

FUELBASE, TAF-ID DATABASES AND OC SOFTWARE: ADVANCED COMPUTATIONAL TOOLS TO PERFORM THERMODYNAMIC CALCULATIONS ON NUCLEAR FUEL MATERIALS

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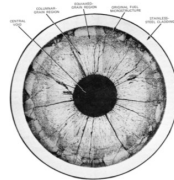


AIM

- To develop a **thermodynamic database** as a **computational tool** to perform thermodynamic calculations on advanced fuel materials using the Calphad method
 - ➔ **Phase diagrams + Thermodynamic properties of the phases**
- To facilitate the **exchange** on the models, review of experimental data, softwares, assessments
....

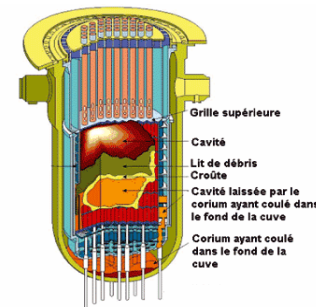
CONTEXT ➔ Fuel materials for Generation 2,3 & 4 reactors

- **Fuels**
 - UO_2 , $(\text{U,Pu,Am,Np})\text{O}_2$, $(\text{U,Th})\text{O}_2$, (U,Pu,Zr,Am,Np) , UN, $(\text{U,Pu})\text{C}$
- **Fission products**
 - Ba, Sr, Mo, Zr, Lanthanides (Ce, La, Nd, Gd), metallic FPs (Pd, Ru, Rh, Te), Volatile (Cs, I, Te)
- **Structural materials**
 - Fe-Cr-Ni, Zr alloys, Fe-Cr-Al-Y, Concrete (SiO_2 -CaO- Fe_xO_y - Al_2O_3 -MgO), SiC, B_4C

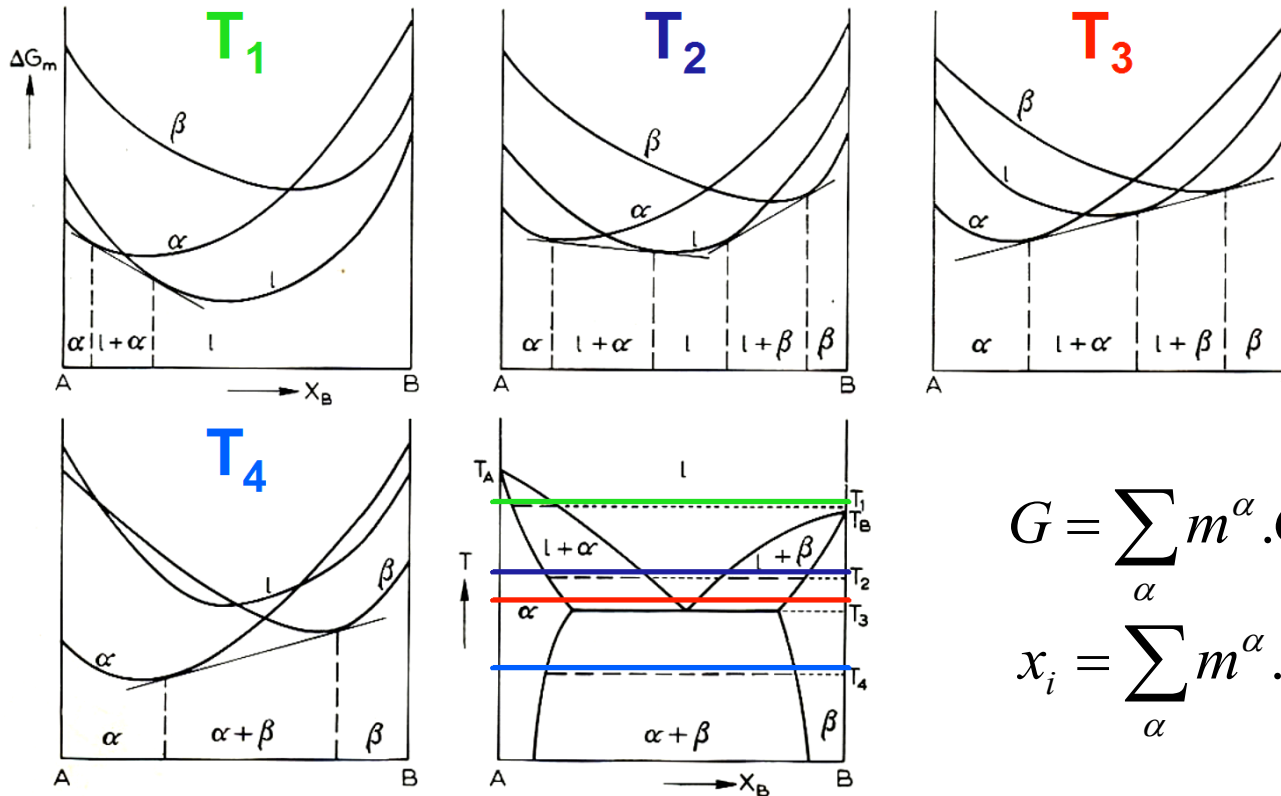


APPLICATIONS

- **Fuel behaviour at high temperature under normal and off-normal conditions**
 - Influence of the **Minor Actinides** on the fuel thermodynamic properties
 - **Fission product** « chemistry »
 - **Solid/liquid** phase transition
 - **Vaporization**
- **Fuel / cladding chemical interaction at high temperature**
- **Fuel fabrication**



The thermodynamic equilibrium is calculated by minimizing the Gibbs energy of the system

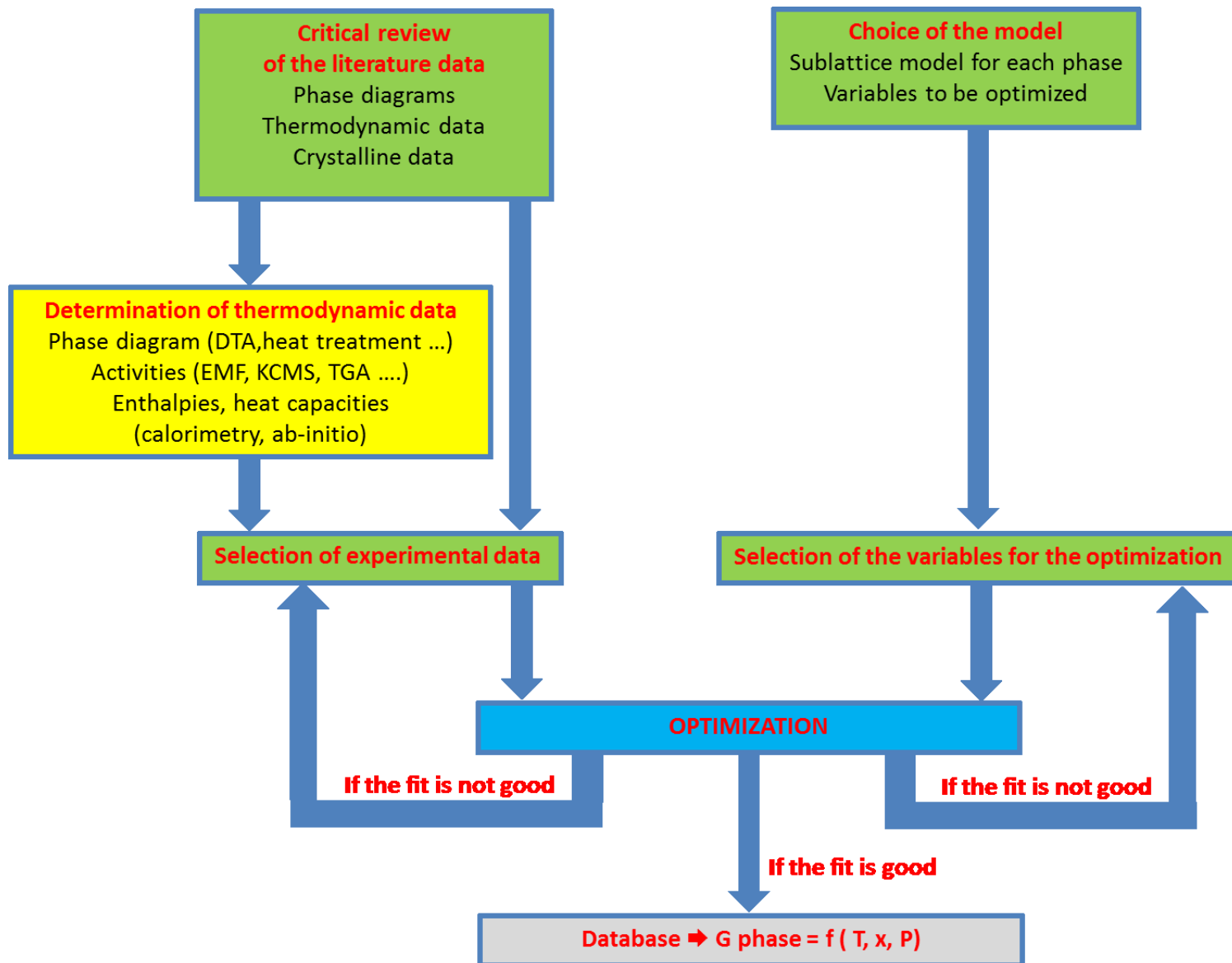


$$G = \sum_{\alpha} m^{\alpha} \cdot G_m^{\alpha}$$

$$x_i = \sum_{\alpha} m^{\alpha} \cdot x_i^{\alpha}$$

➔ $\min(G) = \min \left(\sum_{\alpha} m^{\alpha} G_m^{\alpha} (T, p, x_i^{\alpha} \text{ or } y_k^{(l,\alpha)}) \right)$

CALPHAD METHOD



FUELBASE DATABASE FOR ADVANCED NUCLEAR FUEL MATERIALS (2005-2012)

FUELBASE was a collaboration between CEA, Calcul Thermo, ITU, NRG and ORNL and served as the model for the expanded TAF-ID project

Am	C	Cr	Mo	N	Nb	Np	O	Pu	Re	Ru	Si	Ta	Ti	U	V	W	Zr
Am						Kurata 10	Gotcu 10	Dupin 07						Kurata 10			
	C	Anderson 87	Andersson 88	SGTE	Lee 01		SGTE	CEA 10	Dupin 07		Grobner 96	Frisk 96	Dumitrescu 98	Dupin 09	Huang 91	Jonsson 93	Guillemet 95
		Cr	Frisk 88	Frisk 91			Taylor 90	Dupin 06			Coughanowr 94		Saunders 98	Dupin 05	Lee 92		Zeng 98
			Mo	Frisk 91			Sundman 07	Dupin 05	Dupin 08		Liu 05		Chung 99	Dupin 06			Jerlerud 03
				N			SGTE	Sundman 05			Hillert 92		Jonsson 96	Chevalier 00	Ohtani 91		Ma 04
					Nb			Berche 09			Shao 04			Liu 08			Guillemet 91
						Np	Benes 09	Dupin 08						Kurata 10			
							O	Gueneau 08			Halsted 93		Sundman 05	Gueneau			Liang 01
								Pu	Berche 08	Dupin 08	Dupin 05	Berche 09	Dupin 06	Kurata 99	Berche 09	Berche 08	Kurata 99
									Re		Dupin			Berche 08		Dupin	
										Ru				Dupin 08			
											Si	Vahmas 89	Selfert 00	Berche 09		Vahmas 89	Gueneau 94
												Ta		Berche 09			
													Ti	Rado 06	Saunders 98		Kumar 94
														U	Berche 09	Sundman 07	Chevalier 04



JRC - Institute for Transuranium Elements



2013-2016: Thermodynamics of Advanced Fuels – International Database

➡ The aim is to make available a comprehensive, internationally recognised and quality-assured thermodynamic database for advanced fuels

		Programme Review Group	
Country	Signatory	Representative	Alternate Member
Canada	CNL, RMCC, UOIT	M. Piro	E.C. Corcoran
France	CEA	C. Guéneau (Chair)	J.-C. Dumas
Japan	JAEA, CRIEPI	M. Kurata	T. Ogata
The Netherlands	NRG	R. Hania	G.-J. de Haas
Rep. Of Korea	KAERI	B.-O. Lee	J.-H. Kim
USA	DOE	T. Besmann (Vice-Ch)	P. Turchi

■ The TAF-ID database is being built by **merging existing databases**

■ N. Dupin (consultant) is responsible for maintenance and documentation

■ Coordinated by S. Massara from OECD/NEA ➡ <http://www.oecd-nea.org/science/taf-id>

DATABASES DEVELOPED BY THE PARTNERS

Country	Software	Chemical system	Model
Canada AECL RMC UOIT	<i>FACTSAGE</i>	Fuel $UO_2 + Np, Pu + \text{Coolant } H_2O$ FPs: (Kr), Rb, Sr, Y, Zr, Mo, Tc, Ru, Rh, Pd Te, I, Xe, Cs, Ba, La, Ce, Pr, Nd	302 comp. 17 solutions
France CEA	<i>Thermo-Calc</i>	Fuel $UO_2, MOX+Am,Np,(U,Pu,Zr), (U,Pu)C, (U,Pu)N$ FPs: Ag, Ba, Cs, I, La, Mo, Nb, Ru, Sr, Te Materials: Concrete, B-C, Fe-Cr-Ni, SiC,Ta, W, V	Solutions 561 binaries 30 ternaries
Japan JAEA, CRIEPI	<i>Thermo-Calc</i>	Metallic fuel: Am-Cd-Ce-Fe-Gd-La-Nd-Np-Pr-Pu-U-Y-Zr Oxide fuel: Pu-Zr-O, Fe-B-C-O	Solutions
Netherlands NRG	<i>FACTSAGE</i>	Fuel: (U, Pu, Am, Np, Th)-(C, N, O) FPs: Ag, Ba, Br, Ce, Cs, Eu, I, La, Mo, Nb, Nd, Pd, Rb, Ru, Sb, Sn, Sr, Te, Y, Zr Materials: Fe, Ni, Si, Ti, Ta, W, Zn + Na, H, Pb	727 comp.
USA ORNL LLNL	<i>FACTSAGE</i> <i>Thermo-Calc</i>	$UO_2 + RE: Pu-U-Gd-Ce-La-O$ Metallic fuel: Am-Pu, Mo-Pu, Mo-U, Nb-U, Nb-Zr, Pu-U, Ti-U, U-Zr Materials: Be-Cu-Fe-Nb-Ta-Ti-Zr	C1 solution solutions

- ➔ Different databases with different models.
- ➔ FACTSAGE and Thermo-Calc softwares are used.

THERMOCHEMICAL MODELS

Thermochemical models may be inconsistent between contributors and need to be reconciled

Models with stoichiometric phases and a few solid solutions

TBASE+RMC+UOIT: many compounds are described

- ➔ Associate model for oxide solid solutions (A, AO₂, AO₃ ...)
- ➔ The phase diagrams can not be calculated
- ➔ A solution model for (Mo, Pd, Rh, Ru, Tc)

Models for MOX solid solution with Lanthanides

ORNL: determines oxygen potential versus burnup

- ➔ Ionic three sublattice model for MOX : Compatible with CEA database
- ➔ Phase diagrams can be calculated

Models with a full description of non stoichiometric phases (solid & liquid)

JAEA+CEA+LLNL ➔ The phase diagrams can be calculated

The aims of our project are:

- **Merge the different databases,**
- **Agree on thermodynamic descriptions** for binary and ternary sub-systems
- **Propose experiments** to improve the descriptions

TAF-ID DATABASE (VERSION 5 – JANUARY 2015)

ELEMENTS ➔ Ag-Al-Am-Ar-B-Ba-C-Ca-Ce-Cr-Cs-Fe-Gd-H-He-I-La-Mg-Mo-N-Nb-Nd-Ni-Np-O-Pd-
Pu-Re-Rh-Ru-Si-Sr-Ta-Te-Th-Ti-U-V-W-Zr

BINARY SYSTEMS

Ag-I Ag-O Ag-Ti Ag-Zr
Al-Ca Al-Cr Al-Fe Al-Mg Al-O Al-Si Al-U Al-Zr
Am-Fe Am-Np Am-O* Am-Pu* Am-U Am-Zr
B-C B-Fe B-H B-I B-O B-Pu B-U B-Zr
Ba-H Ba-I* Ba-La* Ba-Mo* Ba-N Ba-O Ba-Ti* Ba-V*
C-Cr C-Fe C-Mo C-N C-Nb C-Ni C-O C-Pu* C-Re C-Si C-Ta C-Ti C-U* C-V C-W C-Zr
Ca-Fe Ca-Mg Ca-O Ca-Si Ca-U* Ca-Zr*
Ce-Cr Ce-Fe Ce-O*
Cr-Cs* Cr-Fe Cr-H Cr-I Cr-La* Cr-Mo Cr-N Cr-Nd* Cr-Ni Cr-O Cr-Pu* Cr-Si Cr-Ti Cr-U* Cr-Zr
Cs-I* Cs-Mo* Cs-Nb* Cs-O Cs-Pu* Cs-Ta* Cs-Te* Cs-Ti* Cs-U* Cs-V* Cs-Zr*
Fe-Nd Fe-Ni Fe-Np Fe-O Fe-Pu Fe-Si Fe-U Fe-Zr
Gd-O Gd-U*
H-I H-O H-Sr
I-Mo I-Sr I-Te
La-Mo* La-Nb* La-O La-Pu* La-Re* La-Ta* La-Te La-Ti* La-U* La-V* La-W*
Mg-O Mg-U* Mg-Zr*
Mo-N Mo-O Mo-Pd Mo-Pu* Mo-Re Mo-Rh* Mo-Ru Mo-Si Mo-Sr* Mo-Te* Mo-Ti Mo-U* Mo-Zr
N-O N-Pu* N-Si N-Ti N-U N-Zr
Nb-O Nb-Pu* Nb-Si Nb-U Nb-Zr
Nd-O* Nd-U*
Ni-O Ni-U
Np-O* Np-Pu* Np-U Np-Zr
O-Pu* O-Ru O-Si O-Sr O-Te O-Th* O-Ti O-U O-Zr
Pd-Rh Pd-Ru* Pd-Tc* Pd-Te* Pd-Zr
Pu-Re* Pu-Ru* Pu-Si* Pu-Ti* Pu-U Pu-W* Pu-Zr
Re-Si Re-U* Re-W
Rh-Ru* Rh-Tc* Rh-Te*
Ru-Te* Ru-U*
Si-Ta Si-Ti Si-U* Si-W Si-Zr
Sr-Ti* Sr-V*
Ta-U*
Ti-U* Ti-Zr
U-W* U-Zr

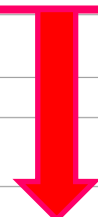
In red*: 72 assessed within our project
In blue: 116 coming from the literature

TERNARY SYSTEMS

Al-Ca-O Al-Cr-O Al-Fe-O Al-Mg-O
Al-O-Si Al-O-U Al-O-Zr
Am-O-Pu
B-C-Fe B-C-U B-C-Zr B-Fe-Zr B-Pu-U
C-Mo-Re C-Mo-Si C-Mo-Ti C-Mo-U C-N-Ti C-N-U
C-O-Pu C-O-U C-Pu-U C-Pu-W C-Re-U C-Re-W
C-Si-Ti C-Si-U C-U-W C-U-Zr
Ca-Fe-O Ca-Mg-O Ca-O-Si Ca-O-U Ca-O-Zr
Cr-Fe-O Cr-Fe-Zr
Cs-Mo-O Cs-O-U Cs-O-Zr
Fe-O-Si Fe-O-U Fe-O-Zr Fe-U-Zr
Gd-O-U
La-O-U
Mg-O-Si Mg-O-U Mg-O-Zr
Mo-O-U Mo-Pd-Rh Mo-Pd-Ru Mo-Rh-Ru
Nb-O-U
Nd-O-U
Ni-O-Si
O-Pu-U O-Pu-Zr O-Si-U O-Si-Zr O-U-Zr
Pd-Rh-Ru
Pu-U-Zr

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home	Introduction	Models	Phases	Systems
Phases described by usual name: ε-Pu... database name: BCC_A2... prototype: W... StrukturBericht: A2...				
Table				
BETA_RHOMBO_B	B	hR105	(B)	
BETA_SIALON	β-Si ₃ N ₄	hP14	(Si ⁴⁺) ₃ (N ³⁻) ₃ (N ³⁻)	
BF_CASI	BCr	oC8	Bf	(Ca) (Si)
BH_MC_SHP	WC	hP2	B _h	(Mo, Re, W) (C)
MoC, WC				
C1_MO2	CaF ₂	cF12	C1	(Al ³⁺ , Am ³⁺ , Am ⁴⁺ , Ca ²⁺ , Np ³⁺ , Np ⁴⁺ , Pu ³⁺ , Pu ⁴⁺ , Th ⁴⁺ , U ³⁺ , U ⁴⁺ , U ⁵⁺ , Zr ²⁺ , Zr ⁴⁺) (O ²⁻ , ∅) ₂ (O ²⁻ , ∅)
UO ₂ , PuO ₂ , ZrO ₂ , AmO ₂ , NpO ₂				
C2_MTE2	FeS ₂	cP12	C2	(Rh,Ru,∅) (Te) ₂
Pyrite				
C4_RUTILE	TiO ₂	tP6	C4	(Ru ⁴⁺ , Ti ⁴⁺) (O ²⁻) ₂
C4_TI2N	TiO ₂	tP6	C4	(Ti) ₂ (C, N)
Described independently of TiO ₂				
C6_B81	NIAs	hP4	B8 ₁	(Pd,Rh) (Pd,Rh,∅) (Te) ₂
Identical model for CdI ₂				
C6_B81_2	CdI ₂	hP3	C6	(Pd,Rh)
Identical model for NIAs				
C11B_AGM2	MoSi ₂	tI6	C11 _b	(Ag) (C)
C11B_MOSI2	MoSi ₂	tI6	C11 _b	(Mo, R)
C12_CASI2	CaSi ₂	hR18	C12	(Ca) (S)
C14_LAVES	MgZn ₂	hP12	C14	(Cr, Fe)
C15_LAVES	MgCu ₂	cF8	C15	(Al, Cr)
C16_THETA	CuAl ₂	tI12	C16	(Ta, Z)
C23_CA2SI	Co ₂ Si	oP12	C23	(Ca) ₂ (C)



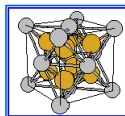
TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home Introduction Models **Phases** Systems

Usual name ZrO₂-Y, PuO₂, UO₂, AmO₂, NpO₂, ThO₂ **Name in the database**
C1_MO2

Crystallography

Prototype CaF₂ **StrukturBericht** C1 **Pearson** cF12 **Space Group** Fm-3m



Characteristics of the different sites for the prototype

Occupation	Multiplicity	Wickoff	Symmetry
F	8	c	-43m
Ca	4	a	m-3m

Thermodynamic model

(Al³⁺, Am³⁺, Am⁴⁺, Ca²⁺, Np³⁺, Np⁴⁺, Pu³⁺, Pu⁴⁺, Th⁴⁺, U³⁺, U⁴⁺, U⁵⁺, Zr²⁺, Zr⁴⁺) (O²⁻, ∅)₂ (O²⁻, ∅)

Assessed systems where the phase is stable

Am-O Ce-O Np-O O-Pu O-Th O-U O-Zr Am-O-Pu C-O-Pu C-O-U Nd-O-U O-Pu-U O-Pu-Zr

A single sublattice model for all the phases with the same crystalline structure

The source of the description is clearly mentioned.

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Home

Introduction

Models

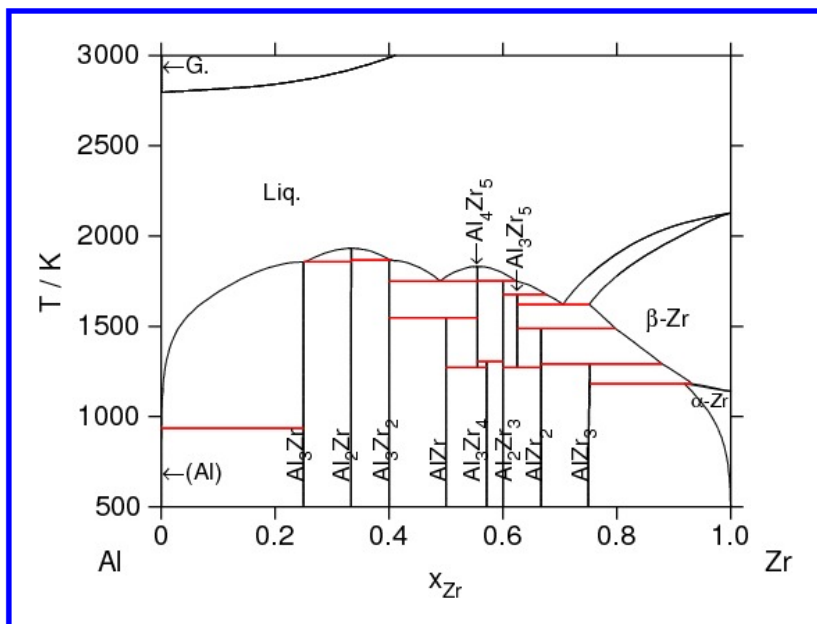
Phases

Systems

TDB

Binary system Al-Zr

Al-O-Zr Al Zr Binary systems Ternary systems Periodic table



Source of the description

T. Wang, Z. Jin, J.-C. Zhao, *J. phase equilibria*, **22** (5), 544-551, 2001.

Comments

The Al₂Zr and AlZr₃ descriptions are slightly modified in order to model them as the phases having the same prototype. The L1₂ phase corresponding to the AlZr₃ phase is rejected by default but restored by default when using the BINARY module of ThermoCalc.

File to calculate the phase diagram

[Al-Zr.TCM](#)

The source of the description is clearly mentioned.

Home
Introduction
Models
Phases
Systems
TDB

Ternary system Cr-Fe-Zr Cr-Fe Cr-Zr Fe-Zr Cr Fe Zr Binary systems Ternary systems Periodic table

Isothermal section at 1500 K

Projection of the monovariant lines of the liquidus

Source of the description

N. Dupin, TAF-ID, 2014 october

Comments

The description recently published by [Yang et al.](#) was not used because of different descriptions for the Fe-Zr and Cr-Zr subsystems. The early description by [Barberis et al.](#) was using a Cr-Zr description with an overestimated enthalpy of formation for the Laves phases.

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Home

Introduction

Models

Phases

Systems

TDB

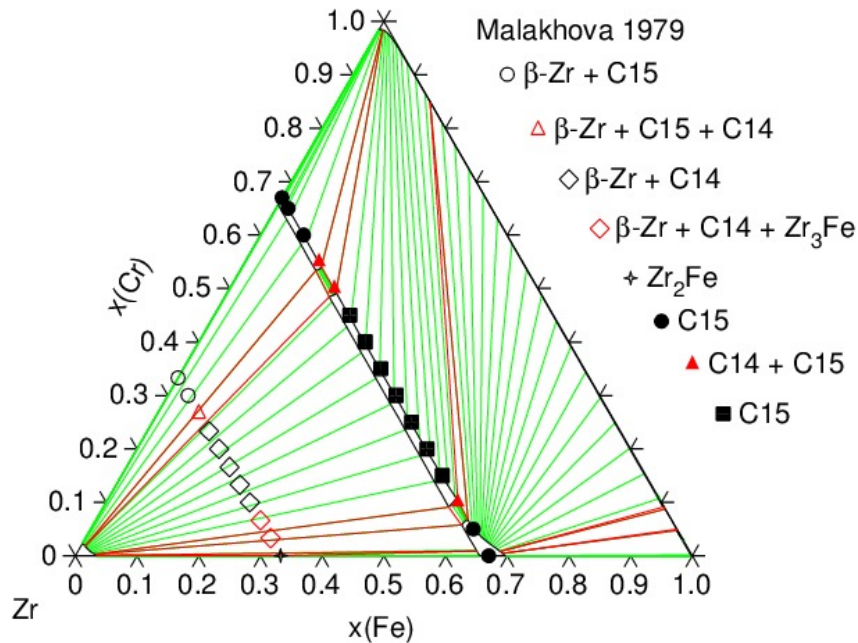
Ternary system Cr-Fe-Zr

Cr-Fe Cr-Zr Fe-Zr Cr Fe Zr Binary systems Ternary systems Periodic table

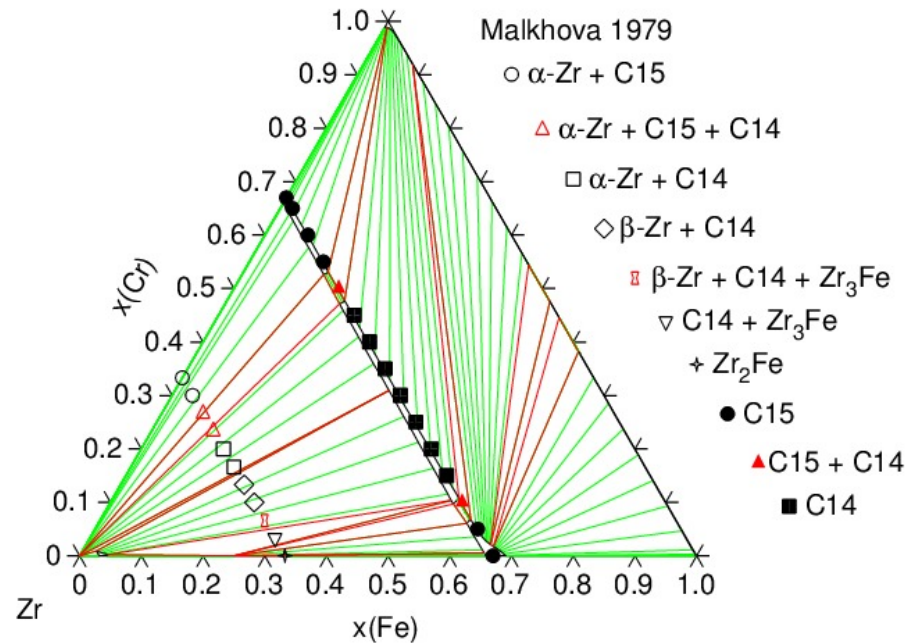
Comparison with experiments

Phase diagram

T = 1148 K



T = 1073 K



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Home

Introduction

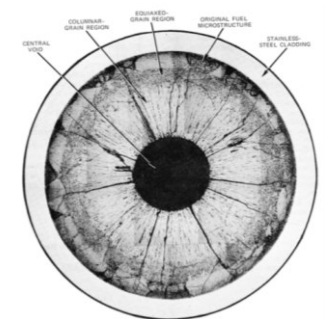
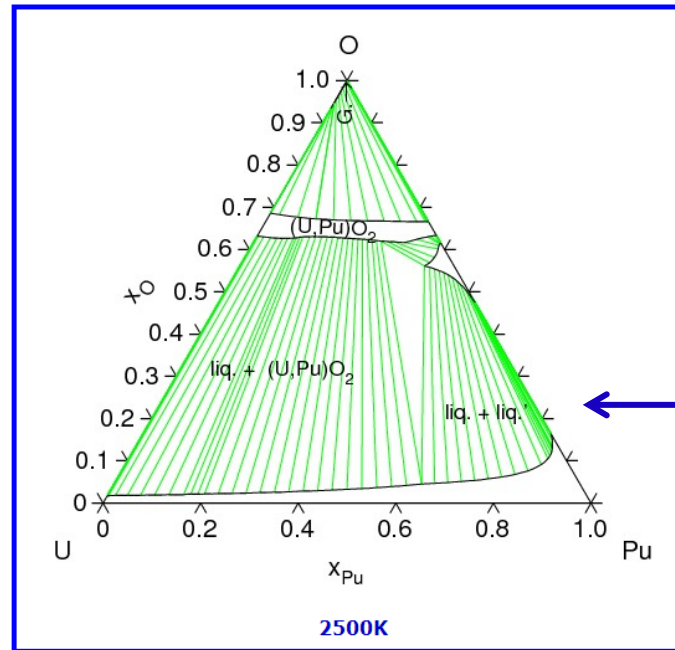
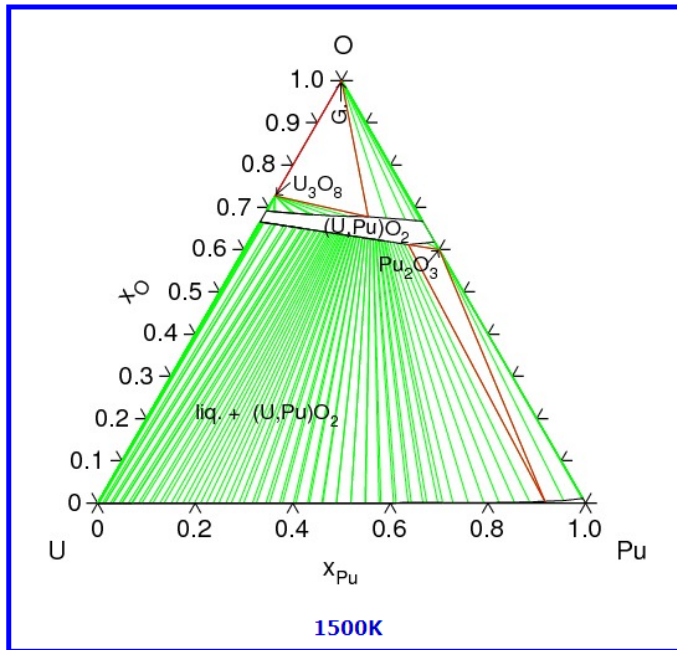
Models

Phases

Systems

Ternary system O-Pu-U

O-Pu O-U Pu-U O Pu U Binary systems Ternary systems Periodic table

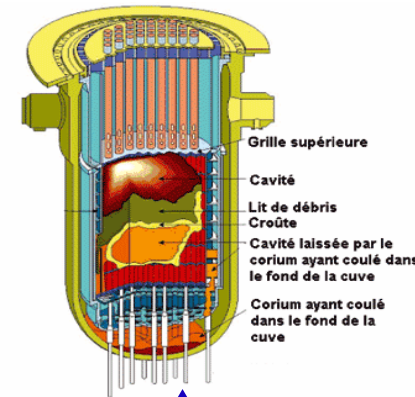


MOX fuel in SFR

-Interaction with steel clad
- Fission product chemistry

Source of the description

C. Guéneau, N. Dupin, B. Sundman, C. Martial, J.C. Dumas, S. Gossé, S. Chatain, F. De Bruycker, D. Manara, R. Konings, Thermodynamic modelling of advanced oxide and carbide nuclear fuels: Description of U-Pu-O-C systems, *J. Nuclear Materials*, **419** (2011) 145-167



Corium (U,Zr,O) forming from UO_2/Zr interaction

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Home

Introduction

Models

Phases

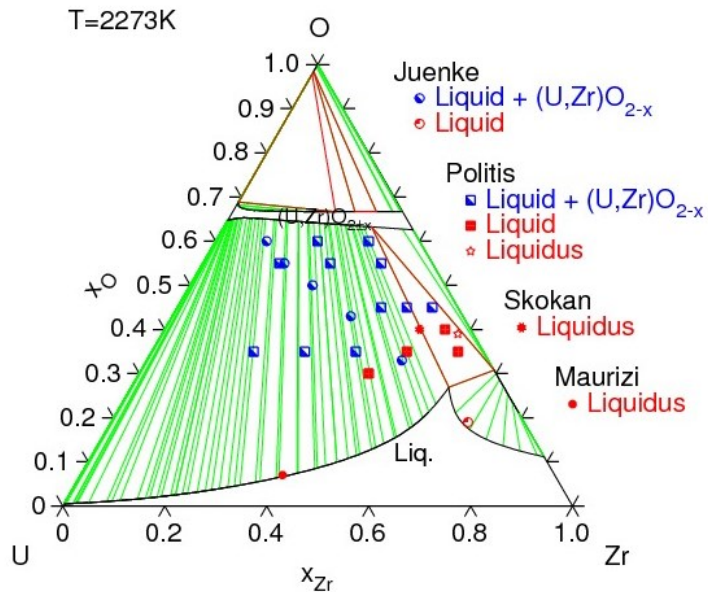
Systems

Ternary system O-U-Zr

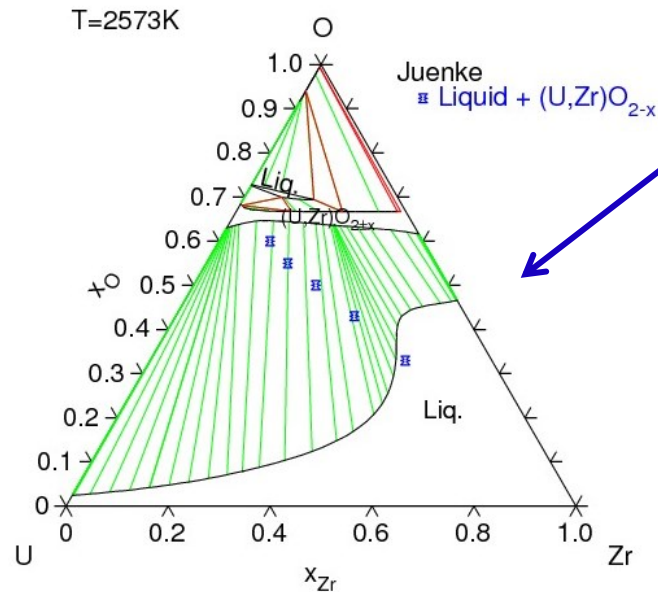
O-U O-Zr U-Zr O U Zr Binary systems Ternary system

Comparison with experiments

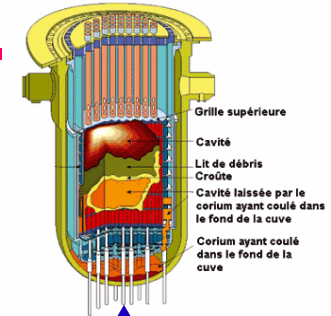
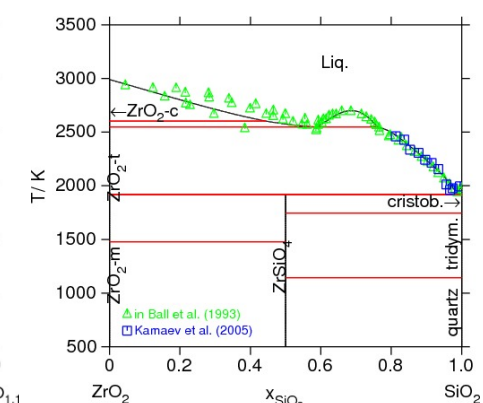
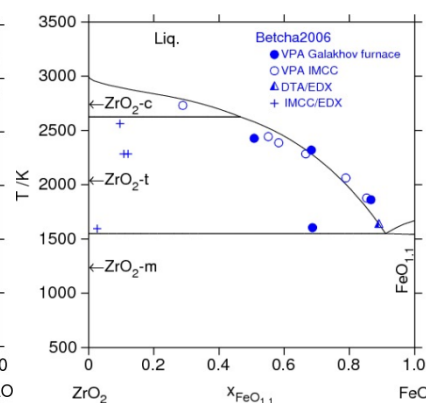
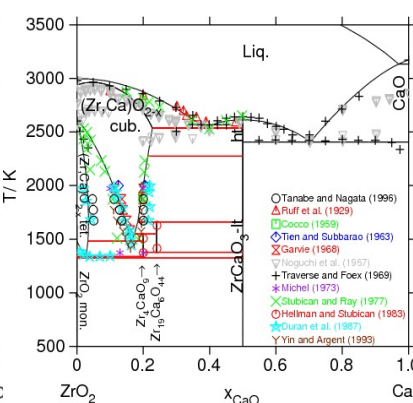
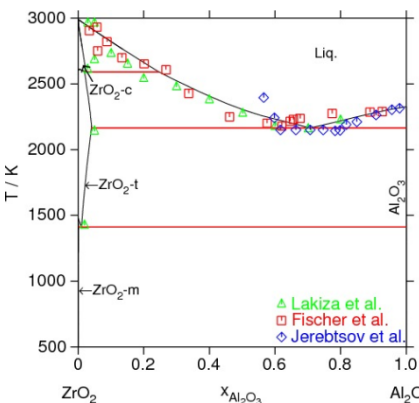
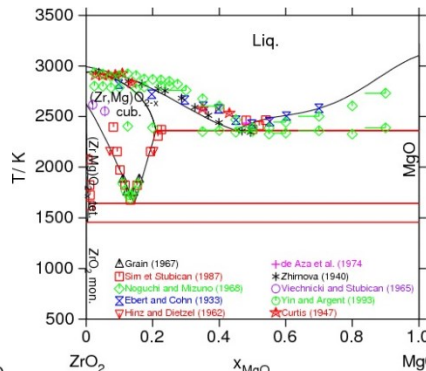
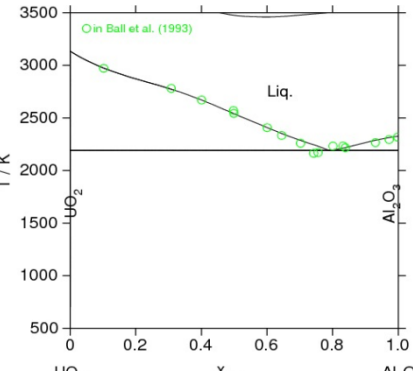
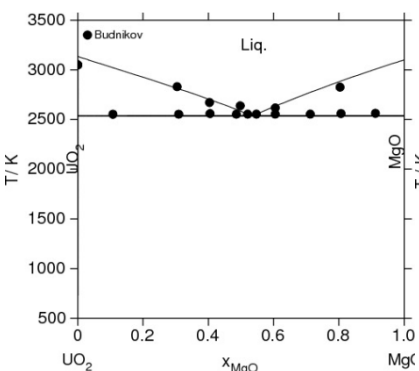
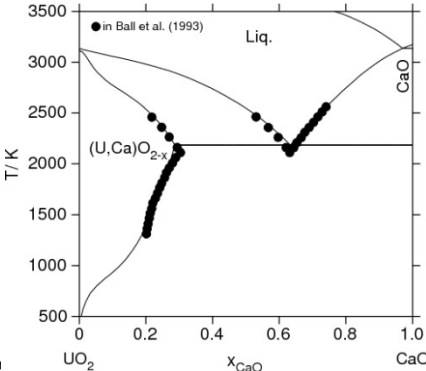
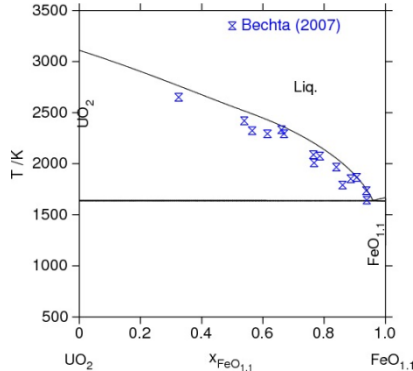
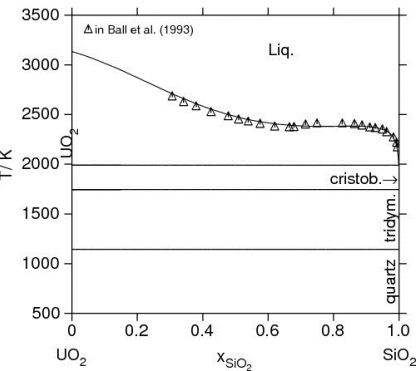
Isothermal section at 2273K



Isothermal section at 2573K



UO₂-CONCRETE AND ZRO₂-CONCRETE INTERACTION



Corium (U,Zr,O,Fe) forming from UO₂/Zr/Fe interaction

UO₂ + ZrO₂ + concrete



Nuclear science > Projects > TAF-ID

TAF-ID

Thermodynamic data

Tools for thermodynamic calculations

Project Organisation

The TAF-ID Versions

Project Signatories

Relevant links

Contact

Thermodynamics of Advanced Fuels – International Database (TAF-ID) Project

TAF-ID public version

The TAF-ID public version contains only data already published in the literature. Currently, the following systems are available in the public version:

- Oxide-Carbide fuel (U-Pu-O-C, released December 2014);
- Metal fuel (U-Pu-Zr, released December 2014).

This version is accessible free of charge to all NEA member countries upon request to the NEA and signature of a [Non-Disclosure Agreement \(NDA\)](#).

- To send to the NEA a signed copy of the Non-Disclosure Agreement (NDA) please [click here](#);
- If you already submitted a signed copy of the NDA and you received a confirmation e-mail, please directly enter the [restricted access zone](#) (password protected | [reminder](#)) and proceed to downloading.

Contact

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Last reviewed: 8 January 2015

TAF-ID working areas

Programme review group

TAF-ID working version

TAF-ID public version

OC: OPEN CALPHAD SOFTWARE (BO SUNDMAN)

- OC is an **open source** software to perform thermodynamic calculations using the CALPHAD method.
- OC uses as input data Databases containing mathematical models of the Gibbs energy as function of temperature, composition and pressure. **OC is compatible with databases in Thermo-Calc format (TDB).**
- A **grid minimizer** is used to provide an initial global minima as a start point for the equilibrium calculation. This solves the problems related to miscibility gaps.
- A **software interface module** is available to compute a thermodynamic equilibrium for given conditions (P, T, N, x_i) to provide input data to other softwares (diffusion, phase field, thermohydraulics, thermal ...).
- Calculations as function of temperature (or composition) can be performed.
- Binary phase diagrams can be calculated.
- A project is in progress to develop a **new assessment module** to develop the Gibbs Energy database.

RESULTS USING OC/TAF-ID ➔ IN-VESSEL CORIUM

In-vessel EPR corium: $n(\text{fe})=0.413601$ $n(\text{o})=0.48623376$ $n(\text{u})=0.19442428$ $n(\text{zr})=0.250339$

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM

Conditions

1:T=2900, 2:P=100000, 3:N(FE)=0.413601, 4:N(O)=0.48623376, 5:N(U)=0.19442428, 6:N(ZR)=0.250339

Degrees of freedom are 0

Some global data, reference state SER

T= 2900.00 K (2626.85 C), P= 1.0000E+05 Pa, V= 0.0000E+00 m3

N= 1.3446E+00 moles, B= 9.9993E+01 g, RT= 2.4112E+04 J/mol

G= -5.6581E+05 J, G/N= -4.2080E+05 J/mol, H= -1.2890E+05 J, S= 1.5066E+02 J/K

Some component data

Component name	Moles	Mole-fr	Chem.pot/RT	Activities	Ref.state
FE	4.1360E-01	0.30760	-9.8791E+00	5.1234E-05	SER (default)
O	4.8623E-01	0.36162	-2.6262E+01	3.9298E-12	SER (default)
U	1.9442E-01	0.14460	-1.6957E+01	4.3218E-08	SER (default)
ZR	2.5034E-01	0.18618	-1.3235E+01	1.7863E-06	SER (default)

Some Phase data

Phase: LIQUID Status: Entered Driving force: 0.0000E+00

Moles 5.8403E-01, Mass 5.1195E-02 kg, Volume 0.0000E+00 m3

Formula Units: 2.2580E-01, Moles of atoms/FU: 2.5865E+00, Molar content:

FE 7.08188E-01 U 1.48903E-01 ZR 1.37959E-01 O 4.94951E-03

Constitution:

Sublattice 1 with 3 constituents and 2.573713 sites

FE+2 7.11711E-01 U+4 1.49644E-01 ZR+4 1.38645E-01

Sublattice 2 with 4 constituents and 2.576578 sites

VA 9.95031E-01 O 1.77141E-07

O-2 4.96842E-03 FEO3/2 1.00000E-12

Phase: C1_MO2 Status: Entered Driving force: 0.0000E+00

Moles 7.6057E-01, Mass 4.8799E-02 kg, Volume 0.0000E+00 m3

Formula Units: 2.7723E-01, Moles of atoms/FU: 2.7435E+00, Molar content:

O 6.35500E-01 ZR 2.23210E-01 U 1.41290E-01 FE 0.00000E+00

Constitution:

Sublattice 1 with 5 constituents and 1.000000 sites

U+4 3.72682E-01 ZR+2 2.49045E-01 U+3 1.49417E-02 U+5 2.51318E-06 ZR+4 3.63329E-01

Sublattice 2 with 2 constituents and 2.000000 sites

O-2 8.71743E-01 VA 1.28257E-01

Sublattice 3 with 2 constituents and 1.000000 sites

VA 1.00000E+00 O-2 4.50893E-08

RESULTS USING OC/TAF-ID ➔ IN-VESSEL CORIUM

In-vessel EPR corium: $n(\text{fe})=0.413601$ $n(\text{o})=0.48623376$ $n(\text{u})=0.19442428$ $n(\text{zr})=0.250339$

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM

Conditions

1:T=3000, 2:P=100000, 3:N(Fe)=0.413601, 4:N(O)=0.48623376, 5:N(U)=0.19442428, 6:N(ZR)=0.250339

Degrees of freedom are 0

Some global data, reference state SER

T= 3000.00 K (2726.85 C), P= 1.0000E+05 Pa, V= 0.0000E+00 m3

N= 1.3446E+00 moles, B= 9.9993E+01 g, RT= 2.4944E+04 J/mol

G= -5.8167E+05 J, G/N= -4.3260E+05 J/mol, H= -9.5706E+04 J, S= 1.6199E+02 J/K

Some component data

Component name	Moles	Mole-fr	Chem.pot/RT	Activities	Ref.state
FE	4.1360E-01	0.30760	-9.9398E+00	4.8219E-05	SER (default)
O	4.8623E-01	0.36162	-2.5505E+01	8.3826E-12	SER (default)
U	1.9442E-01	0.14460	-1.7408E+01	2.7536E-08	SER (default)
ZR	2.5034E-01	0.18618	-1.3671E+01	1.1550E-06	SER (default)

Some Phase data

Phase: LIQUID Status: Entered Driving force: 0.0000E+00

Moles 8.1749E-01, Mass 5.7516E-02 kg, Volume 0.0000E+00 m3

Formula Units: 1.4424E-01, Moles of atoms/FU: 5.6677E+00, Molar content:

O 5.92126E-01 ZR 2.42115E-01 U 1.62142E-01 FE 3.61699E-03

Constitution:

Sublattice 1 with 3 constituents and 2.311727 sites

ZR+4 5.93602E-01 U+4 3.97530E-01 FE+2 8.86791E-03

Sublattice 2 with 4 constituents and 3.982264 sites

O-2 8.42740E-01 O 1.13229E-06

VA 1.57259E-01 FEO3/2 1.00000E-12

Phase: OXID_LIQUID#2 Status: Entered Driving force: 0.0000E+00

Moles 5.2710E-01, Mass 4.2477E-02 kg, Volume 0.0000E+00 m3

Formula Units: 2.1570E-01, Moles of atoms/FU: 2.4437E+00, Molar content:

FE 7.79057E-01 U 1.17385E-01 ZR 9.94327E-02 O 4.12613E-03

Constitution:

Sublattice 1 with 3 constituents and 2.433628 sites

FE+2 7.82284E-01 U+4 1.17871E-01 ZR+4 9.98447E-02

Sublattice 2 with 4 constituents and 2.435431 sites

VA 9.95860E-01 O 4.95523E-07

O-2 4.13966E-03 FEO3/2 1.00000E-12

RESULTS USING OC/TAF-ID ➔ EX-VESSEL CORIUM

Ex-vessel corium: mass. % Al₂O₃ 1.8 CaO 32.4 SiO₂ 24.6 UO₂ 38.8 ZrO₂ 18.4

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM

Conditions

1:N(AL)=.0353, 2:N(CA)=0.57776, 3:N(SI)=0.40943, 4:N(U)=0.114062, 5:N(ZR)=.0844, 6:N(O)=1.85, 7:T=1700, 8:P=100000

Degrees of freedom are 0

Some global data, reference state SER

T= 1700.00 K (1426.85 C), P= 1.0000E+05 Pa, V= 0.0000E+00 m³

N= 3.0710E+00 moles, B= 1.0006E+02 g, RT= 1.4135E+04 J/mol

G= -1.2386E+06 J, G/N= -4.0334E+05 J/mol, H= -8.9264E+05 J, S= 2.0353E+02 J/K

Some component data

Component name Moles Mole-fr Chem.pot/RT Activities Ref.state

AL 3.5300E-02 0.01149 -3.9744E+01 5.4895E-18 SER (default)

CA 5.7776E-01 0.18814 -3.8105E+01 2.8250E-17 SER (default)

O 1.8500E+00 0.60242 -2.0816E+01 9.1189E-10 SER (default)

SI 4.0943E-01 0.13332 -3.7248E+01 6.6559E-17 SER (default)

U 1.1406E-01 0.03714 -5.3410E+01 6.3717E-24 SER (default)

ZR 8.4400E-02 0.02748 -5.1673E+01 3.6212E-23 SER (default)

Some Phase data

Phase: OXID_LIQUID#2 Status: Entered Driving force: 0.0000E+00

Moles 2.3195E+00, Mass 5.4779E-02 kg, Volume 0.0000E+00 m³

Formula Units: 2.1708E-01, Moles of atoms/FU: 1.0685E+01, Molar content:

O 5.89762E-01 SI 1.71915E-01 ZR 1.45910E-07 U 7.88385E-08

CA 2.23105E-01 AL 1.52180E-02

Phase: CAUO4_S2 Status: Entered Driving force: 0.0000E+00

Moles 7.6863E-03, Mass 4.3825E-04 kg, Volume 0.0000E+00 m³

Formula Units: 1.2810E-03, Moles of atoms/FU: 6.0000E+00, Molar content:

O 6.66667E-01 U 1.66667E-01 ZR 0.00000E+00 AL 0.00000E+00

CA 1.66667E-01 SI 0.00000E+00

Phase: RANKINITE Status: Entered Driving force: 0.0000E+00

Moles 6.4009E-02, Mass 1.5384E-03 kg, Volume 0.0000E+00 m³

Formula Units: 5.3341E-03, Moles of atoms/FU: 1.2000E+01, Molar content:

O 5.83333E-01 SI 1.66667E-01 ZR 0.00000E+00 AL 0.00000E+00

CA 2.50000E-01 U 0.00000E+00

Phase: C1_MO2 Status: Entered Driving force: 0.0000E+00

Moles 1.0150E-01, Mass 8.6351E-03 kg, Volume 0.0000E+00 m³

Formula Units: 3.3828E-02, Moles of atoms/FU: 3.0004E+00, Molar content:

O 6.66706E-01 CA 2.17836E-02 AL 9.10416E-07 SI 0.00000E+00

U 3.07356E-01 ZR 4.15360E-03

Phase: C1_MO2_ZRO2#2 Status: Entered Driving force: 0.0000E+00

Moles 5.7823E-01, Mass 3.4665E-02 kg, Volume 0.0000E+00 m³

Formula Units: 2.0633E-01, Moles of atoms/FU: 2.8024E+00, Molar content:

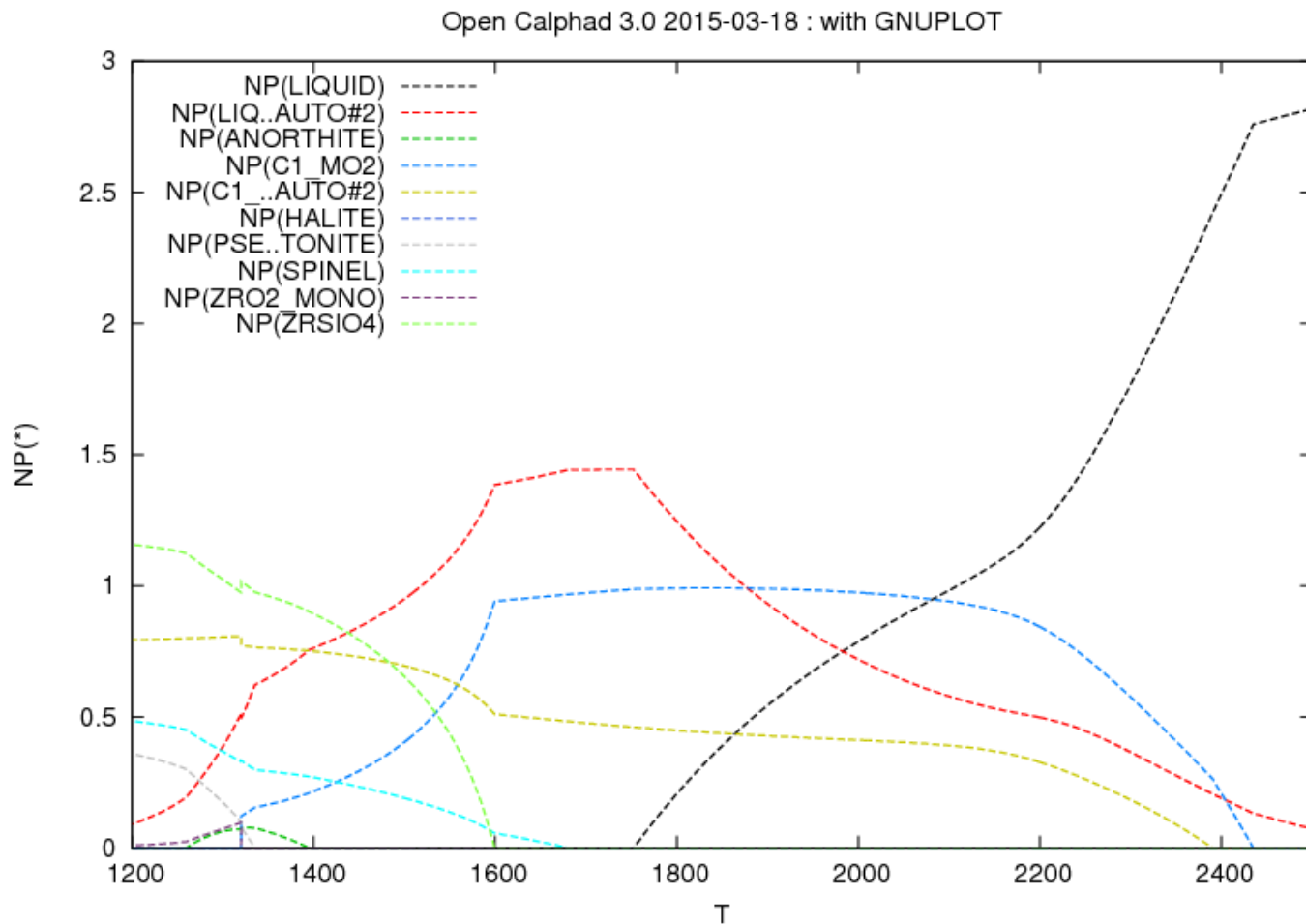
O 6.43166E-01 U 1.41095E-01 AL 2.42748E-06 SI 0.00000E+00

ZR 1.45233E-01 CA 7.05034E-02

RESULTS USING OC/TAF-ID

Ex-VESSEL corium:

$N(O)=1.85$, $N(U)=0.255$, $N(ZR)=0.196$, $N(Fe)=0.141$, $N(CR)=.032$, $N(SI)=0.279$, $N(AL)=.05$, $N(CA)=.088$



SUMMARY

- **The Working Version 5 of TAF-ID database is available for the participants of the TAF-ID project**
- **A public version restricted to only published work is available for all the member countries of OECD/NEA since december 2014**
 - ➔ <https://www.oecd-nea.org/science/taf-id/taf-id-public/>
- **The TAF-ID database will be available in Thermo-Calc and FACTSAGE formats**
 - **A software to convert the databases from both codes is being developed**
- **The TAF-ID project may be extended for 3 years**
- **OC is an open source software for CALPHAD calculations, compatible with Thermo-Calc format (TDB)**
- **Both OC and TAF-ID are operational computational tools to perform thermodynamic calculations on corium systems for severe accident applications**