmer, L.M. McUmber, R.W. Aeschlimann and B.W. Spencer,
ANL-NT TECHNICAL MEMORUNDUM Nø 88, October 1998.

[2001Pun]L
"AEAT"
AEA,
ENTHALPY Private communication

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