

Přehled SW pro výpočty fázových rovnováh

SW pro metodu CALPHAD

	Thermo- Calc	MTDATA	Chem- Sage	Lucas program package	PD-pp program package
Trade mark					PD-pp
required user education	M.S. engineer, * advanced thermody- misticist	M.S. engineer	M.S. engineer	very advanced thermodynamicist and good programer	M.S. engineer or thermo- dynamicist
U T I L I T Y	calculation of equilibria	Yes	Y	Y	Y
	Data bank	Y	Y	Y	N
	Graphical output	Y	Y	Y	N
	extracting of TD-parameters from exp. results	* Y	N	N	Y
hardware & software requirement	UNIX (VAX)	VAX (UNIX) 386/486 MSDOS PCs	PC ≥ 386	PC ≥ 486 (DOS)	PC ≥ 286 (+MS) WIN.
Origin	Sweden	UK	AACHEN	STUTGARD	CZECH R.
price [DM]	10000-15000 (annual)	9000-13000 (annual)	9400-8000,- 2000-1000,- (multi lic.)	-publication -reference [Lucas]	TD-parameters (* .pat file)

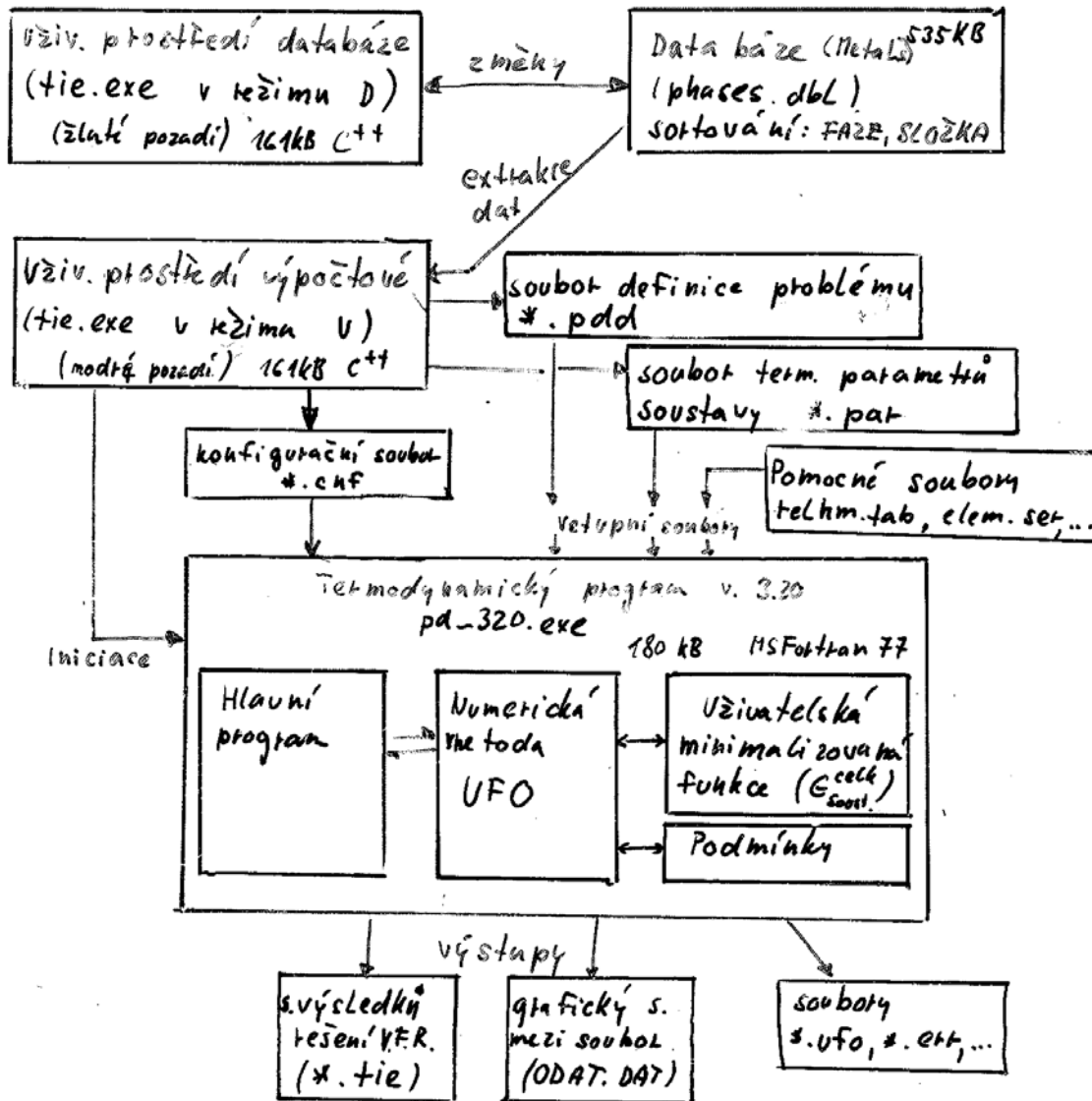


<http://www.computerherm.com/>

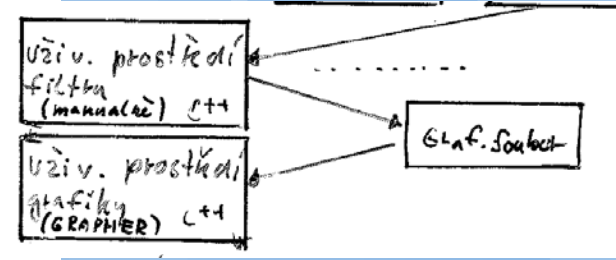


<http://gtt.mch.rwth-aachen.de/gtt-web/factsage>

PD-PP (Phase diagram programme package)



- PD-pp:
- 4 phases, 8 comp.
 - activities, chem. pot., phase ratio, ...)
 - sublattice model (4. subl.)
 - integral. cond.
 - Linear constraints



ThermoCalc

Databáze: KP, Geo, SALT, SLAG, ION, Fe-data

DATA
(databáze
a tvorba TPS)

POLY-3
(výpočet FD)

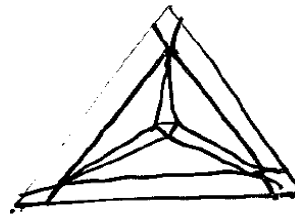
Num. metoda pro řešení integrační podm FR
(není prezentováno)

POST (Grafika)

GES, TABULATE,
ata.

Parrot
(assessment FD)

Uset modals



Pozn.: "DIKTRA" - modul pro výpočty difúzních koeficientů z TP.

ThermoCalc 2015b (graphical mode)

Thermo-Calc 2015b - My Project FeC OK.tcu

File Tools Window Help

New Open Save Switch to Console Mode

Project Configuration

My Project
Binary Calculator 1
Plot Renderer 1

Plot Renderer 1

Save Diagram Show Triangular Show Grid Switch Axes Retain Labels

Binary Calculator 1

Tie lines: 1 Legend style: None

X Axis

Axis variable: Composition C Mass percent

Axis type: Linear

Limits: 0.0 to 10.0 step 2.0 Automatic scaling

Y Axis

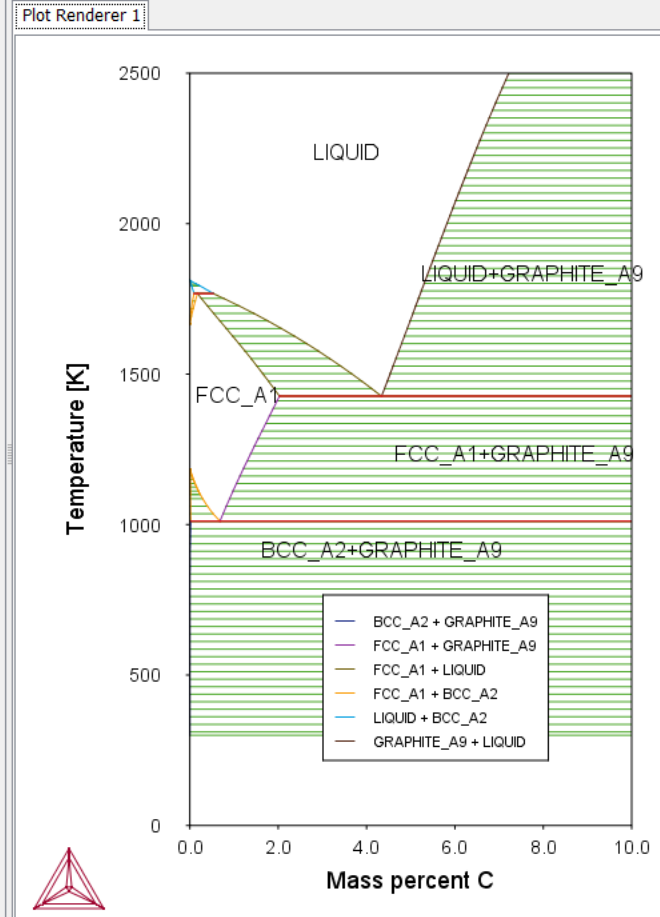
Axis variable: Temperature Kelvin

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 Automatic scaling

Add Predecessor Perform Create New Successor

Results



Event Log

CS Čeština (Česká republika) České (QWERTY) nápověda



11:57 8.11.2017

ThermoCalc 2015b (console mode)

Thermo-Calc 2015b - My Project FeC OK.tcu

File Tools Window Help

New Open Save Switch to Graphical Mode

Console

Console 1

```
AMBIGUOUS COMMAND, USE HELP
TDB_USER:get
ELEMENTS .....
SPECIES .....
PHASES .....

*** ERROR 1184 IN GZDIS2
*** PARTITIONED PHASES HAVE DIFFERENT NUMBER OF COMPOSITION SETS
If you read from a database the database manager may have to rearrange
the type codes for the phases B2_BCCVA and A2_BCCVA
to correct this error. Remind him that TYPE_DEFINITIONS are executed
in the order they appear in the TDB file.
ERROR 1184 RESET
PARAMETERS ...
FUNCTIONS ....
-OK-
TDB_USER:pol
NO SUCH COMMAND, USE HELP
TDB_USER:poly3
NO SUCH COMMAND, USE HELP
TDB_USER:?
AMEND_SELECTION      EXIT                NEW_DIRECTORY_FILE
APPEND_DATABASE      GET_DATA           REJECT
BACK                 GOTO_MODULE       RESTORE
DATABASE_INFORMATION HELP              SET_AUTO_APPEND_DATABASE
DEFINE_ELEMENTS      INFORMATION        SWITCH_DATABASE
DEFINE_SPECIES       LIST_DATABASE
DEFINE_SYSTEM        LIST_SYSTEM
TDB_USER:go poly

POLY version 3.32
POLY_3:s-c t=1000 n=2 p=1e5 x(cr)=0.5
```

Console Results

Results Console 1

Plot 1

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12:02 8.11.2017

Výpočtové SW a DATABASES pro chemickou termodynamiku

Name	Host	Content	Access Mode
FACT	École Polytechnique de Montréal	Integrated thermochemical database which couples software with thermodynamic data.	online, PC and web
THERDAS	Lehrstuhl für Theoretische Hüttenkunde	Databank system for thermochemical data	PC-disks, non-commercial
Thermoalloy	THERMODATA http://thermodata.online.fr/anglais.html	Properties of multicomponent systems, and phase diagrams	Transpac, Internet
Thermo-Calc	Royal Institute of Technology	Software for thermodynamic and phase diagram calculations, specially designed for systems with strongly non-ideal phases.	PC and workstation

DATABASES pro chemickou termodynamiku

Name	Host	Content	Access Mode
Thermophysical and Thermochemical Property Database	JICST. factual databases (JOIS-F)	thermophysical and related data for inorganic and low molecular weight compounds and up to 3-component systems.	planned for WWW, subscript. Note: this service is temporary down
<u>KINDAS</u>	Lehrstuhl für Theoretische Hüttenkunde	Database of kinetic properties and with calculation programs	PC-disks, commercial
<u>THERDAS</u>	Lehrstuhl für Theoretische Hüttenkunde	Databank system for thermochemical data	PC-disks, non-commercial
Thermocomp	<u>THERMODATA</u>	Thermodynamic properties of elements and substances in inorganic chemistry, and their reactions.	Transpac, Internet

Další užitečné linky

ThermoCalc (Švédsko):

<http://www.thermocalc.com/>

MTData (Velká Británie): <http://www.npl.co.uk/advanced-materials/measurement-techniques/modelling/mtdata>

FactSage (Canada+SRN) <http://www.factsage.com/> (i příklady diagramů), **Downloady:**
<http://www.crct.polymtl.ca/fact/download.php#>

Pandat (USA, Japan, Corea): <http://www.computherm.com/home.html>

THERMODATA (Francie) <http://thermodata.online.fr>

VLXE (polymery) free: <http://www.vlxe.com>

Diagramy:

ASM : <http://www.asminternational.org/asmenterprise/apd/default.aspx> , **MSI** (lze koupit si diagram)

Databaze

STGE <http://www.crct.polymtl.ca/sgte/index.php>

Assessment

Kniha: <http://www.springerlink.com/content/100270622k03v066/>

Diskuse

<http://thermodata.online.fr/nuclea.html>