

Přehled SW pro výpočty fázových rovnováh



MetSW pro metody 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)

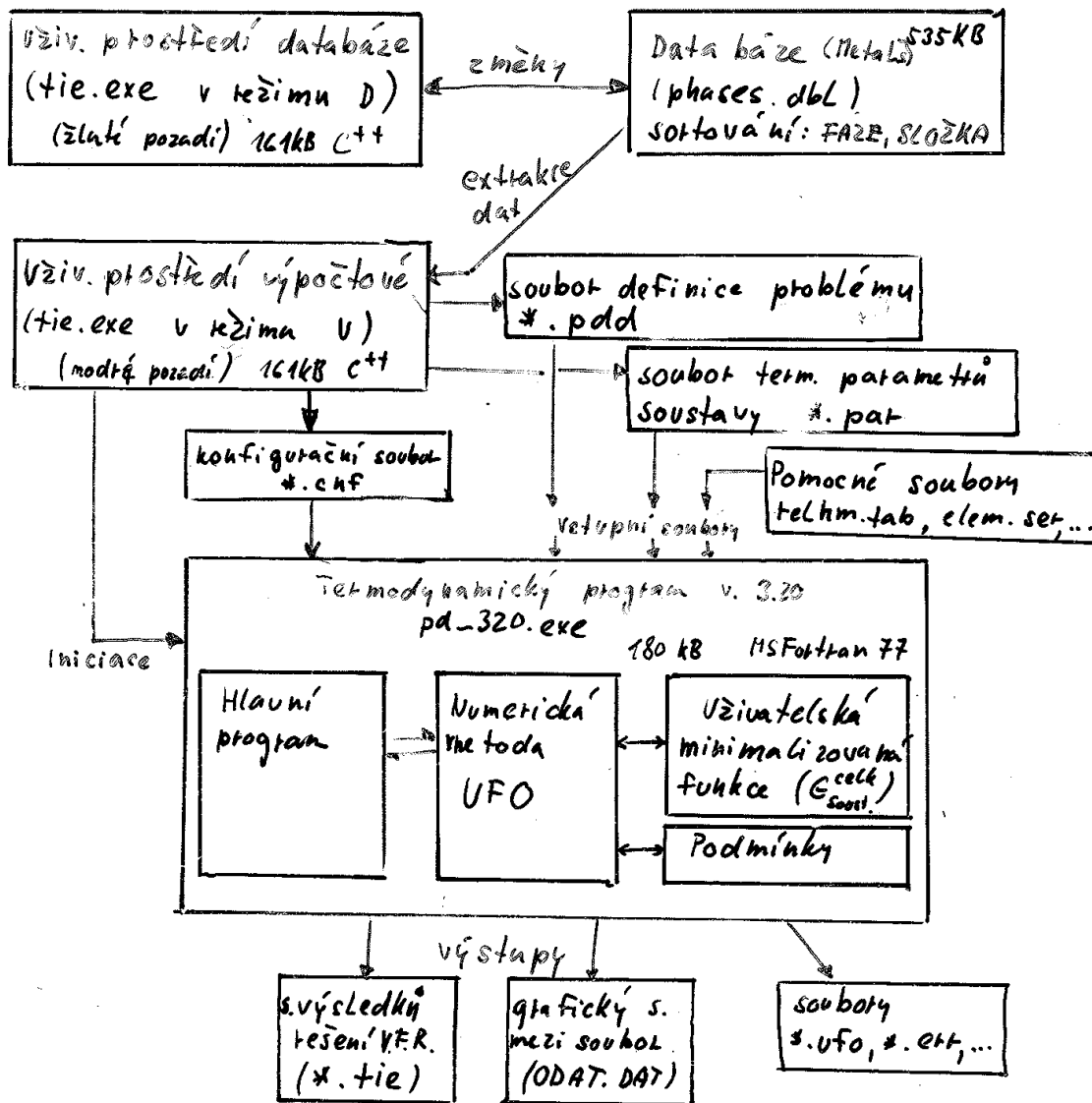


<http://www.computerherm.com/>



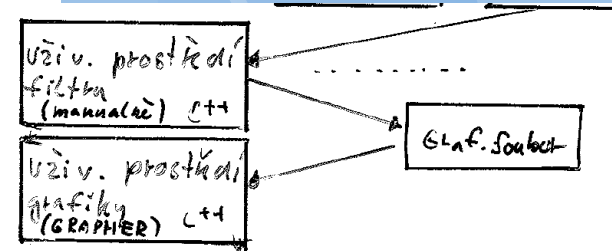
<http://gtt.mch.rwth-aachen.de/gtt-web/factsage>

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)

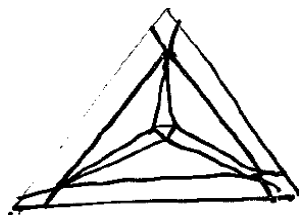
Num. metoda pro řešení integrační podm FR
(není prezentováno)

POST (Grafika)

GES, TABULATE,
ata.

Parrot
(assessment FD)

Uset modals



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

Výpočtové SW a DATABASES pro chemickou termodynamiku

Name	Host	Content	Access Mode
<u>F*A*C*T</u>	École Polytechnique de Montréal	Integrated thermochemical database which couples software with thermodynamic data.	online, PC and web
<u>THERDAS</u>	Lehrstuhl für Theoretische Hüttenkunde	Databank system for thermochemical data	PC-disks, non-commercial
Thermoalloy	<u>THERMODATA</u> http://thermodata.online.fr/anglais.html	Properties of multicomponent systems, and phase diagrams	Transpac, Internet
<u>Thermo-Calc</u>	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, Korea): <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>