The Software Tools (basic information)

		Thermo-Calc	MTDATA	Chem-Sage	Lucas program package	PD-pp program package	F.A.C.T.
Trade mark						PD_pp	
required USER education		M.S. engineer, * advanced thermodynamicist	M.S. engineer	M.S. engineer	very advanced thermodynamicist and good programer	M.S. engineer or thermodynamicist	M.S. eng.
UTILITY	calculation of equilibria	Yes	Y	Y	Y	Y	Y
	Data bank	Y	Y	Y	N	N	Y
	Graphical output	Y	Y	Y	Y	N	Y
	extracting of TD-parameters from exp. results	*Y	N	N	Y	N	N
hardware & software requirement		UNIX (VAX)	VAX (UNIX) 386/486 MSDOS PCs	PC ≥ 386	PC ≥ 486 (DOS)	PC ≥ 286 ~~(DOS)~~ WIN.	PC - Intel
Origin		Sweden	UK	AACHEN	STUTGARD	CZECH R.	CANADA
price [DM]		~~15 000~~ 15 000 (~~annual~~)	9 000 - 13 000 (annual)	9400 - 8000,- / 2 000 - 1000,- (multi lic.)	- publication - reference [Lukas]	TD-parameters (*.par file)	?

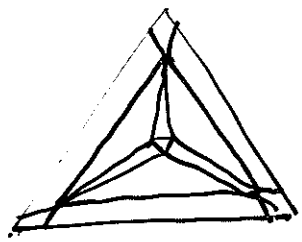
Thermo-Calc

... Sundman: Thermo-Calc Users' Guide (version L), Royal Inst. of Technology, Stockholm (1997)

Rysy: Fortran 77, přístup interaktivní nebo pomocí maker, vícesl. model, ionic model, associate model, ordering model, ...

Moduly souboru programů Thermo-Calc

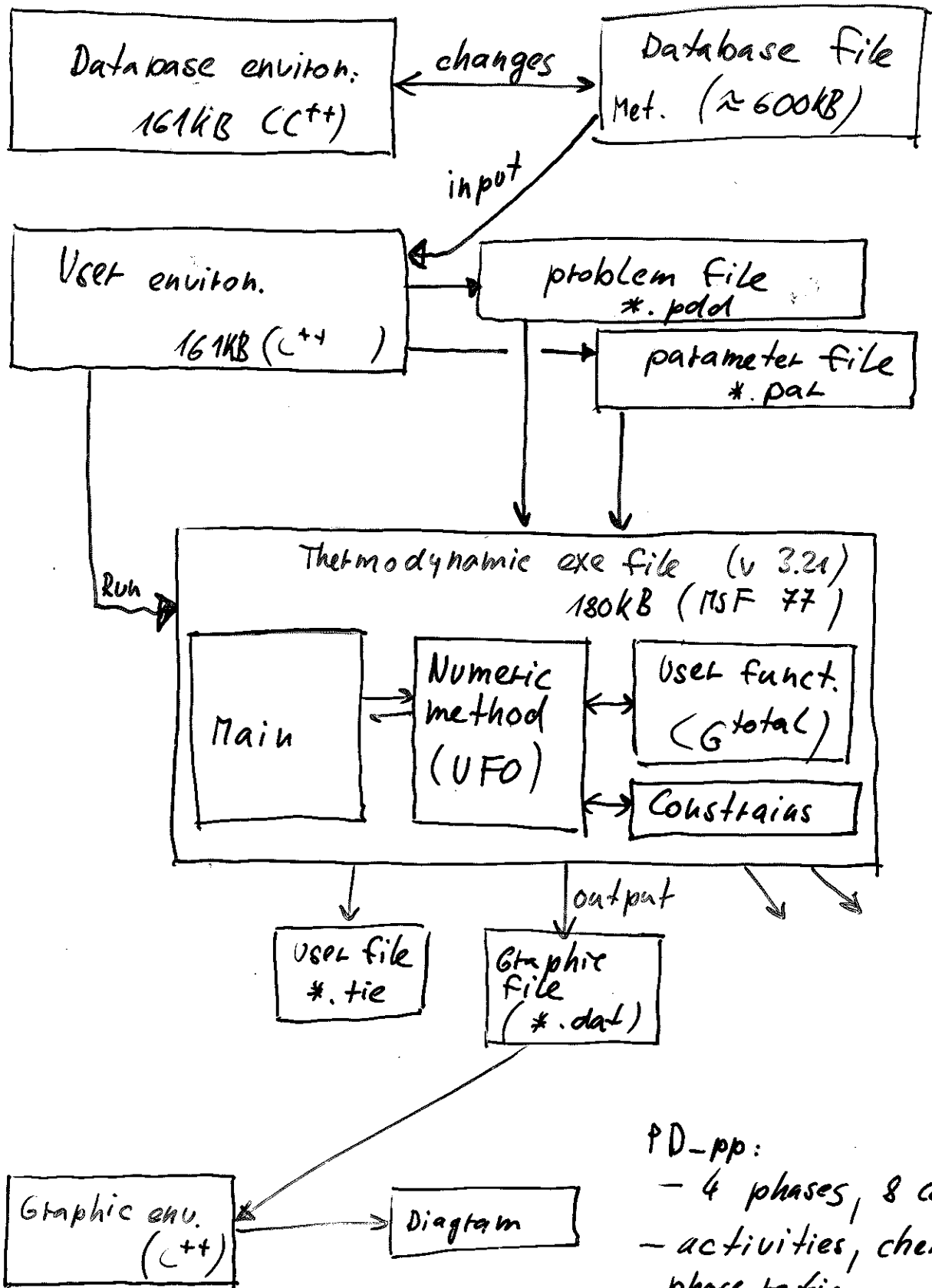
- DATA (databáze a tvorba TPS) — Databáze: KP, GEO, SALT, SLAG, ION, Fe-data
- POLY-3 (výpočet FD)
  - Num. metoda pro řešení integračních podm FR (není presentováno)
  - POST (Grafika)
- GES, TABULATE, ata.
- Parrot (assessment FD)
- User modules



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

PD_pp

Phase Data_programme package



PD_pp:

- 4 phases, 8 comp.
- activities, chem. pot., phase ratio, ...)
- sublatice model (4. subl.)
- integral. cond.
- Linearly constrains

FIG. 1
Print screen of the user / PD-pp interface (verze 3.10)

```
                EQUILIBRIUM COMPUTING ENVIRONMENT

      CONFIGURATION            fecrc.fdc

      INPUT FILES
          problem              FERCC.PDD
          parameters           fecrc.par

      OUTPUT FILES
          equilibrium          FECRC.TIE
          errors               OERR.ERR
          variables            FECRC.VAR
          numeric method       OUFO.UFO

      STRATEGY (type y or n)
          using last equilibrium solution     y
          using last problem solution         n
          activity evaluation                 y

                        press <PgDn> for next page

  F1-Help  F3-View  F4-Edit  F5-Go  F6-Print  F7-Save  F10-Exit
```

FIG. 2
Example of input file *.PDD (verze 3.10)

```
PROBLEM DEFINITION DATA
number of elements: 3 (max.8)                    base element: Fe
system  (elements): Fe-Cr-C
number of coexisting phases: 3(max.4)          number of TIE:  1
phase 1=Fe-gamma  phase 2=M7C3       phase 3=M23C6      phase 4=

 1 TIE:                                  equilibrium temperature= 1273.00K
global content      guess of equilibrium concentrations
     [%]           phase 1 [%]    phase 2 [%]    phase 3 [%]    phase 4 [%]
Cr   45.00000      10.000000000   50.000000000   60.000000000
C     5.00000       0.500000000    8.500000000    5.500000000

 end of FECRC.PDD
```

SOPOUŠEK J., KROUPA A., DOJIVA R., VŘEŠŤÁL J. : CALPHAD 17, 1993, 229.

PD_pp
Phase diagram - programme package

FIG. 3
Fragment of file *.PAR.

Verze 3.1

```
      PARAMETERS OF THE Fe-C                          SYSTEM      PD_310.exe

Source: Per Gustafson: A Thermodynamic Evaluation of the Fe-C System,
        Scand. J. of Metall. 14, (1985) 259-267.

*****PHASE:Fe-gamma  *****
Model: Number of sublattices: 2 (max.4)
        Number of components:  3
       Sublattice Stoich.coef.     Schematic view
         1             1.0          Fe @@ @@
         2             1.0          @@ C  Va
THERMODYNAMIC PARAMETERS:
 Reference level parameters:
Fe:C
 1 59595.43 287.269 -4.22982D-8 -48.9643 2639958.5 -2.643D8 1.2D10
Fe:Va
 1 -237.57 132.416 -3.75752D-3 -5.89269D-8 -24.6643 77358.5 0.0  0.0
  Interaction parameters of the first order:   included(Y/N):[Y]
              L0                      L1                  L2
Fe:C ,Va
        -34671.0  0.0   0.0       0.0   0.0   0.0       0.0   0.0   0.0

$
  Interaction parameters of high order:        included(Y/N):[N]
MAGNETIC PARAMETERS:                           included(Y/N):[N]

*****PHASE:Fe-alpha    *****
Model: Number of ..................etc.
```

FIG. 4
Example of output file *.TIE

PD_310.exe

```
 SYSTEM: Fe-Cr-C                                          DATE 9/28/1992
EQUILIBRIUM:  Fe-gamma     M7C3       M23C6
Number of TIE:   1                              >>computed values<<
TIME 14:20: 8.87

 1 TIE:
T=1273.00[K] G syst.=  -63970.160001413O100[J] MAX INT*)NFV= 217
global cont.[%]    Fe-gamma        M7C3           M23C6
 Fe  50.0000       88.92617198     26.71823404    33.40926516
 Cr  45.0000       10.76886549     64.43949264    61.03805063
 C    5.0000        0.30496253      8.84227333     5.55268421
phase ratio [ ]:    .28910345       .43080737      .28008918
phase ener. [J]: -641333E+05    -.634807E+05   -.645545E+05

 Elem.  Chem.pot.[J mol-1]   activity
 C          -53354.21          .04316
TIME 14:20:27.82
```

*)minimization method message (5).