Vysoká škola báňská – Technická univerzita Ostrava
Fakulta metalurgie a materiálového inženýrství

POČÍTAČOVÁ SIMULACE A MODELOVÁNÍ V MATERIÁLOVÉM INŽENÝRSTVÍ

Příloha

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OBSAH

1. Aplikace software DICTRA v oblasti tepelného zpracování slitin

Čas ke studiu: 6 hodin

Cíl Po prostudování tohoto odstavce budete umět

- Využívat program DICTRA v praktických cvičeních
- Pochopíte postup programování při praktických aplikacích MI
- Naučíte se pracovat s modulem FE v programu DIGIMAT

Výklad

1.1 Definice systému: načítání dat

Aby bylo možné provést simulaci v DICTRA, jsou k tomu potřeba jak termodynamické databáze, tak kinetické databáze. Termodynamická databáze je normální databáze Thermo-Calc, zatímco kinetická databáze obsahuje informace o mobilitě (pohybu) atomů jednotlivých složek v různých fázích.

Je doporučeno, aby byl problém definován co nejjednodušší s co nejmenším počtem složek a fází.

Jak definovat systém?

Definovat systém, znamená zvolit složky a získat termodynamické a/nebo kinetické údaje o těchto složkách z příslušné databáze. Tato část popisuje, jak to provést v DATA modulu.

Předpokladem je, že se musíte nacházet v DATA modulu. Pro vstup použijte příkaz GOTO_MODULE DAT.

Chcete-li definovat systém, postupujete takto:

1. Pomocí SWITCH_DATABASE vyberete databázi.
2. Použijte DEFINE_ELEMENTS a vypište seznam prvků, které chcete do vašeho systému zahrnout. (Chcete-li zobrazit prvky, které jsou k dispozici v aktuální databázi, použijte LIST_DATABASE ELEMENTS.)
3. Fáze z databáze, které nepotřebujete, zrušíte pomocí REJECT PHASE *.
4. Obnovení fází, které by měly být zahrnuty do simulace, se provádí pomocí RESTORE PHASE.
5. Pomocí GET_DATA načtete databázi a odešlete termodynamické údaje o vašem systému do pracovního prostředí GIBBS a DICTRA.
6. Pomocí APPEND_DATABASE vyberte databázi, ze které chcete načíst kinetická data.
7. Definujte prvky a určete, zda chcete odmítnout nebo obnovit všechny fáze. Udělejte to přesně stejným způsobem jako pro termodynamická data (viz předchozí krok 2, 3 a 4).
8. Pomocí GET_DATA načtete údaje z databáze a přidáte kinetická data k termodynamickým údajům, která již existují v GIBBS a DICTRA pracovním prostředí.

Chcete-li přidat termodynamická nebo kinetická dat z další databáze, opět použijete APPEND_DATABASE. Pokud jste získali veškeré údaje, které potřebujete, můžete přistoupit k DICTRA modulu.

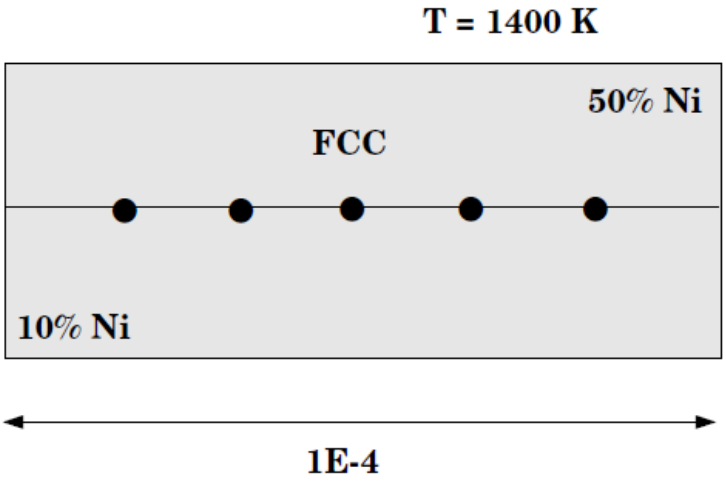
Po spuštění simulace a dokončení výpočtů můžete vytvořit obrázek či tabelovat výsledky v modulu post-procesoru, který se nazývá POST modul. Diagram je uveden v okně "DICTRA - graf" (obr. 4.2).

1.1 DIFUZE V JEDNOFÁZOVÉM SYSTÉMU

Řešené úlohy

Příklad 1.1: Homogenizace binární slitiny Fe-Ni

Příklad se zabývá homogenizací binární slitiny Fe-Ni. Předpokládáme lineární koncentrační profil Ni, který je naznačený na obr. 1.1.



Obr. 1.1 Lineární koncentrační profil v binární slitině Fe-Ni

♦ Řešení

Začneme tím, že přejdeme do databáze MODUL pomocí příkazu *SYS: goto_module* a načteme *data*. Aktuální databáze je označena *TCS Steels/Fe-Alloys Database v7.0*, ve které jsou definovány krystalografická mřížka *fcc*, krystalografická mřížka *bcc*, *vakance* a *sigma* fáze a je odmítnuta krystalografická mřížka *fcc_A1*. Pro termodynamická data využijme *TCFE databázi*. Pro konkrétní systém Fe-Ni použijeme databázi *tcfe7*. Jedná se o databázi TCS Steels/Fe-Alloys Database verze 7.0. Nyní musíme definovat systém, se kterým chceme pracovat, tj. prvky *Fe* a *Ni*. Dále vyloučíme termodynamická data pro fáze, které nejsou potřeba. Pro výpis fází použijeme *. Obnovíme termodymamická data pro fázi *fcc* a získáme data z databázového souboru. MOBILITA / DIFUZIVITA data jsou uložena v samostatném souboru databáze, který nyní načteme. Vstoupíme do DICTRA MONITORu, kde budeme nastavovat náš systém. Nastavíme hlavní a okrajové podmínky: teplotu (*T*). Začneme zadáním šířky regionu, kterou je austenit. Nastavíme krok v daném regionu. Pro jednoduchost používáme stejnou vzdálenosti kroku. Potvrdíme aktivní fáze v regionu. Pro danou fázi zadáme počátečních obsah Ni. Předpokládáme lineární změnu v regionu. Okrajová podmínka bude uzavřený systém. Dále nastavíme čas simulace. Zadání příkladu uložíme do souboru.

V další části provedeme samotný výpočet.

Posledním krokem bude grafický výstup, tj. vykreslení koncentračního profilu Ni (obr. 1.2). Znovu vstoupíme do DICTRA MONITORu a načteme uložená data.

```
SYS: goto_module
MODULE NAME: data
THERMODYNAMIC DATABASE module
Current database: TCS Steels/Fe-Alloys Database v7.0
VA DEFINED
L12_FCC B2_BCC     B2_VACANCY
HIGH_SIGMA         DICTRA_FCC_A1 REJECTED
```

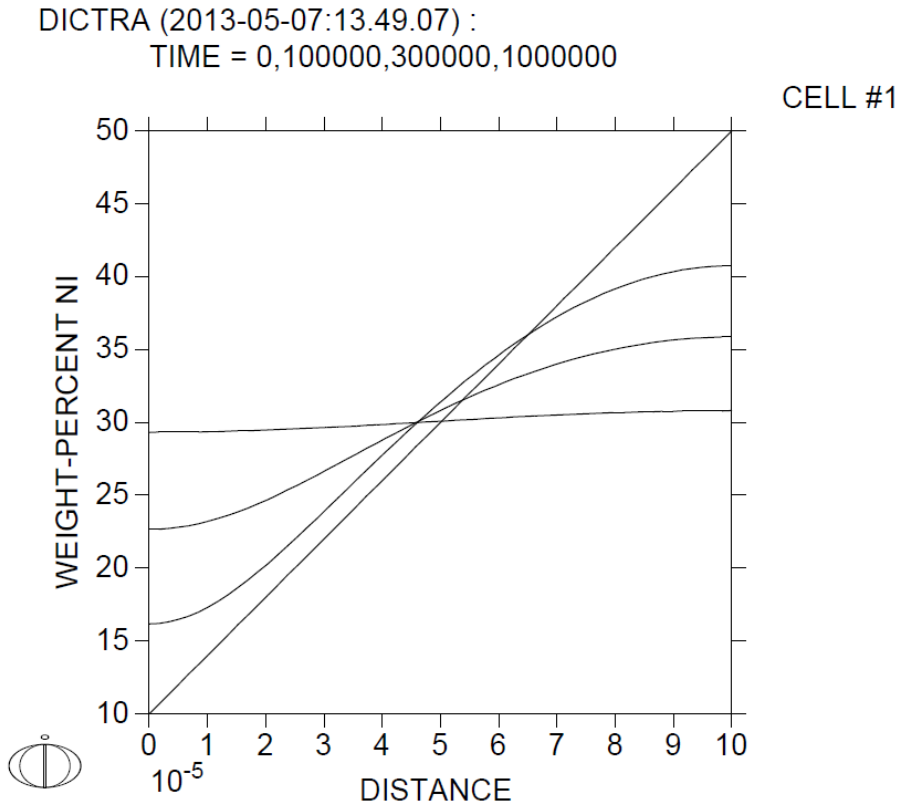
```
TDB_TCFE7: switch_database
Use one of these databases
TCFE7 = TCS Steels/Fe-Alloys Database v7.0
TCFE6 = TCS Steels/Fe-Alloys Database v6.2
TCFE5 = TCS Steels/Fe-Alloys Database v5.0
TCFE4 = TCS Steels/Fe-Alloys Database v4.1
TCFE3 = TCS Steels/Fe-Alloys Database v3.1
…
DATABASE NAME /TCFE7/: tcfe7
TDB_TCFE7: define_system
ELEMENTS: fe ni
FE      NI DEFINED
TDB_TCFE7:
TDB_TCFE7: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
LIQUID:L               BCC_A2           FCC_A1
HCP_A3  A1_KAPPA KAPPA
LAVES_PHASE_C14        NBNI3            NI3TI
REJECTED
TDB_TCFE7:
TDB_TCFE7: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
PHASES: fcc
FCC_A1 RESTORED
TDB_TCFE7:
TDB_TCFE7: get_data
REINITIATING GES5 .....
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
List of references for assessed data
'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
-OKTDB_
TCFE7:
TDB_TCFE7: append_database
Use one of these databases
…
MOBFE1 = TCS Steels/Fe-Alloys Mobility Database v1.0
MOBFE2 = TCS Steels/Fe-Alloys Mobility Database v2.0
MOBNI2 = TCS Ni-Alloys Mobility Database v2.4
MOBNI1 = TCS Ni-Alloys Mobility Database v1.0
MOBAL2 = TCS Al-Alloys Mobility Database v2.0
MOBAL1 = TCS Al-Alloys Mobility Database v1.0
MOBTI1 = TCS Ti-Alloys Mobility Database v1.0
…
DATABASE NAME /TCFE7/: mobfe2
Current database: TCS Steels/Fe-Alloys Mobility Database v2.0
TCS Steel Mobility Database Version 2.0 from 2011-12-09.
VA DEFINED
APP: define_system
ELEMENTS: fe ni
FE      NI DEFINED
APP: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
BCC_A2  FCC_A1        HCP_A3
LIQUID:L REJECTED
APP:
APP: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
```

```
PHASES: fcc
FCC_A1 RESTORED
APP:
APP: get_data
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
List of references for assessed data
'This parameter has not been assessed'
'B. Jönsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jönsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
-OKAPP:
APP: goto_module
MODULE NAME: dictra_monitor
NO TIME STEP DEFINED
DIC>
DIC> set_condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: global
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> enter_region
REGION NAME : austenite
DIC>
DIC> enter_grid_coordinates
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: linear
NUMBER OF POINTS /50/: 60
DIC>
DIC> enter_phase_in_region
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter_compositions
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weight_percent
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 10
VALUE OF LAST POINT : /0/: 50
DIC>
DIC> set_simulation_time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
```

```
DIC> @@
DIC> @@ SAVE THE SETUP ON FILE
DIC> @@
DIC> save_workspaces exa1 Y
DIC>
DIC> set_interactive
--OK---
DIC>DIC> CPU time 4 seconds


SYS: goto_module
MODULE NAME: dictra_monitor
NO TIME STEP DEFINED
DIC>
DIC> read_workspaces exa1
OK
DIC>
DIC> simulate_reaction
Automatic start values will be set
Old start values kept
Automatic start values will be set
Automatic start values will be set
Old start values kept
Automatic start values will be set
U-FRACTION IN SYSTEM:      FE = .709680021906033      NI = .290319978093967
TOTAL SIZE OF SYSTEM:      1E-04 [m]
U-FRACTION IN SYSTEM:      FE = .709680021906033      NI = .290319978093967
TOTAL SIZE OF SYSTEM:      1E-04 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906033 NI = .290319978093967
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10100000E-04 DT = 0.10000000E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906033 NI = .290319978093967
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.40101000E-02 DT = 0.40000000E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906033 NI = .290319978093967
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1.6040101 DT = 1.6000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906033 NI = .290319978093967
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 358.59620 DT = 356.99219 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906033 NI = .290319978093967
TOTAL SIZE OF SYSTEM: 1E-04 [m]
:
:
:
TIME = 582424.61 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906034 NI = .290319978093966
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 682424.61 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906034 NI = .290319978093966
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 782424.61 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906034 NI = .290319978093966
```

```
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 882424.61 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906036 NI = .290319978093964
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 982424.61 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906037 NI = .290319978093963
TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 1000000.0 DT = 17575.389 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680021906037 NI = .290319978093963
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME       0.0000000
DELETING TIME-RECORD FOR TIME       0.10000000E-06
DELETING TIME-RECORD FOR TIME       0.10100000E-04
DELETING TIME-RECORD FOR TIME       0.40101000E-02
DELETING TIME-RECORD FOR TIME       1.6040101
DELETING TIME-RECORD FOR TIME       358.59620
DELETING TIME-RECORD FOR TIME       1072.5806
DELETING TIME-RECORD FOR TIME       2500.5493
DELETING TIME-RECORD FOR TIME       5356.4868
DELETING TIME-RECORD FOR TIME       11068.362
DELETING TIME-RECORD FOR TIME       22492.112
DELETING TIME-RECORD FOR TIME       45339.612
DELETING TIME-RECORD FOR TIME       91034.611
DELETING TIME-RECORD FOR TIME       182424.61
DELETING TIME-RECORD FOR TIME       282424.61
DELETING TIME-RECORD FOR TIME       382424.61
DELETING TIME-RECORD FOR TIME       482424.61
DELETING TIME-RECORD FOR TIME       582424.61
DELETING TIME-RECORD FOR TIME       682424.61
DELETING TIME-RECORD FOR TIME       782424.61
DELETING TIME-RECORD FOR TIME       882424.61
KEEPING TIME-RECORD FOR TIME        982424.61
AND FOR TIME                        1000000.0
WORKSPACE RECLAIMED
DIC>
DIC> set_interactive
--OK---
DIC>DIC> CPU time 3 seconds


SYS: goto_module
MODULE NAME: dictra_monitor
NO TIME STEP DEFINED
DIC> read_workspaces exa1
OK
DIC>
DIC> post_processor
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : x
VARIABLE : distance
INFO: Distance is set as independent variable
DISTANCE : /GLOBAL/: global
POST-1:
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : y
```

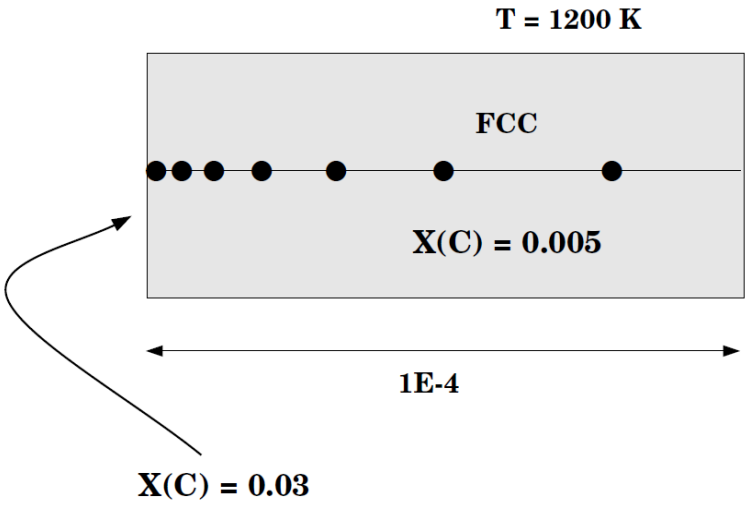
```
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: set_plot_condition
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: plot_diagram SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set_interactive
--OK---
POST-1: CPU time 0 seconds
```



Obr. 1.2 Koncentrační profil Ni v binární slitině Fe-Ni

Příklad 1.2: Nauhličování binární slitiny Fe-C

Jedná se o jednoduchou binární simulaci s jedinou fázovou oblastí. Porovnáme naše numerické simulace s analytickým erf řešením. Z tohoto důvodu byla vytvořena zvláštní databáze ERF.TDB, ve které je difuzní koeficient nastaven jako proměnná nezávislá na koncentraci Příklad je v manuálu DICTRA označen jako a4a.



Obr. 1.3 Nauhličování binární slitiny Fe-C

♦ Řešení

```
SYS: @@
SYS: @@ NAČTEME DATA Z DATABÁZE
SYS: @@
SYS: go da
SYS: go da
THERMODYNAMIC DATABASE module
Current database: TCS Steels/Fe-Alloys Database v7.0
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE7: sw ptern
Current database: TCS Public Ternary Alloys TDB v1.3
VA DEFINED
TDB_PTERN: def-system fe,c
FE C DEFINED
TDB_PTERN: rej-ph *
LIQUID:L FCC_A1 BCC_A2
HCP_A3 GRAPHITE CEMENTITE
M7C3 M23C6 V3C2
REJECTED
TDB_PTERN: rest-ph fcc
FCC_A1 RESTORED
TDB_PTERN: get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
List of references for assessed data
'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
-425, also in NPL Report DMA(A)195 Rev. August 1990'
'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
C-FE'
-OKTDB_
PTERN:
```

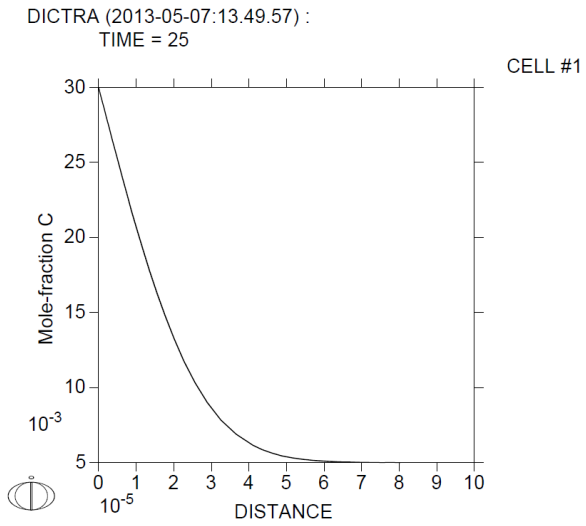
```
TDB_PTERN: append user exa4.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command
VA DEFINED
TDB_APP: def-system fe,c
FE C DEFINED
TDB_APP: rej-ph *
FCC_A1 REJECTED
TDB_APP: rest-ph fcc
FCC_A1 RESTORED
TDB_APP: get
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
-OKTDB_
APP:
TDB_APP: @@
TDB_APP: @@ PŘEJDEME DO DICTRA MODULE A NADEFINUJEME ŘEŠENÝ PROBLÉM
TDB_APP: @@
TDB_APP: go d-m
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
G(ZZDICTRA_GHOST,FE;0)-H298(BCC_A2,FE;0)
L(ZZDICTRA_GHOST,C,FE;0)
NO TIME STEP DEFINED
*** ENTERING ZZDICTRA_GHOST AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ZADÁME HLAVNÍ PODMÍNKU, KTEROU JE TEPLOTA T
DIC> @@
DIC> set-cond glob T 0 1200; * N
DIC>
DIC> @@
DIC> @@ ZADÁME REGION, KTERÝM JE OCEL (steel)
DIC> @@
DIC> enter-region
REGION NAME : steel
DIC>
DIC> @@
DIC> @@ ZADEJTE MŘÍŽKU
DIC> @@ UHLÍK VSTUPUJE DO SYSTÉMU Z DOLNÍ HRANICE, A PROTO POTŘEBUJEME NA
       TÉTO HRANICI VÍCE BODŮ. Z TOHOTO DŮVODU POUŽÍVÁME V TOMTO PŘÍPADĚ
       GEOMETRICKOU MŘÍŽKU.
DIC> @@
DIC> enter-grid
REGION NAME : /STEEL/: steel
WIDTH OF REGION /1/: 1E-4
TYPE /LINEAR/: geometric
NUMBER OF POINTS /50/: 32
VALUE OF R IN THE GEOMETRICAL SERIE : 1.11
DIC>
DIC> @@
DIC> @@ ZADEJTE FÁZE V REGIONU
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
```

```
DIC>
DIC>
DIC> @@
DIC> @@ ZADEJTE POČÁTEČNÍ SLOŽENÍ VE FÁZI FCC
DIC> @@
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.005
VALUE OF LAST POINT : /0/: 0.005
DIC>
DIC>
DIC> @@
DIC> @@ NASTAVTE FIX SLOŽENÍ JAKO MEZNÍ HODNOTU
DIC> @@
DIC> set-condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: state-variable-value
State variable expression #1 : /N=1/: n=1
State variable expression #2 : x(c)=0.03
DIC>
DIC>
DIC> @@
DIC> @@ NASTAVTE ČAS SIMULACE
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 100
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> save exa4 Y
DIC>
DIC> set-inter
--OK---
DIC>DIC> CPU time 1 seconds


SYS:SYS:SYS:SYS:
SYS:
SYS: @@ exa4_run.DCM
SYS:
SYS: @@
SYS: @@ SOUBOR PRO VÝPOČET PŘÍKLADU A4
SYS: @@
SYS:
SYS: @@
SYS: @@ ZADEJTE DICTRA MONITOR A NAČTĚTE ULOŽENÝ SOUBOR ENTER
SYS: @@
SYS: go d-m
NO TIME STEP DEFINED
DIC> read exa4
OK
DIC>
DIC> @@
```

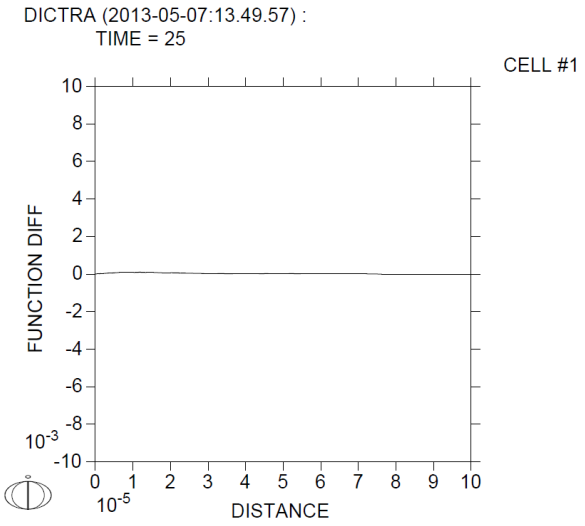
```
DIC> @@ ZAČNĚTE VÝPOČET
DIC> @@
DIC> sim
Automatic start values will be set
Old start values kept
Automatic start values will be set
Automatic start values will be set
Old start values kept
Automatic start values will be set
U-FRACTION IN SYSTEM: C = .00502512562814071 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: C = .00502512562814071 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
9 GRIDPOINT(S) ADDED TO CELL #1 REGION: STEEL
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00508348834679687 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: STEEL
TIME = 0.10100000E-04 DT = 0.10000000E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00508354928077668 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.12015107E-01 DT = 0.12005007E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0051359752161144 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.36025121E-01 DT = 0.24010014E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00519775380828899 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
:
:

:
:
TIME = 52.281132 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0111746068103599 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 62.281132 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0117364028934144 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 72.281132 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .012254676640172 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 82.281132 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0127382032368992 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 92.281132 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0131931543537021 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 100.00000 DT = 7.7188676 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0135276709326239 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10100000E-04
DELETING TIME-RECORD FOR TIME 0.12015107E-01
DELETING TIME-RECORD FOR TIME 0.36025121E-01
DELETING TIME-RECORD FOR TIME 0.84045150E-01
DELETING TIME-RECORD FOR TIME 0.18008521
DELETING TIME-RECORD FOR TIME 0.37216532
DELETING TIME-RECORD FOR TIME 0.75632555
DELETING TIME-RECORD FOR TIME 1.5246460
DELETING TIME-RECORD FOR TIME 3.0612869
DELETING TIME-RECORD FOR TIME 6.1345688
DELETING TIME-RECORD FOR TIME 12.281132
DELETING TIME-RECORD FOR TIME 22.281132
```

```
DELETING TIME-RECORD FOR TIME 32.281132
DELETING TIME-RECORD FOR TIME 42.281132
DELETING TIME-RECORD FOR TIME 52.281132
DELETING TIME-RECORD FOR TIME 62.281132
DELETING TIME-RECORD FOR TIME 72.281132
DELETING TIME-RECORD FOR TIME 82.281132
KEEPING TIME-RECORD FOR TIME 92.281132
AND FOR TIME 100.00000
WORKSPACE RECLAIMED
DIC>
DIC> @@
DIC> @@ VÝPOČET JE UKONČEN
DIC> @@
DIC>
DIC> set-inter
--OK---
DIC>DIC> CPU time 1 seconds


SYS:SYS:
SYS:
SYS: @@ exa4_plot.DCM
SYS:
SYS: @@
SYS: @@ SOUBOR PRO GRAFICKÝ VÝSTUP PŘÍKLADU
SYS: @@
SYS:
SYS: @@
SYS: @@ JDI DO DICTRA MONITORU A NAČTI ULOŽENÝ SOUBOR S VÝSLEDKY
SYS: @@
SYS: go d-m
NO TIME STEP DEFINED
DIC> read exa4
OK
DIC>
DIC> @@
DIC> @@ JDI DO POST PROCESORU
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ VYKRESLI PROFIL SLOŽENÍ
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y x(c)
POST-1: s-p-c time 25
POST-1:
POST-1: @@
POST-1: @@ ZADEJTE ANALYTICKÉ ŘEŠENÍ, S NÁZVEM ERFSOL
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: function
NAME: erfsol
FUNCTION: 0.03-0.025*erf(gd/sqrt(4*dc(fcc,c,c,fe)*25));
POST-1:
POST-1: @@
POST-1: @@ POROVNEJ ANALYTICKÉ A NUMERICKÉ ŘEŠENÍ
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: table
NAME: aaa
```

```
Variable(s) x(c) erfsol
POST-1:
POST-1: s-d-a y aaa
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: set-axis-text
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Mole-fraction C
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ VYKRESLI ROZDÍLY OBOU ŘEŠENÍ
POST-1: @@
POST-1: enter func diff=x(c)-erfsol;
POST-1: s-d-a y diff
POST-1: s-s-s y n -1e-2 1e-2
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set-interactive
--OK---

POST-1: CPU time 0 seconds
```



Obr. 1.4 Množství uhlíku v závislosti na vzdálenosti od povrchu



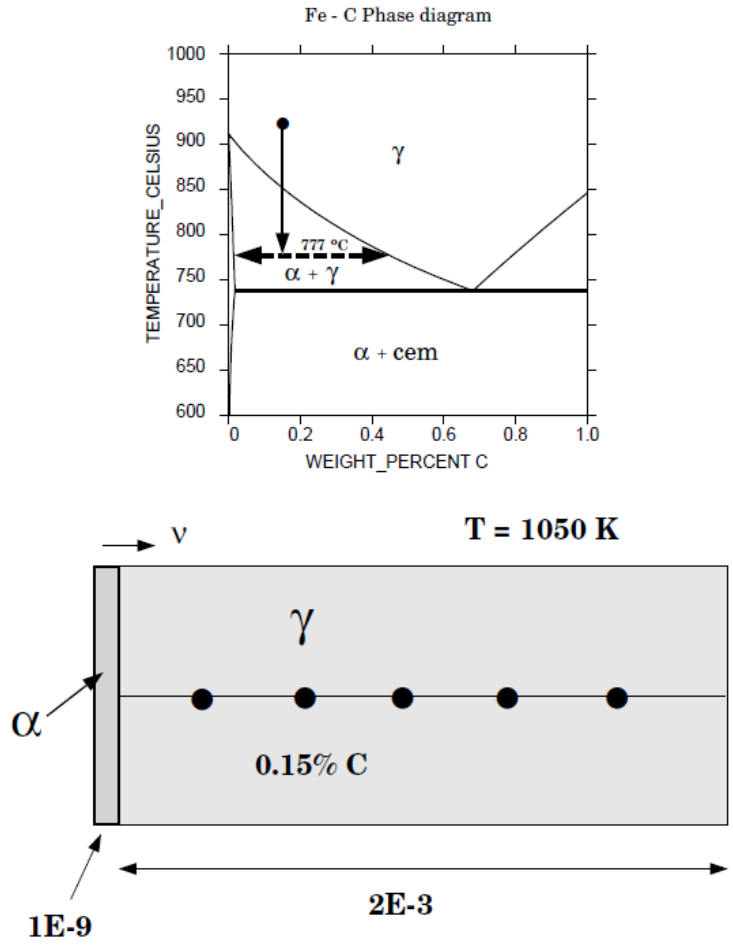
Obr. 1.5 Porovnání numerické simulace s analytickým erf řešením

1.2 PROBLÉMY POHYBU ROZHRANÍ

Řešené úlohy

Příklad 1.3: Transformace γ na α v v binární slitině Fe-C

Výchozí stav tvoří austenit o tloušťce 2 mm. Složení austenitu je Fe – 0,15 hm. % C. Po austenitizaci vzorku bylo provedeno ochlazení z teploty 1050 K. Systém je považovaný za uzavřený, takže není potřeba stanovit žádnou okrajovou podmínku (uzavřený systém je Default). Očekává se růst feritu do austenitu. Z tohoto důvodu začneme s tenkou oblastí u feritu přilehlého k austenitu (příklad b1a).



Obr. 1.6 Nauhličování binární slitiny Fe-C

```
SYS: @@
SYS: @@ ZAČNEME VSTUPEM DO MODULU DATABÁZE.
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: TCS Steels/Fe-Alloys Database v7.0
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ PRO NAČTENÍ TERMODYNAMICKÝCH DAT VYUŽIJEME DATABÁZI SSOL.
```

```
TDB_TCFE7: @@
TDB_TCFE7: sw ptern
Current database: TCS Public Ternary Alloys TDB v1.3
VA DEFINED
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ DEFINUJTE, SE KTERÝM SYSTÉMEM BUDETE PRACOVAT.
TDB_PTERN: @@
TDB_PTERN: def-sys fe c
FE C DEFINED
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ VYLUČTE TERMODYNAMICKÁ DATA PRO FÁZE, KTERÉ NEJSOU POTŘEBA.
TDB_PTERN: @@
TDB_PTERN: rej ph * all
LIQUID:L FCC_A1 BCC_A2
HCP_A3 GRAPHITE CEMENTITE
M7C3 M23C6 V3C2
REJECTED
TDB_PTERN: res ph fcc bcc
FCC_A1 BCC_A2 RESTORED
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ NAČTĚTE DATA Z DATABÁZOVÉHO SOUBORU.
TDB_PTERN: @@
TDB_PTERN: get
REINITIATING GES5 .....

ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
List of references for assessed data
'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
-425, also in NPL Report DMA(A)195 Rev. August 1990'
'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
C-FE'
'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
-OKTDB_
PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ MOBILITY/DIFFUSIVITY DATA JSOU ULOŽENA V SAMOSTATNÉM SOUBORU.
TDB_PTERN: @@ K načtení dat přidej databázi MOBILITY.
TDB_PTERN: @@
TDB_PTERN: append
Use one of these databases
TCFE7 = TCS Steels/Fe-Alloys Database v7.0
TCFE6 = TCS Steels/Fe-Alloys Database v6.2
TCFE5 = TCS Steels/Fe-Alloys Database v5.0
TCFE4 = TCS Steels/Fe-Alloys Database v4.1
TCFE3 = TCS Steels/Fe-Alloys Database v3.1
TCFE2 = TCS Steels/Fe-Alloys Database v2.1
TCFE1 = TCS Steels/Fe-Alloys Database v1.0
FEDAT = TCS/TT Steels Database v1.0
TCNI6 = TCS Ni-Alloys Database v6.0
TCNI5 = TCS Ni-Alloys Database v5.1
TCNI4 = TCS Ni-Alloys Database v4.0

……
DATABASE NAME /PTERN/: pfrib
Current database: Fridberg Dilute Fe-Alloys MDB v1.0
FE VA DEFINED
APP: def-sys fe c
FE C DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 REJECTED
APP: res ph fcc bcc
```

```
FCC_A1 BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
-OKAPP:
APP: @@
APP: @@ VSTUPTE DO DICTRA MONITORU, VE KTERÉM NASTAVÍTE VÁŠ SYSTÉM.
APP: @@
APP: go d-m
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED

G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
G(ZZDICTRA_GHOST,FE;0)-H298(BCC_A2,FE;0)
L(ZZDICTRA_GHOST,C,FE;0)
NO TIME STEP DEFINED
*** ENTERING ZZDICTRA_GHOST AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ZADEJTE HLAVNÍ PODMÍNKU, TJ. TEPLOTU T.
DIC> @@
DIC> set-condition global T 0 1050; * N
DIC>
DIC> @@
DIC> @@ ZAČNEME ZADÁNÍM OBLASTI FERITU A AUSTENITU, RESP. FÁZÍ BCC A FCC.
       FERITICKÁ OBLAST SE PŘEDPOKLÁDÁ, ŽE JE NA POČÁTKU VELMI TENKÁ, 1E-9
       M.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ DO OBLASTÍ (REGIONŮ) ZADEJTE MŘÍŽKU.
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: linear
NUMBER OF POINTS /50/: 10
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: linear
NUMBER OF POINTS /50/: 50
DIC>
DIC> @@
DIC> @@ DO OBLASTÍ (REGIONŮ) ZADEJTE AKTIVNÍ FÁZE.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
```

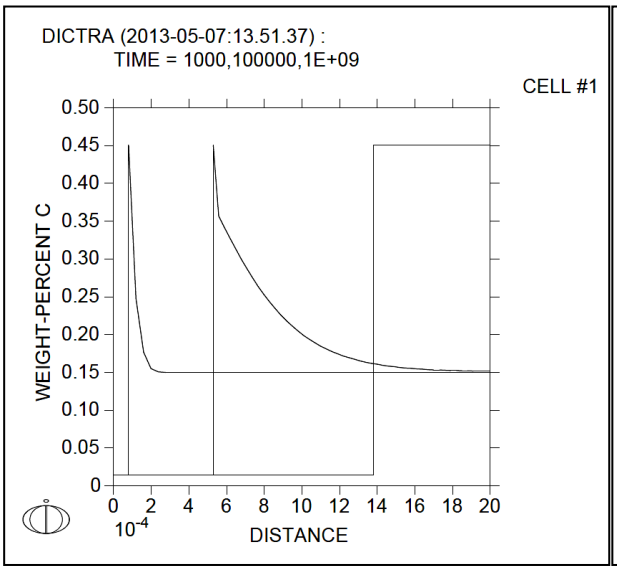
```
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ZADEJTE VSTUPNÍ SLOŽENÍ V MŘÍŽCE BCC.
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.01
VALUE OF LAST POINT : /0/: 0.01
DIC>
DIC> @@
DIC> @@ ZADEJTE VSTUPNÍ SLOŽENÍ V FCC.
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0/: 0.15
DIC>
DIC> @@
DIC> @@ OKRAJOVÁ PODMÍNKA BUDE UZAVŘENÝ SYSTÉM.
DIC> @@
DIC>
DIC> @@
DIC> @@ NASTAVTE ČAS SIMULACe.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /100000000/: 1e8
INITIAL TIMESTEP : /1E-07/: 1E-5
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-5
DIC>
DIC>
DIC> @@
DIC> @@ V TOMTO PŘÍPADĚ POUŽIJEME IMPLICITNĚ INTEGRAČNÍ ČAS (1) MÍSTO
       PŘESNĚJŠÍ, ALE MÉNĚ STABILNÍ LICHOBĚŽNÍKOVÉ METODY, KTERÁ JE METODOU
       VÝCHOZÍ.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES : /ACTIVITIES/:
```

```
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ ULOŽ NASTAVENÍ DO NOVÉHO SOUBORU A OPUSŤ DICTRA
DIC> @@
DIC> save exb1a Y
DIC>
DIC> set-inter
--OK---

DIC>DIC> CPU time 1 seconds
SYS:SYS:SYS:SYS:
SYS:
SYS: @@ exb1a_run.DCM
SYS:
SYS: @@
SYS: @@ PRŮBĚŽNÝ SOUBOR b1a
SYS: @@
SYS:
SYS: @@
SYS: @@ VSTUP DO DICTRA MONITORU A NAČTI ULOŽENÝ SOUBOR
SYS: @@
SYS: go d-m
NO TIME STEP DEFINED
DIC> read exb1a
OK
DIC>
DIC> @@
DIC> @@ ZAČÁTEK SIMULACE
DIC> @@
DIC> simulate
Automatic start values will be set
Old start values kept
Automatic start values will be set
Old start values kept
Automatic start values will be set
Trying old scheme 3
Automatic start values will be set
Old start values kept
Automatic start values will be set
Old start values kept
Automatic start values will be set
U-FRACTION IN SYSTEM: C = .00698495590385911 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
U-FRACTION IN SYSTEM: C = .00698495590385911 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
1.37555273486720901E-024
TIME = 0.10000000E-04 DT = 0.10000000E-04 SUM OF SQUARES = 0.13755527E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS 4.7520732 AND 4.7520732
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.47521732E-04
U-FRACTION IN SYSTEM: C = .00698495582692675 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE
CPU time used in timestep 0 seconds
5 GRIDPOINT(S) ADDED TO CELL #1 REGION: FERRITE
1.01085912387231901E-020
TIME = 0.30000000E-04 DT = 0.20000000E-04 SUM OF SQUARES = 0.10108591E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.72520790E-07 AND 0.72520790E-07
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.47521733E-04
U-FRACTION IN SYSTEM: C = .00698495582793217 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
CPU time used in timestep 0 seconds
26 GRIDPOINT(S) ADDED TO CELL #1 REGION: FERRITE
3.53936379252091046E-017
TIME = 0.70000000E-04 DT = 0.40000000E-04 SUM OF SQUARES = 0.35393638E-16
:
```

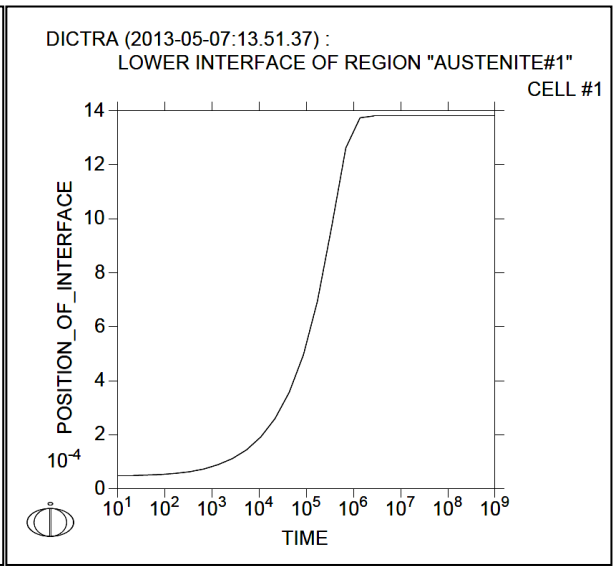
```
:
:
:
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-04
DELETING TIME-RECORD FOR TIME 0.30000000E-04
DELETING TIME-RECORD FOR TIME 0.70000000E-04
DELETING TIME-RECORD FOR TIME 0.15000000E-03
DELETING TIME-RECORD FOR TIME 0.31000000E-03
DELETING TIME-RECORD FOR TIME 0.63000000E-03
DELETING TIME-RECORD FOR TIME 0.12700000E-02
DELETING TIME-RECORD FOR TIME 0.25500000E-02
DELETING TIME-RECORD FOR TIME 0.51100000E-02
DELETING TIME-RECORD FOR TIME 0.10230000E-01
DELETING TIME-RECORD FOR TIME 0.20470000E-01
DELETING TIME-RECORD FOR TIME 0.40950000E-01
DELETING TIME-RECORD FOR TIME 0.81910000E-01
DELETING TIME-RECORD FOR TIME 0.16383000
DELETING TIME-RECORD FOR TIME 0.32767000
DELETING TIME-RECORD FOR TIME 0.65535000
DELETING TIME-RECORD FOR TIME 1.3107100
DELETING TIME-RECORD FOR TIME 2.6214300
DELETING TIME-RECORD FOR TIME 5.2428700
DELETING TIME-RECORD FOR TIME 10.485750
DELETING TIME-RECORD FOR TIME 20.971510
DELETING TIME-RECORD FOR TIME 41.943030
DELETING TIME-RECORD FOR TIME 83.886070
DELETING TIME-RECORD FOR TIME 167.77215
DELETING TIME-RECORD FOR TIME 335.54431
DELETING TIME-RECORD FOR TIME 671.08863
DELETING TIME-RECORD FOR TIME 1342.1773
DELETING TIME-RECORD FOR TIME 2684.3546
DELETING TIME-RECORD FOR TIME 5368.7091
DELETING TIME-RECORD FOR TIME 10737.418
DELETING TIME-RECORD FOR TIME 21474.836
DELETING TIME-RECORD FOR TIME 42949.673
DELETING TIME-RECORD FOR TIME 85899.346
DELETING TIME-RECORD FOR TIME 171798.69
DELETING TIME-RECORD FOR TIME 343597.38
DELETING TIME-RECORD FOR TIME 687194.77
DELETING TIME-RECORD FOR TIME 1374389.5
DELETING TIME-RECORD FOR TIME 2748779.1
DELETING TIME-RECORD FOR TIME 5497558.1
DELETING TIME-RECORD FOR TIME 10995116.
DELETING TIME-RECORD FOR TIME 21990233.
DELETING TIME-RECORD FOR TIME 43980465.
DELETING TIME-RECORD FOR TIME 87960930.
DELETING TIME-RECORD FOR TIME 0.17592186E+09
DELETING TIME-RECORD FOR TIME 0.27592186E+09
DELETING TIME-RECORD FOR TIME 0.37592186E+09
DELETING TIME-RECORD FOR TIME 0.47592186E+09
DELETING TIME-RECORD FOR TIME 0.57592186E+09
DELETING TIME-RECORD FOR TIME 0.67592186E+09
DELETING TIME-RECORD FOR TIME 0.77592186E+09
DELETING TIME-RECORD FOR TIME 0.87592186E+09
KEEPING TIME-RECORD FOR TIME 0.97592186E+09
AND FOR TIME 0.10000000E+10
WORKSPACE RECLAIMED
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SIMULACE BYLA UKONČENA
DIC> @@
DIC>
DIC> set-inter
--OK---

DIC>DIC> CPU time 5 seconds


SYS:
SYS: @@ exb1a_plot.DCM
```

```
SYS:
SYS: @@
SYS: @@ SOUBOR PRO GENEROVÁNÍ GRAFICKÉHO VÝSTUPU Z PŘÍKLADU b1a
SYS: @@
SYS:
SYS: @@
SYS: @@ VSTUP DO DICTRA MONITORU A NAČTI ULOŽENÝ SOUBOR VÝSLEDKŮ
SYS: @@
SYS: go d-m
NO TIME STEP DEFINED
DIC> read exb1a
OK
DIC>
DIC> @@
DIC> @@ JDI DO POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ GRAF ZÁVISLOSTI OBSAHU UHLÍKU NA VZDÁLENOSTI PŘI RŮZNÝCH ČASECH
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ GRAF ZÁVISLOSTI POZICE BCC/FCC ROZHRANÍ
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:
```

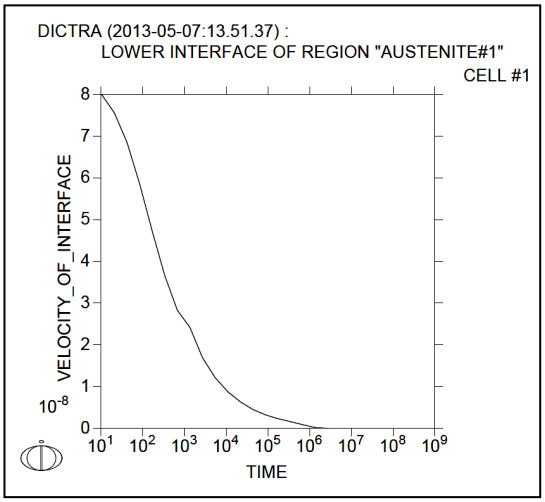
```
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ SESTROJÍ RYCHLOST BCC / FCC ROZHRANÍ
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set-inter
--OK---

POST-1: CPU time 0 seconds
```



Obr. 1.7 Graf závislosti obsahu uhlíku na vzdálenosti při různých časech



Obr. 1.8 Graf závislosti bcc/fcc rozhraní na čase



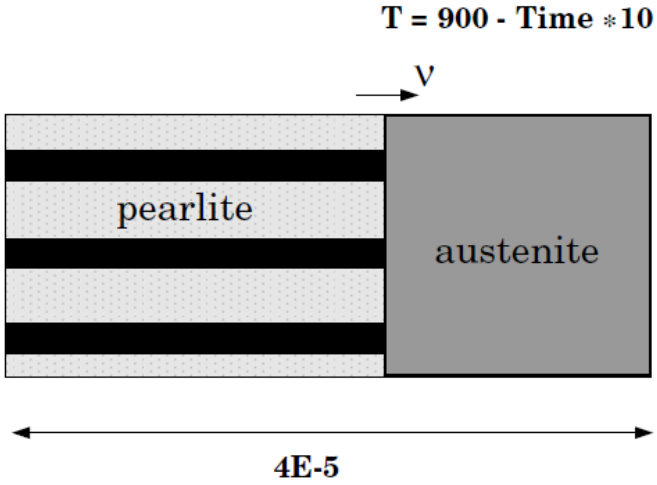
Obr. 1.9 Rychlost pohybu BCC / FCC rozhraní v závislosti na čase

1.3 KOOPERATIVNÍ RŮST

Řešené úlohy

Příklad 1.4: Růst perlitu ve slitině Fe-Mn-C

V tomto příkladu budeme řešit výpočtu růstu perlitu v oceli Fe - 0.50 hm. % C - 0.91 hm. % Mn.



Obr. 1.10 Růst perlitu do austenitu

```
SYS: @@
SYS: @@ NAČTETE DATA Z  DATATÁZE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: TCS Steels/Fe-Alloys Database v7.0
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE7: sw tcfe7
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ DEFINUJTE SYSTÉM
TDB_TCFE7: @@
TDB_TCFE7: def-sys fe c mn
FE C MN
DEFINED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ ZACHOVAT POUZE FÁZE AUSTENIT, FERIT A CEMENTIT.
TDB_TCFE7: @@
TDB_TCFE7: rej-ph /all
GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 KSI_CARBIDE
A1_KAPPA KAPPA FE4N_LP1
FECN_CHI LAVES_PHASE_C14 G_PHASE
REJECTED
TDB_TCFE7: rest-ph fcc,bcc,cem
FCC_A1 BCC_A2 CEMENTITE
RESTORED
TDB_TCFE7:
```

```
TDB_TCFE7: @@
TDB_TCFE7: @@ ZADEJTE TERMODYNAMICKÁ DATA
TDB_TCFE7: @@
TDB_TCFE7: get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
List of references for assessed data
'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
-FE'
'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
1989); C-FE-MN'
'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'P. Villars and L.D. Calvert (1985). Pearson´s handbook of
crystallographic data for intermetallic phases. Metals park, Ohio.
American Society for Metals; Molar volumes'
-OKTDB_
TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ PŘIDEJTE KINETICKÁ DATA Z DATABÁZE MOBILITY
TDB_TCFE7: @@
TDB_TCFE7: append mobfe2
Current database: TCS Steels/Fe-Alloys Mobility Database v2.0
TCS Steel Mobility Database Version 2.0 from 2011-12-09.
VA DEFINED
APP: def-sys fe c mn
FE C MN
DEFINED
APP: rej-ph /all
BCC_A2 CEMENTITE FCC_A1
FE4N_LP1 HCP_A3 LIQUID:L
REJECTED
APP: rest-ph bcc,fcc,cem
BCC_A2 FCC_A1 CEMENTITE
RESTORED
APP: get
ELEMENTS .....
SPECIES ......
PHASES .......
PARAMETERS ...
FUNCTIONS ....
List of references for assessed data
'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jönsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Bae et al.: Z. Metallkunde 91(2000)672-674; fcc Fe-Mn
Mn-Ni'
'B. Jönsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jönsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'Assessed from data presented in Landholt-Börnstein, Vol. 26, ed. H.
Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
-OKAPP:
APP: @@
APP: @@ OK, VŠECHNA TERMODYNAMICKÁ A KINETICKÁ DATA BYLA NAČTENA
APP: @@ PŘEJDĚTE DO DICTRA MONITORU A ZADEJTE VÁŠ PROBLÉM
APP: @@
APP: go d-m
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
```

```
G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
G(ZZDICTRA_GHOST,FE;0)-H298(BCC_A2,FE;0)
G(ZZDICTRA_GHOST,MN;0)-H298(CBCC_A12,MN;0)
L(ZZDICTRA_GHOST,C,FE;0)
L(ZZDICTRA_GHOST,C,MN;0)
L(ZZDICTRA_GHOST,FE,MN;0)
NO TIME STEP DEFINED
*** ENTERING ZZDICTRA_GHOST AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ NASTAVTE PODMÍNKY ZÁVISLÉ NA T
DIC> @@
DIC> set-cond glob t 0 900-time*10; * n
DIC>
DIC> @@
DIC> @@ ZADEJTE OBLASTI (REGIONY)
DIC> @@
DIC> enter-reg pearlite
DIC>
DIC> @@
DIC> @@ ZADEJTE MALÁ INICIAČNÍ MÍSTA MŘÍŽKY V PERLITICKÉ OBLASTI
DIC> @@
DIC> enter-grid pearlite 5e-10 lin 5
DIC>
DIC> @@
DIC> @@
DIC> @@ ZADEJTE DO PERLITICKÉ OBLASTI FÁZE BCC A CEM A UPŘESNĚTE, ŽE BUDOU
       PŘÍTOMNY VE FORMĚ LAMELÁRNÍ. NASTAVTE JEJICH STAV JAKO AKTIVNÍ.
       SPOUSTA OTÁZEK TAKTO KE HODNOTY PARAMETRŮ PŘÍTOMNÝCH V PERLIT RŮSTU
       MODEL TAK, POVRCHOVÉ NAPĚTÍ, OPTIMÁLNÍ TEMPO RŮSTU FACTOR, HRANICE
       DIFUZNÍ KOEFICIENTY. UHLÍK (C) SE UVNITŘ PROGRAMU CHOVÁ ZVLÁŠTNÍM
       ZPŮSOBEM, POKUD JE AUTOMATICKY ZAPSÁNA DIFUZE C, VYPOČÍTÁ SE PODLE
       ROVNICE PRO SMÍŠENÉ HRANICE A ŠIŘENÍ V OBJEMU. MÁTE NA VÝBĚR MEZI
       MANUÁLNÍ NEBO AUTOMATICKÉ SPUŠTĚNÍ HODNOT PRO VŠECHNY PROMĚNNÉ KROMĚ
       RYCHLOSTI RŮSTU, ZKUSÍME HODNOTU 1E-6DIC.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /PEARLITE/: pearlite
PHASE TYPE /MATRIX/: lam
Eutectiod reaction is "GAMMA" ==> "ALPHA" + "BETA"
Enter name of "ALPHA" phase /BCC_A2/: bcc_a2
Enter name of "BETA" phase /CEMENTITE/: cementite
Enter name of "GAMMA" phase /FCC_A1/: fcc_a1
Enter "ALPHA"/"BETA" surface tension
LOW TIME LIMIT /0/: 0
Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Enter "ALPHA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Enter "BETA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Optimum growth condition factor /2/: 2
```

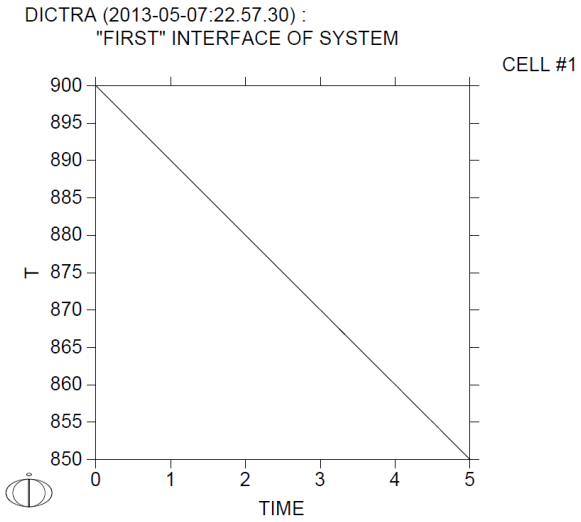
```
Name of dependent element /FE/: fe
INPUT OF DIFFUSION DATA
Growth model (VOLUME/BOUNDARY/KIRKALDY) for element C /BOUNDARY/: boundary
DF(C) = /value/AUTOMATIC/MIXED/: auto
Growth model (VOLUME/BOUNDARY/KIRKALDY) for element MN /BOUNDARY/: boundary
DF(MN) = /value/MIXED/: 5.4e-14
DQ(MN): 155000
Automatic start values for the S0 determination /Y/: Y
Growth rate V: 1E-6
Automatic start values on other variables /Y/: Y
DIC>
DIC> @@
DIC> @@ INITIATE THE COMPOSITION RECORDS FOR THE 'PEARLITE'
DIC> @@
DIC> enter-composition
REGION NAME : /PEARLITE/: pearlite
DIC>
DIC> @@
DIC> @@ NYNÍ BUDEME POKRAČOVAT DEFINICÍ MATRICE, DO KTERÉ PERLIT POROSTE.
       ZAČNEME ZADÁNÍM NÁZEVU REGIONU, OZNAČÍME HO AUSTENIT.
DIC> @@
DIC> @@
DIC> enter-region austenite
ATTACH TO REGION NAMED /PEARLITE/:
ATTACHED TO THE RIGHT OF PEARLITE /YES/:
DIC> @@
DIC> @@ URČETE, JAKÁ FÁZE FCC BUDE V OBLASTI "AUSTENIT" K DISPOZICI A JAKÝ
       TYP FÁZE "MATRICE" TO JE A JEHO PŮVODNÍ STAV AKTIVNÍ.
DIC> @@
DIC> enter-phase act austenite matrix fcc
DIC>
DIC> @@
DIC> @@ V OBLASTI AUSTENITU POTŘEBUJETE MÍT TAKÉ PROSTOROVOU MŘÍŽKU. JAKO
       HODNOTY GEOMETRICKÉHO FAKTORU MŘÍŽKY VYBERTE VELIKOST 4E-5, TYP
       MŘÍŽKY 'GEOMETRICAL', BODY MŘÍŽKY '30' X '1.5'.
DIC> @@
DIC> enter-grid austenite 4e-5 geo 30 1.5
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ZADEJTE POČÁTEČNÍ KONCENTRAČNÍ PROFIL VE FÁZI FCC V AUTENITICKÉ
       OBLASTI. KONCENTRACE MUSÍ BÝT DÁNA V Y-FRAKCÍCH.
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /MN/: fe
COMPOSITION TYPE /MOLE_FRACTION/: site-fraction
PROFILE FOR MN
TYPE /LINEAR/: lin 9.29232973E-3 9.29232973E-3
PROFILE FOR C
TYPE /LINEAR/: lin 2.3384332E-2 2.3384332E-2
DIC>
DIC> @@
DIC> @@ NYNÍ JSTE DOKONČILI ZADÁNÍ MATRICE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SPECIFIKUJTE KULOVOU GEOMETRII '2'
```

```
DIC> @@
DIC> enter-geo 2
DIC>
DIC> @@
DIC> @@ ZADEJTE ČAS SIMULACE
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 5
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /.5/: 0.1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ ULOŽTE NASTAVENÍ DO NOVÉHO SOUBORU A UKONČETE PROGRAM
DIC> @@
DIC> save exe1 Y
DIC>
DIC> set-inter
--OK---
DIC>DIC> CPU time 4 seconds

SYS: @@
SYS: @@ VSTUPTE DO DICTRA MONITORU
SYS: @@
SYS: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ OTEVŘETE SOUBOR S NASTAVENÍM
DIC> @@
DIC> read exe1
OK
DIC>
DIC> @@
DIC> @@ ZAČNĚTE SIMILACI
DIC> @@
DIC> simulate
Automatic start values will be set
Automatic start values will be set
Old start values kept
Automatic start values will be set
Trying old scheme 4
Automatic start values will be set
Automatic start values will be set
Old start values kept
Automatic start values will be set
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399292
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399292
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
17 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76465982E-05 AND 0.76465982E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.50076466E-09
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399294
MN = .00929232973121272
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE
CPU time used in timestep 1 seconds
4 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10100000E-04 DT = 0.10000000E-04 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76466217E-05 AND 0.76466217E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.57723088E-09
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399294
:
```

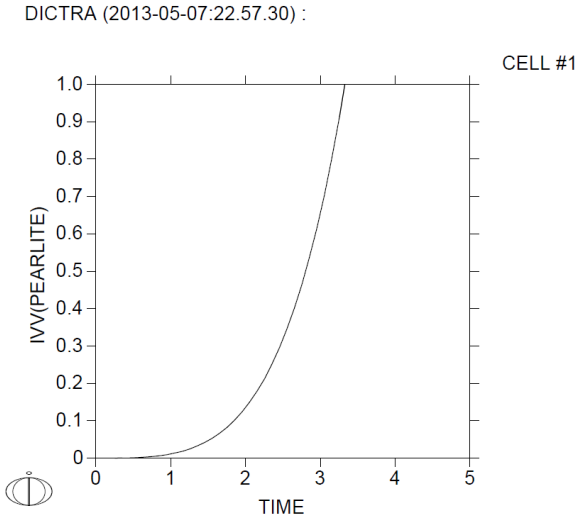
```
:
:
:
CPU time used in timestep 0 seconds
TIME = 4.6271825 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030519 FE = .990707670399278
MN = .00929232973122924
TOTAL SIZE OF SYSTEM: 2.67696400106E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 4.7271825 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030519 FE = .990707670399278
MN = .00929232973122924
TOTAL SIZE OF SYSTEM: 2.67696400106E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 4.8271825 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030519 FE = .990707670399278
MN = .00929232973122924
TOTAL SIZE OF SYSTEM: 2.67696400106E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 4.9271825 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030519 FE = .990707670399278
MN = .00929232973122924
TOTAL SIZE OF SYSTEM: 2.67696400106E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 5.0000000 DT = 0.72817470E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030519 FE = .990707670399278
MN = .00929232973122924
TOTAL SIZE OF SYSTEM: 2.67696400106E-13 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 3.2527350
DELETING TIME-RECORD FOR TIME 3.3261725
DELETING TIME-RECORD FOR TIME 3.3261825
DELETING TIME-RECORD FOR TIME 3.3271825
DELETING TIME-RECORD FOR TIME 3.4271825
DELETING TIME-RECORD FOR TIME 3.5271825
DELETING TIME-RECORD FOR TIME 3.6271825
DELETING TIME-RECORD FOR TIME 3.7271825
DELETING TIME-RECORD FOR TIME 3.8271825
DELETING TIME-RECORD FOR TIME 3.9271825
DELETING TIME-RECORD FOR TIME 4.0271825
DELETING TIME-RECORD FOR TIME 4.1271825
DELETING TIME-RECORD FOR TIME 4.2271825
DELETING TIME-RECORD FOR TIME 4.3271825
DELETING TIME-RECORD FOR TIME 4.4271825
DELETING TIME-RECORD FOR TIME 4.5271825
DELETING TIME-RECORD FOR TIME 4.6271825
DELETING TIME-RECORD FOR TIME 4.7271825
DELETING TIME-RECORD FOR TIME 4.8271825
KEEPING TIME-RECORD FOR TIME 4.9271825
AND FOR TIME 5.0000000
WORKSPACE RECLAIMED
DIC>
DIC> @@
DIC> @@ SIMULACE JE UKONČENA
DIC> @@
DIC>
DIC> set-inter
--OK---
DIC>DIC> CPU time 14 seconds

SYS:SYS:
SYS:
SYS: @@ exe1_plot.DCM
SYS:
SYS: @@
SYS: @@ SOUBOR PRO GRAFICKÝ VÝSTUP
SYS: @@
SYS:
SYS: @@
SYS: @@ JDI DO DICTRA MONITORU A NAČTI SOUBOR VÝSLEDKŮ
SYS: @@
```

```
SYS: go d-m
NO TIME STEP DEFINED
DIC> read exe1
OK
DIC>
DIC> @@
DIC> @@ JDI DO POST PROCESSORU
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ SESTROJ ZAVILOST TEPLOTY JAKO FUNKCI ČASU.
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y t
POST-1: s-p-c interface first
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NYNÍ ZNÁZORNĚTE PODÍL PERLITU VS. ČAS.
POST-1: @@
POST-1: s-d-a y ivv(pearlite)
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ MEZILAMELÁRNÍ VZDÁLENOST JAKO FUNKCE ČASU.
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : lamellar-sp
IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
CONDITION /INTEGRAL/: interface
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PODÍVEJME SE NA MEZILAMELÁRNÍ VZDÁLENOST VS. TEPLOTA.
POST-1: @@
POST-1: s-d-a x t
POST-1:
```

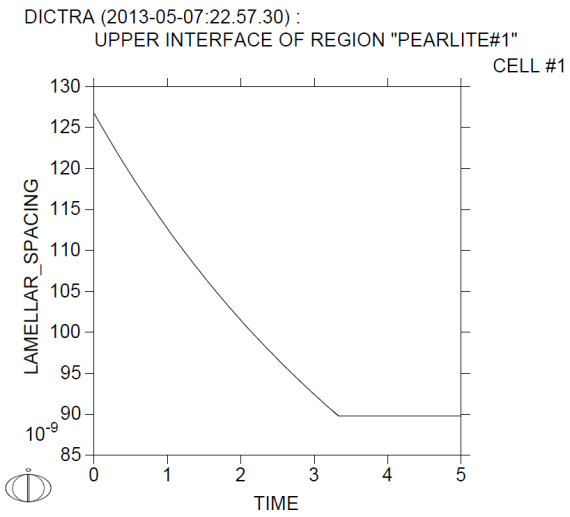
```
POST-1: s-p-c interface pearlite upper
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ A MNOŽSTVÍ UHLÍKU VE FERITU V ZÁVISLOSTI NA TEPLOTĚ.
POST-1: @@
POST-1: s-d-a y w(bcc,c)
POST-1:
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ KONEČNĚ, PODÍVEJME SE NA RYCHLOST ROZHRANÍ VS. TEPLOTA.
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x velocity
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1: set-ax-ty x log
POST-1: s-s-s x n 1e-6 1e-4
POST-1:
POST-1: plot SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1: CPU time 0 seconds
```



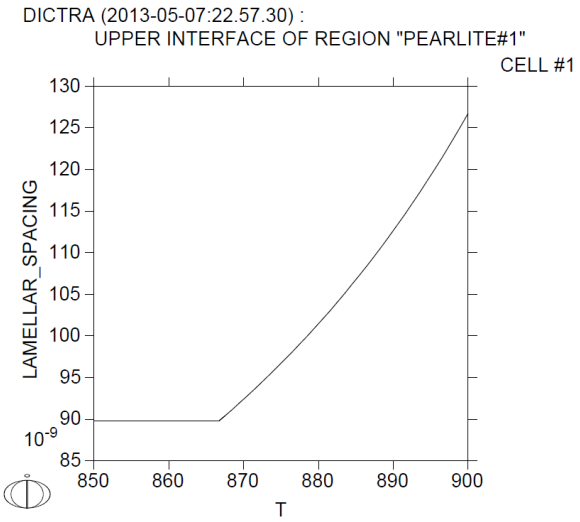
Obr. 1.11 Závislost teploty jako funkce času



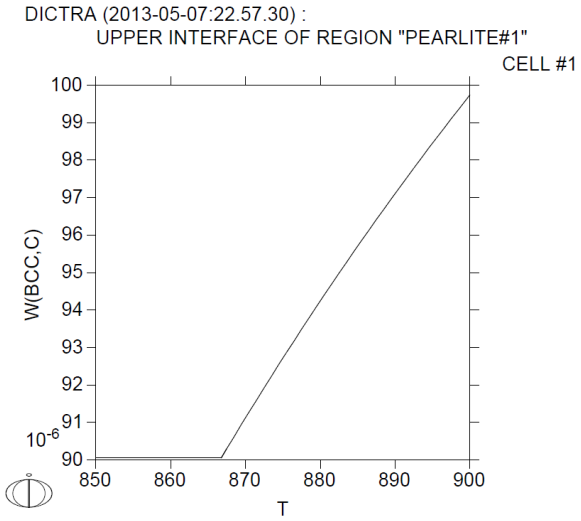
Obr. 1.12 Podíl perlitu vs. čas



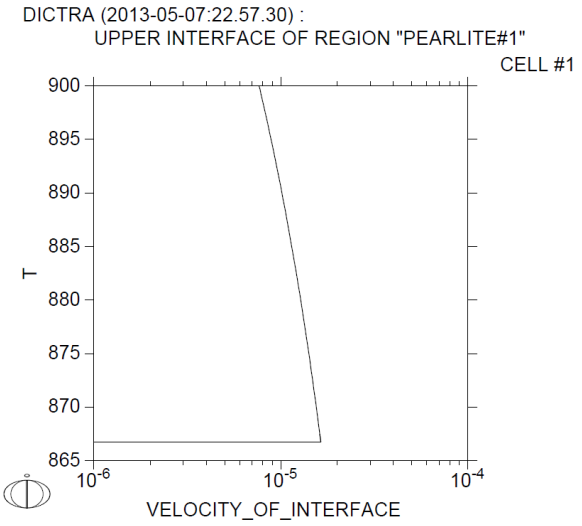
Obr. 1.13 Mezilamelární vzdálenost. jako funkce času



Obr. 1.14 Mezilamelární vzdálenost vs. teplota



Obr. 1.15 Množství uhlíku ve feritu. v závislosti na teplotě



Obr. 1.16 Rychlost rozhraní vs. teplota

2. MODELOVÁNÍ KŘIVEK SOLIDU A LIKVIDU V BINÁRNÍM SYSTÉMU

Výpis programu pro QBASIC:

```
10 REM Vypocet rozdelovacich koeficientu binarnich soustav
12 DIM T(50), M(20)
14 CLS:SCREEN 0,1:COLOR 0,3:WIDTH 40
16 LOCATE 6,10:PRINT CHR$(213)+STRING$(19,205)+CHR$(184)
18 LOCATE 7,10:PRINT CHR$(179)+STRING$(19,32)+CHR$(179)
20 LOCATE 8,10:PRINT CHR$(179)+"D O B R Y  D E N ! "+CHR$(179)
22 LOCATE 9,10:PRINT CHR$(179)+STRING$(19,32)+CHR$(179)
24 LOCATE 10,10:PRINT CHR$(212)+STRING$(19,205)+CHR$(190)
26 COLOR 4,0:LOCATE 13,2:PRINT"VYPOCET ROZDELOVACICH KOEFICIENTU"
28 LOCATE 15,10:PRINT"BINARNICH SOUSTAV"
30 COLOR 14,0:LOCATE 19,2:PRINT "ZADEJTE VASE PRIJMENI A JMENO:"
32 LOCATE 20,10:INPUT J$
34 CLS:WIDTH 80
36 COLOR 14,2:INPUT "ZAKLADNI  PRVEK :";A$
38 INPUT "PRIMESOVY PRVEK :";B$
40 PRINT:PRINT:COLOR 0,5
42 PRINT "TEPLOTA TANI ZAKLADNIHO PRVKU ";A$;"    [st.Celsia]  :";:INPUT T1
44 PRINT "TEPLOTA EUTEKTIKA NEBO PERITEKTIKA  [st.Celsia]  :";:INPUT T2
46 PRINT "MOLARNI ENTALPIE TANI ZAKLADNIHO PRVKU ";A$;" [J/mol]:";:INPUT H1
48 R=8.314:T0=273.16
49 FOR I=1 TO 8:X(I)=0:Y(I)=0:W(I)=0:Z(I)=0:NEXT I
50 PRINT:PRINT:COLOR 0,11:PRINT"S  O  L  I  D  U  S"
52 COLOR 0,7:INPUT "POCET BODU SOLIDU   :";N
54 FOR I=1 TO N
56 PRINT "BOD SOLIDU CISLO ";I;":  XS = ,  TS = ";:INPUT X(I),Y(I)
58 NEXT I
60 PRINT:PRINT:COLOR 0,4:PRINT "L  I  K  V  I  D  U  S"
62 COLOR 0,7:INPUT "POCET BODU LIKVIDU  :";M
64 FOR I=1 TO M
66 PRINT "BOD LIKVIDU CISLO ";I;": XL = ,  TL = ";:INPUT W(I),Z(I)
68 NEXT I
70 COLOR 0,2:PRINT "---------------------------------------"
72 IF N>=M THEN N5=N:GOTO 76
74 N5=M
76 CLS
78 S$=A$+" - "+B$
80 LOCATE 1,60:COLOR 14,2:PRINT "SOUSTAVA :";S$
82 PRINT:COLOR 13,0:LOCATE 3,13:PRINT "T A B U L K A   Z A D A N Y C H   H O D N O T"
84 PRINT:COLOR 0,11:PRINT "    S  O  L  I  D  U  S      ";
86 LOCATE 5,39:COLOR 0,4:PRINT "    L  I  K  V  I  D  U  S    "
88 PRINT:COLOR 0,7
90 PRINT "BOD      XS [MOL.%]     TS [C]        ";
92 PRINT "BOD      XL [MOL.%]     TL [C]":PRINT
94 FOR I=1 TO N5+1
96 PRINT USING "##       ###.####       ####.#        ";I;X(I);Y(I);
98 PRINT USING "##       ###.####       ####.#";I;W(I);Z(I)
100 NEXT I
102 PRINT:COLOR 0,6:PRINT "VOLBA REZIMU :VYPOCET       = 1"
104 PRINT "             ZMENA  SOLIDU = 2"
106 PRINT "             ZMENA LIKVIDU = 3"
108 PRINT "             NOVA SOUSTAVA = 4"
110 PRINT "             KONEC PRACE   = 5";:INPUT B5
112 ON B5 GOTO 114,234,240,14,232
114 REM Vypocet parametru solidu a likvidu
116 FOR I=1 TO 8:IF X(I)=0 THEN P=I-1:GOTO 120
118 M(I)=X(I):N(I)=Y(I):NEXT I
120 GOSUB 246
122 C$=D$:A1=D1:B1=D2
124 PRINT:COLOR 0,11
126 PRINT USING "ROVNICE  SOLIDU : TS = #######.#### XS^2 + #####.#### ";A1;B1;
128 PRINT USING "XS + ####.#  \    \";T1;C$
130 IF C$<>"O" THEN PRINT P$
```

```
132 IF A1=0 OR B1=0 THEN PRINT "NEVHODNE ZVOLENE BODY SOLIDU":GOTO 234
134 FOR I=1 TO 10:IF W(I)=0 THEN P=I-1:GOTO 138
136 M(I)=W(I):N(I)=Z(I):NEXT I
138 GOSUB 246
140 A2=D1:B2=D2
142 PRINT:COLOR 0,4
144 PRINT USING "ROVNICE LIKVIDU : TL = #######.#### XL^2 + #####.#### ";A2;B2;
146 PRINT USING "XL + ####.#  \    \";T1;D$
148 IF D$<>"O" THEN PRINT P$
150 IF A2=0 OR B2=0 THEN PRINT "NEVHODNE ZVOLENE BODY LIKVIDU":GOTO 240
152 IF B1>0 GOTO 156
154 A3=-A1:B3=-B1:GOTO 158
156 A3=A1:B3=B1
158 IF B2>0 GOTO 162
160 A4=-A2:B4=-B2:GOTO 164
162 A4=A2:B4=B2
164 P2=R*(T1+T0)^2/H1
166 COLOR 0,15:PRINT "STISKNETE <Enter>";:INPUT K$
168 IF C$<>"O" THEN INPUT "ZMENA BODU  SOLIDU ? Y/N";Y$:IF Y$="Y" THEN 76
170 IF D$<>"O" THEN INPUT "ZMENA BODU LIKVIDU ? Y/N";Z$:IF Z$="Y" THEN 76
172 REM Vypocet jednoho radku
174 DATA 0.01,0.1,1,10,100,200,500
176 RESTORE
178 FOR I=1 TO 7:READ T(I):IF T2>T1 THEN T(I)=-T(I)
180 NEXT I
182 COLOR 0,13:CLS
184 COLOR 11,0:LOCATE 3,10
186 PRINT "T A B U L K A   V Y P O C T E N Y C H   H O D N O T"
188 LOCATE 5,5:COLOR 14,2
190 PRINT "DELTA T TEPLOTA   X(SOL.)    X(LIQ.)   K 0  ";
192 PRINT "   DTH    DTH/DT"
194 LOCATE 6,5:PRINT " [K]    [ST. C]   [MOL %]    [MOL. %]  [ - ]";
196 PRINT "   [K]    [ - ] "
198 LOCATE 7,5:FOR J=1 TO 60:PRINT "-";:NEXT J:PRINT
200 COLOR 15,1
202 FOR I=1 TO 7
204 LOCATE 8+I,5
206 IF ABS(T(I))>ABS(T1-T2) THEN T(I)=T1-T2
208 S=(-B3+SQR(B3^2+4*A3*ABS(T(I))))/2/A3
210 L=(-B4+SQR(B4^2+4*A4*ABS(T(I))))/2/A4
212 T=T1-T(I):K=S/L:D=P2*(L-S)/100:E=D/T(I)
214 PRINT USING "####.##  ####.#  ###.###### ###.####  #.####";T(I);T;S;L;K;
216 PRINT USING "  ####.#  ##.###";D;E
218 IF T(I)=T1-T2 THEN 222
220 NEXT I
222 PRINT:PRINT:COLOR 0,6:PRINT "VOLBA REZIMU : NOVA SOUSTAVA   = 1"
224 PRINT "              ZMENA BODU      = 2"
226 PRINT "              TISK VYSLEDKU   = 3"
228 PRINT "              KONEC PRACE     = 4";:INPUT B6
230 ON B6 GOTO 14,76,298,232
232 END
234 COLOR 0,11:PRINT "ZMENA BODU NA  SOLIDU :"
236 PRINT "ZADEJ CISLO BODU,  XS = , TS = ";:INPUT I,X(I),Y(I)
238 GOTO 76
240 COLOR 0,7:PRINT "ZMENA BODU NA LIKVIDU :"
242 PRINT "ZADEJ CISLO BODU,  XL = , TL = ";:INPUT I,W(I),Z(I)
244 GOTO 76
246 REM Regrese parabolicke funkce
248 S2=0:S3=0:S4=0:S8=0:S9=0
250 FOR I=1 TO P
252 S2=S2+M(I)^2:S3=S3+M(I)^3:S4=S4+M(I)^4
254 S8=S8+(N(I)-T1)*M(I)^2:S9=S9+(N(I)-T1)*M(I)
256 NEXT I
258 J1=S4*S2-S3^2:D1=(S8*S2-S9*S3)/J1:D2=(S4*S9-S3*S8)/J1
260 REM Test konzistence rovnic
262 H2=ABS(T2-T1):A5=H2/10000:A6=2*H2/100:G=0
264 FOR I=1 TO 8:IF M(I)>G THEN G=M(I)
```

```
266 NEXT I
268 P$="PRUBEH KRIVKY NEODPOVIDA FYZIKALNIMU SMYSLU !"
270 A8=2*H2/G:IF D2>0 GOTO 274
272 D3=-D1:D4=-D2:GOTO 276
274 D3=D1:D4=D2
276 IF D4>A6 GOTO 282
278 IF D3<(A5-D4/100) GOTO 292
280 D$="O":RETURN
282 IF D4>=A8 GOTO 288
284 IF D3<(D4^2/(-4*H2)) GOTO 294
286 D$="O":RETURN
288 IF D3<(D4/(-2*G)) GOTO 296
290 D$="O":RETURN
292 D$="?A?":RETURN
294 D$="?B?":RETURN
296 D$="?C?":RETURN
298 REM Tisk vysledku na tiskarne
299 OPEN "SYS"+A$+B$+".VYS" FOR OUTPUT AS #3
300 PRINT #3,"Vypocet rovnovaznych rozdelovacich koeficientu systemu : ";S$
302 PRINT #3,"*****************************************************************"
304 PRINT #3,
306 PRINT #3,"Vstupni hodnoty : Teplota tani         ";A$;
308 PRINT #3,USING "   ####.# °C";T1
310 PRINT #3,"                 Peritekticka teplota    ";
312 PRINT #3,USING "   ####.# °C ";T2
314 PRINT #3,"                 Entalpie tani        ";A$;
316 PRINT #3,USING " ######.# J/mol";H1
318 PRINT #3,
320 PRINT #3,"Solidus    XS [mol. %]     TS [°C]   ";
322 PRINT #3,"Likvidus   XL [mol. %]     TL [°C]"
324 FOR I=1 TO N5
326 IF X(I)=0 GOTO 334
328 IF W(I)=0 GOTO 338
330 PRINT #3,USING "          ###.######      ####.#     ";X(I);Y(I);
332 PRINT #3,USING "          ###.####       ####.#";W(I),Z(I):GOTO 342
334 PRINT #3,"              -            -         ";
336 PRINT #3,USING "          ###.####       ####.#";W(I),Z(I):GOTO 342
338 PRINT #3,USING "          ###.######      ####.#     ";X(I);Y(I);
340 PRINT #3,"              -            -"
342 NEXT I
344 PRINT #3,:PRINT #3,"V y p o c t e n e   h o d n o t y :"
346 FOR I=1 TO 7:PRINT #3,"-----";:NEXT I:PRINT #3,:PRINT #3,
348 PRINT #3,USING "Rovnice solidu  : TS  =########.####  XS ^2  +  ";A1;
350 PRINT #3,USING "######.####  XS  +  ####.#";B1,T1
352 PRINT #3,USING "Rovnice likvidu : TL  =  ######.####  XL ^2  +  ";A2;
354 PRINT #3,USING "  ####.####  XL  +  ####.#";B2,T1
358 PRINT #3,
360 PRINT #3,"   DT     Teplota        XS          XL    ";
362 PRINT #3,"      ko         DTH       DTH/DT"
364 PRINT #3," [ K ]    [°C]      [mol. %]    [mol. %]";
366 PRINT #3,"    [ - ]       [ K ]     [ - ]"
368 FOR I=1 TO 73:PRINT #3,"-";:NEXT I:PRINT #3,
370 GOSUB 392
372 FOR I=1 TO A
374 S=(-B3+SQR(B3^2+4*A3*ABS(T(I))))/2/A3
376 L=(-B4+SQR(B4^2+4*A4*ABS(T(I))))/2/A4
378 T=T1-T(I):K=S/L
380 D=P2*(L-S)/100:E=D/T(I)
382 PRINT #3,USING "####.##   ####.##   ###.######   ###.####";T(I);T;S;L;
384 PRINT #3,USING "   ##.######   ####.##    ##.###";K;D;E
386 NEXT I
388 PRINT #3,
390 CLS:GOTO 222
392 REM Vypocet teplotnich intervalu
394 T5=ABS(T1-T2)
396 IF T1<T2 THEN T3=T1-3000:T$=STR$(T3):D1=LEN(T$):GOTO 400
398 T$=STR$(T1):D1=LEN(T$)
```

```
400 FOR I=1 TO D1
402 IF MID$(T$,I,1)="." THEN P1=D1-I
404 NEXT I
406 IF P1=0 THEN J=1 ELSE J=0
408 FOR I=P1+1 TO D1-1
410 A$(J)=RIGHT$(T$,I)
412 A(J)=VAL(A$(J)):B(J)=A(J)
414 J=J+1
416 NEXT I
418 A=1:B=0
420 FOR I=.01 TO .07 STEP .02
422 IF T1>T2 THEN T(A)=I ELSE T(A)=-I
424 T=T1-T(A):A=A+1
426 NEXT I
428 FOR I=.1 TO .7 STEP .2
430 IF A(0)=0 THEN B=1
432 IF I>=A(B) GOTO 452
434 IF T1>T2 THEN T(A)=I ELSE T(A)=-I
436 T=T1=T(A):A=A+1
438 NEXT I
440 FOR I=1 TO 9 STEP 2
442 IF I>=T5 THEN T=T2:T(A)=T1-T2:GOTO 500
444 IF I>=A(B) GOTO 464
446 IF T1>T2 THEN T(A)=I ELSE T(A)=-I
448 T=T1-T(A):A=A+1
450 NEXT I
452 IF B(1)=0 THEN A(B)=A(B)+.1
454 FOR I=A(B) TO 1 STEP .2
456 IF T1>T2 THEN T(A)=I ELSE T(A)=-I
458 T=T1-T(A):A=A+1
460 NEXT I
462 IF A(0)<>0 THEN A(B)=A(B)+1
464 IF B(1)=0 THEN A(B)=1
466 FOR I=A(B) TO 10 STEP 2
468 IF I>=T5 THEN T=T2:T(A)=T1-T2:GOTO 500
470 IF T1>T2 THEN T(A)=I ELSE T(A)=-I
472 T=T1-T(A):A=A+1
474 NEXT I
476 IF A(0)<>0 THEN B=B+1
478 IF B(1)=0 THEN A(B)=0
480 IF B(1)=0 AND B(2)=0 THEN A(B+1)=100
482 FOR I=A(B)+10 TO A(B+1) STEP 10
484 IF I>=T5 THEN T=T2:T(A)=T1-T2:GOTO 500
486 IF T1>T2 THEN T(A)=I ELSE T(A)=-I
488 T=T1-T(A):A=A+1
490 NEXT I
492 IF T1>T2 THEN K5=50 ELSE K5=-50
494 T(A)=T(A-1)+K5:T=T1-T(A)
496 IF ABS(T(A))>=T5 THEN T=T2:T(A)=T1-T2:GOTO 500
498 PRINT A,T(A),T:A=A+1:GOTO 494
500 RETURN
```

3. MODELOVÁNÍ PROCESU SMĚROVÉ KRYSTALIZACE A ZONÁLNÍHO TAVENÍ

Výpis programu pro QBASIC:

```
 CLS : SCREEN 9
 DIM C(202, 10), A(200), B(200)
  FOR I = 0 TO 160 STEP 3: LINE (320 - 2 * I, 175 - I)-(320 + 2 * I, 175 + I), 12, BF: NEXT
  COLOR 15, 1: LOCATE 9, 19: Z$ = " KONCENTRACNI PROFILY SMEROVE KRYSTALIZACE "
  FOR I = 1 TO 43: PRINT MID$(Z$, I, 1); : SOUND 0, 0: FOR K = 1 TO 300: NEXT K: SOUND 80, 2: NEXT: LOCATE
        11, 30: PRINT " A ZONALNIHO TAVENI ": FOR I = 1 TO 10000: NEXT
80 CLS : RR = 18: PP = 35: LINE (130, 223)-(510, 320), 15, B
  COLOR , 1: LOCATE RR, PP - 16: PRINT " Volba rezimu : "; : PRINT "1...smerova krystalizace": LOCATE RR + 1, PP:
        PRINT "2...zonalni taveni"
  LOCATE RR + 2, PP: PRINT "3...schematicke znazorneni": LOCATE RR + 3, PP: PRINT "4...ukonceni prace":
        LOCATE RR + 4, PP: PRINT "5...koncentracni profily"
130 V$ = INKEY$: P = VAL(V$): ON P GOSUB 500, 1000, 2000, 5000, 6500: GOTO 130
  GOTO 80
500 REM SMEROVA KRYSTALIZACE
  CLS : LINE (70, 48)-(570, 78), 4, BF: LINE (69, 47)-(571, 79), 15, B
  LOCATE 5, 21: COLOR 15, 4: PRINT " S M E R O V A  K R Y S T A L I Z A C E ":  COLOR 15, 1
  GOSUB 3000
  GOSUB 6000
  GOSUB 4000
  QQ$ = "SKZT" + RIGHT$(STR$(K1), 1)
  PRINT "  1.PRUCHOD  ": PRINT
  FOR J = 1 TO N: C3 = C1 * K1: C(0, J) = C3: W(J) = C1: L(J) = L1
  PRINT " BOD  KONCENTRACE "
  PRINT USING "###  ##.#####  "; 0; C3;
  FOR X = 1 TO L1
  C3 = -C1 * L1 * ((1 - X / L1) ^ K1 - (1 - (X - 1) / L1) ^ K1): C(X, J) = C3
  IF INT(X / 10) = X / 10 THEN PRINT
  IF INT(X / 2) = X / 2 THEN PRINT USING "###  ##.#####  "; X; C3;
  NEXT X
  IF J = N THEN PRINT : GOTO 860
  L2 = L1 * (1 - M1 / 100)
  C2 = C1 * (1 - (1 - L2 / L1) ^ K1) * L1 / L2
  PRINT : PRINT : L = INT(L2): C1 = C2
  PRINT "  "; J + 1; ".PRUCHOD  ": PRINT : P$ = STR$(J + 1)
  PRINT "Nova delka ingotu  L("; P$; ")="; L
  PRINT "Prumerna koncentrace  C("; P$; ")="; C2
  PRINT : L1 = L: NEXT
860 LOCATE 24, 1: PRINT " Tisk vysledku?...T  Zmena hodnot?...Z  Konec?...K "
870 V$ = INKEY$: IF V$ = "k" OR V$ = "K" GOTO 80
  IF V$ = "z" OR V$ = "Z" THEN ERASE C: GOTO 500
  IF V$ = "t" OR V$ = "T" THEN GOSUB 1500
  GOTO 870
  RETURN
1000 REM zonalni taveni
   CLS : LINE (70, 48)-(570, 78), 15, BF: LINE (71, 49)-(569, 77), 4, B
   LOCATE 5, 21: COLOR 15, 4: PRINT "  Z O N A L N I  T A V E N I  ":  COLOR 15, 1
   GOSUB 3000
   LOCATE 16, 12: INPUT "Delka zony.....B  ="; B1
   GOSUB 6050
   GOSUB 4000
   LOCATE 12, 19: PRINT "Delka zony.....B  ="; B1: PRINT : PRINT
   PRINT "  1.PRUCHOD  ": PRINT : PRINT " BOD  KONCENTRACE "
   S1 = 0: A(0) = K1 * C1: C(0, 1) = K1 * C1: L(1) = L1
   PRINT USING " ###  ##.#####  "; 0; C1 * K1;
   FOR X = 1 TO (L1 - B1)
   C2 = C1 + (EXP(-K1 * X / B1) - EXP(-K1 * (X - 1) / B1)) * B1 * C1 * (1 / K1 - 1)
   A(X) = C2: C(X, 1) = C2: S1 = S1 + C2
   IF INT(X / 2) * 2 = X THEN PRINT USING "###  ##.#####  "; X; C2;
   NEXT X: S8 = C1 * (L1 - B1) + C1 * B1 * (1 / K1 - 1) * (EXP(-K1 * (L1 / B1 - 1)) - 1)
   C4 = (C1 * L1 - S8) / B1
   FOR Z = 1 TO B1
```

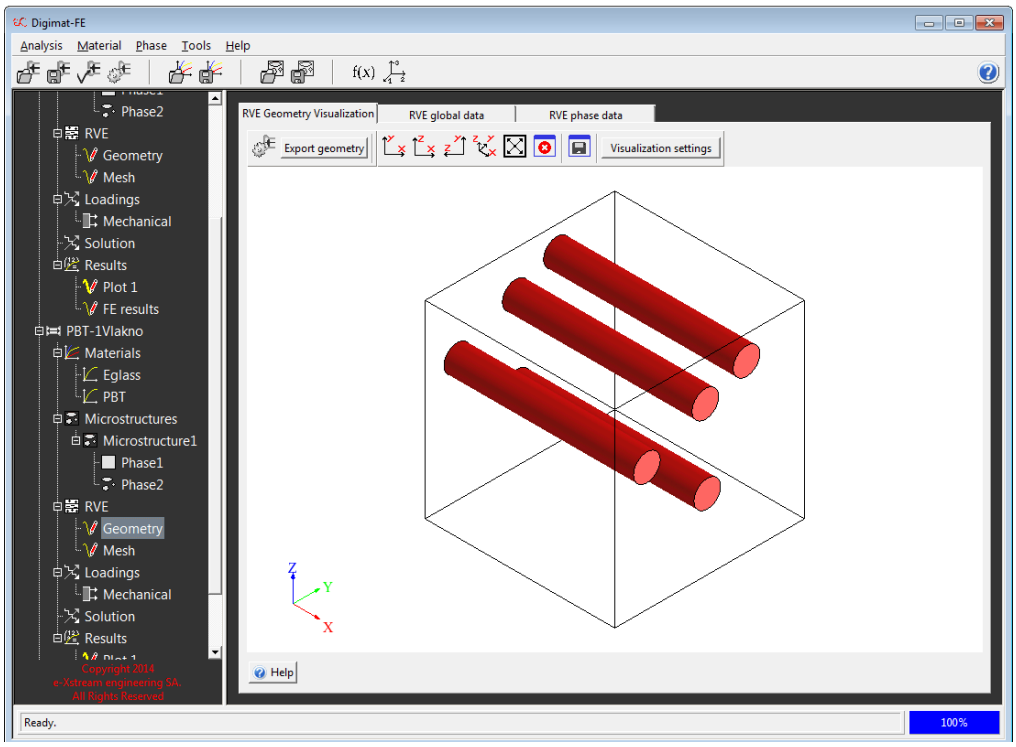
```
   C3 = -C4 * B1 * ((1 - Z / B1) ^ K1 - (1 - (Z - 1) / B1) ^ K1)
   S1 = S1 + C3: X = Z + L1 - B1: A(X) = C3: C(X, 1) = C3
   IF INT(X / 2) * 2 = X THEN PRINT USING "###  ##.#####   "; X; C3;
   NEXT Z: PRINT : Q1 = 2 * K1 / (2 * B1 + K1)
   FOR H = 2 TO N: L = INT(L1 * (1 - M1 / 100)): L(H) = L
   PRINT "   "; H; ".PRUCHOD   ": PRINT : P$ = STR$(H)
   PRINT "Nova delka ingotu      L("; P$; ")="; L: PRINT : PRINT " BOD   KONCENTRACE "
   L2 = L: S3 = 0: S4 = 0
   FOR X = 0 TO B1: S3 = S3 + A(X): NEXT X: B(0) = K1 * S3 / B1: C(0, H) = B(0)
   REM  Vypocet suma c(n-1){x+b}
   FOR X = 0 TO L2 - B1: S3 = S3 + A(B1 + X): C5 = Q1 * (S3 - S4): B(X) = C5: S4 = S4 + C5: C(X, H) = C5
   IF INT(X / 2) * 2 = X THEN PRINT USING "###  ##.#####   "; X; C5;
   NEXT X: C9 = (S3 - S4) / B1
   FOR Z = 1 TO B1
   C5 = -C9 * B1 * ((1 - Z / B1) ^ K1 - (1 - (Z - 1) / B1) ^ K1)
   S4 = S4 + C5: X = Z + L2 - B1: B(X) = C5: C(X, H) = C5
   IF INT(X / 2) * 2 = X THEN PRINT USING "###  ##.#####   "; X; C5;
   NEXT Z: PRINT : FOR X = 0 TO L1
   A(X) = 0: A(X) = B(X): B(X) = 0: NEXT X: L1 = L2: PRINT : PRINT : NEXT H
   LOCATE 24, 1: PRINT " Tisk vysledku?...T    Zmena hodnot?...Z    Konec?...K "
1475 V$ = INKEY$: IF V$ = "k" OR V$ = "K" THEN ERASE A, B: GOTO 80
   IF V$ = "z" OR V$ = "Z" THEN ERASE A, B, C: GOTO 1000
   IF V$ = "t" OR V$ = "T" THEN GOSUB 1500
   GOTO 1475
   RETURN
1500 REM tisk vysledku
   OPEN "SKZT.PRN" FOR OUTPUT AS #3
   IF B1 <> 0 THEN PRINT #3, "              ZONALNI TAVENI S ODVODEM MATERIALU": GOTO 1520
   PRINT #3, "           SMEROVA KRYSTALIZACE S ODVODEM MATERIALU"
1520 PRINT #3, "           ----------------------------------------"
   PRINT #3, "KONCENTRACNI PROFILY": PRINT #3, :
   PRINT #3, "Zadane hodnoty:"
   PRINT #3, "Vychozi koncentrace.......C0   = "; C0
   PRINT #3, "Vychozi delka ingotu......L0   = "; L0
   PRINT #3, "Rozdelovaci koeficient....K    = "; K1$
   PRINT #3, "Odvedena cast ingotu......M[%] = "; M1
   PRINT #3, "Pocet pruchodu............N    = "; N
   IF B1 <> 0 THEN PRINT #3, "Delka zony.................B    ="; B1
   FOR J = 1 TO N
   PRINT #3, : PRINT #3, : PRINT #3, "  "; J; ".PRUCHOD": PRINT #3, "---------------"
   PRINT #3, "Delka ingotu          L("; J; ")="; L(J)
   IF B1 = 0 THEN PRINT #3, "Prumerna koncentrace   C("; J; ")="; W(J)
   PRINT #3, : PRINT #3, "BOD   KONCENTRACE"
   FOR I = 0 TO L0 STEP 1
   IF C(I, J) = 0 GOTO 1685
   PRINT #3, USING "###.#####  "; C(I, J);
   NEXT I
1685 PRINT #3, : NEXT J
   COLOR 15, 1: RETURN
2000 REM
   CLS : LINE (0, 0)-(639, 349), 7, BF
   LINE (70, 48)-(570, 78), 9, BF: LINE (69, 47)-(571, 79), 4, B: LOCATE 5, 14
   COLOR 15, 8: PRINT " S C H E M A   S M E R O V E   K R Y S T A L I Z A C E "
   GOSUB 2300
   LINE (120, 170)-(520, 200), 4, BF
   FOR I = 1 TO 5000: NEXT: FOR L = 120 TO 515: FOR QW = 1 TO 100000: NEXT
   LINE (L, 170)-(L + 5, 200), 14, BF: LINE (120, 170)-(L, 200), 1, BF: FOR J = 1 TO 120: NEXT: NEXT: LINE (515,
         170)-(520, 200), 1, BF: FOR I = 1 TO 5000: NEXT
   REM ZONA
   LINE (0, 0)-(639, 349), 7, BF
   LINE (70, 48)-(570, 78), 2, BF: LINE (69, 47)-(571, 79), 4, B: LOCATE 5, 18
   COLOR 15, 9: PRINT " S C H E M A   Z O N A L N I H O   T A V E N I "
   GOSUB 2300
   LINE (120, 170)-(520, 200), 1, BF
   FOR I = 1 TO 5000: NEXT: FOR L = 150 TO 515: FOR QQ = 1 TO 100000: NEXT
   LINE (L, 170)-(L + 5, 200), 14, BF: LINE (L - 30, 170)-(L - 1, 200), 4, BF: LINE (L - 31, 170)-(L - 36, 200), 14, BF:
         LINE (L - 37, 170)-(L - 42, 200), 1, BF
```

```
    NEXT: LINE (478, 170)-(520, 200), 1, BF: FOR I = 1 TO 5000: NEXT
    COLOR 15, 1: GOTO 80
2300 LINE (80, 250)-(190, 270), 4, BF: LOCATE 19, 14: PRINT "tavenina"
    LINE (250, 250)-(370, 270), 1, BF: LOCATE 19, 36: PRINT "krystal"
    LINE (430, 250)-(540, 270), 14, BF: LOCATE 19, 58: PRINT "rozhrani"
    RETURN
    RETURN
3000 REM
    LOCATE 11, 12: INPUT "Vychozi koncentrace.......C0  ="; C1: C0 = C1
    LOCATE 12, 12: INPUT "Vychozi delka ingotu......L0  ="; L1: L0 = L1
    LOCATE 13, 12: INPUT "Rozdelovaci koeficient....K   ="; K1: K1$ = STR$(K1)
    LOCATE 14, 12: INPUT "Odvedena cast ingotu......M(%)="; M1
    LOCATE 15, 12: INPUT "Pocet pruchodu............N   ="; N
    RETURN
4000 REM
    LOCATE 6, 8: PRINT "Zadane hodnoty:": PRINT
    LOCATE 7, 19: PRINT "Vychozi koncentrace.......C0   ="; C1: C0 = C1
    LOCATE 8, 19: PRINT "Vychozi delka ingotu......L0   ="; L1: L0 = L1
    LOCATE 9, 19: PRINT "Rozdelovaci koeficient....K    ="; K1
    LOCATE 10, 19: PRINT "Odvedena cast ingotu......M[%] ="; M1
    LOCATE 11, 19: PRINT "Pocet pruchodu............N    ="; N
    RETURN
5000 END
6000 CLS : LINE (130, 10)-(505, 30), 5, B
    LOCATE 2, 21: PRINT "SMEROVA KRYSTALIZACE S ODVODEM MATERIALU"
    LOCATE 4, 30: PRINT "KONCENTRACNI PROFILY"
    RETURN
6050 CLS : LINE (130, 10)-(505, 30), 5, B
    LOCATE 2, 21: PRINT "   ZONALNI TAVENI S ODVODEM MATERIALU   "
    LOCATE 4, 30: PRINT "KONCENTRACNI PROFILY"
    RETURN
6500 M5 = 200 / L0: L3 = INT(M5 * L0): L0 = L3
    J = 0: A8 = 40: A7 = .00001: A9 = .0001: K = 8
    IF K1 >= .2 THEN A5 = 1: A6 = 10: A7 = .01: A8 = 90: A9 = .1: K = 5
    IF K1 >= .4 THEN A7 = .1: A9 = 1: K = 4
    CLS : KEY OFF: SCREEN 9: COLOR 15, 1
    FOR I = 20 TO 300 STEP A8
    IF K1 >= .4 AND I = 200 GOTO 6545
    LINE (100, I)-(550, I)
6545 NEXT I
    LINE (100, 99 + A6)-(550, 99 + A6)
    FOR I = 100 TO 550 STEP 45
    LINE (I, 20)-(I, 300 - A6)
    NEXT I
    FOR I = 12 TO 77 STEP 11
    IF J = 1 THEN I = I + 1
    LOCATE 23 - A5, I: PRINT J
    J = J + .2: NEXT I
    DATA 100,0,10,1,1,2,0.1,1,0.01,0,0.001,-1,0.0001,-2,0.00001,-3
    FOR I = 1 TO 8: READ N2(I), N1(I): NEXT I
    LOCATE 2, 20
    IF B1 <> 0 THEN PRINT "KONCENTRACNI PROFILY ZONALNIHO TAVENI": GOTO 6602
    PRINT "KONCENTRACNI PROFILY SMEROVE KRYSTALIZACE"
6602 IF K1 > 1 THEN LL = 10
    LOCATE LL + 4, 16: PRINT "K ="; K1: LOCATE LL + 5, 16: PRINT "L0="; L(1)
    IF B1 <> 0 THEN LOCATE LL + 6, 16: PRINT "B ="; B1
    LOCATE 7 + A5, 30: PRINT "C0 = 1": LOCATE 7, 5: PRINT "C"
    LOCATE 8, 5: PRINT "^"
    LINE (35, 100)-(35, 140)
    IF K1 >= .4 THEN A8 = 180: GOTO 6655
    IF K1 >= .2 GOTO 6645
    FOR I = 1 TO 8: LOCATE 2 + 2.8 * (I - 1), 8 + N1(I): PRINT N2(I): NEXT I
    GOTO 6665
6645 FOR I = 2 TO 5: LOCATE 2 + 6.3 * (I - 2), 8 + N1(I): PRINT N2(I): NEXT I
    GOTO 6665
6655 LOCATE 2, 11: PRINT "3"
    FOR I = 3 TO 4: LOCATE 8 + 12.6 * (I - 3), 8 + N1(I): PRINT N2(I): NEXT I
```

```
6665 N2 = N2(K): L = K - 1
    FOR I = 1 TO 66
    IF K1 >= .4 AND N2 > 3 GOTO 6710
    IF K1 >= .2 AND N2 > 9 GOTO 6710
    C5 = LOG(N2) / LOG(10): Y = 100 + A6 - C5 * A8
    N2 = N2 + N2(K)
    IF N2 >= N2(L) THEN K = K - 1: N2 = N2(K): L = K - 1
    LINE (100, Y)-(110, Y): LINE (540, Y)-(550, Y)
    NEXT I
6710 FOR J = 1 TO N
    FOR I = 0 TO L0
    IF B1 <> 0 THEN C2 = C(I, J): X = 100 + 45 * M5 * I / 20: GOTO 6725
    C2 = -C0 * L0 * ((1 - I / L0) ^ K1 - (1 - (I - 1) / L0) ^ K1): X = 100 + 45 * I / 20
6725 IF C2 = 0 GOTO 6765
    IF C2 < A7 GOTO 6750
    C = LOG(C2) / LOG(10): Y = 100 + A6 - C * A8
    IF B1 <> 0 AND X > 178 AND X < 185 THEN Z = INT(Y / 13.5): LOCATE Z + 1, 20: PRINT J: GOTO 6745
    IF B1 = 0 AND I = 35 THEN Z = INT(Y / 13.5): LOCATE Z + 1, 20: PRINT J
6745 CIRCLE (X, Y), 1
6750 NEXT I
    L1 = L0 * (1 - M1 / 100): C1 = C0 * (1 - (1 - L1 / L0) ^ K1) * L0 / L1: C0 = C1: L0 = INT(L1)
6765 NEXT J
    LOCATE 24, 40: PRINT "PODIL TUHE FAZE  G  ----->"
    COLOR 14, 1: LOCATE 23, 1
    END
```

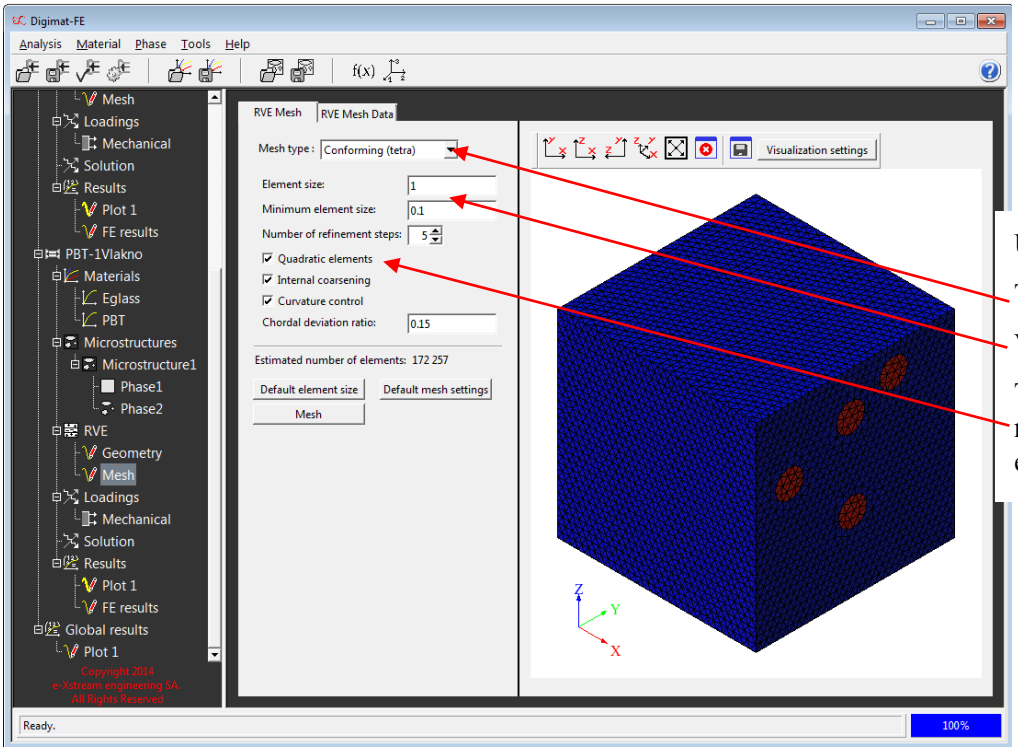
4. APLIKACE MODULU FE V PROGRAMU DIGIMAT

Modul FE-Solver



Generování struktury

Generování sítě



Uživatel nastaví jen:

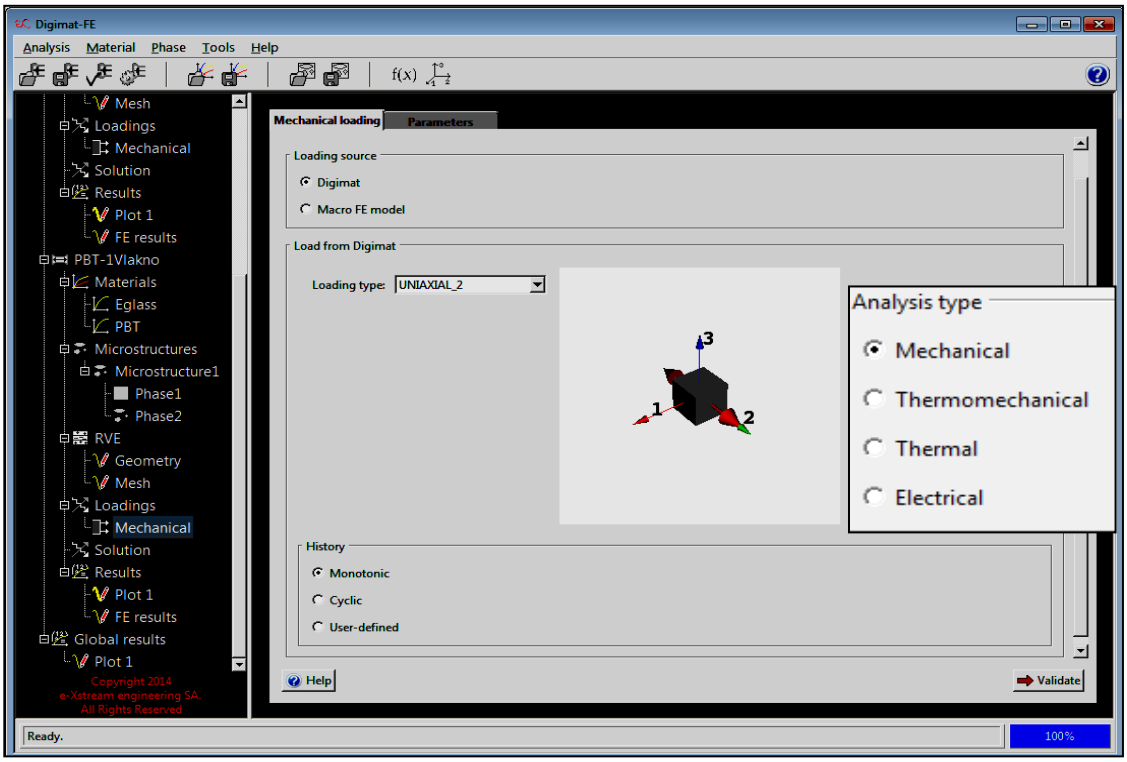
Typ sítě

Velikost elementů

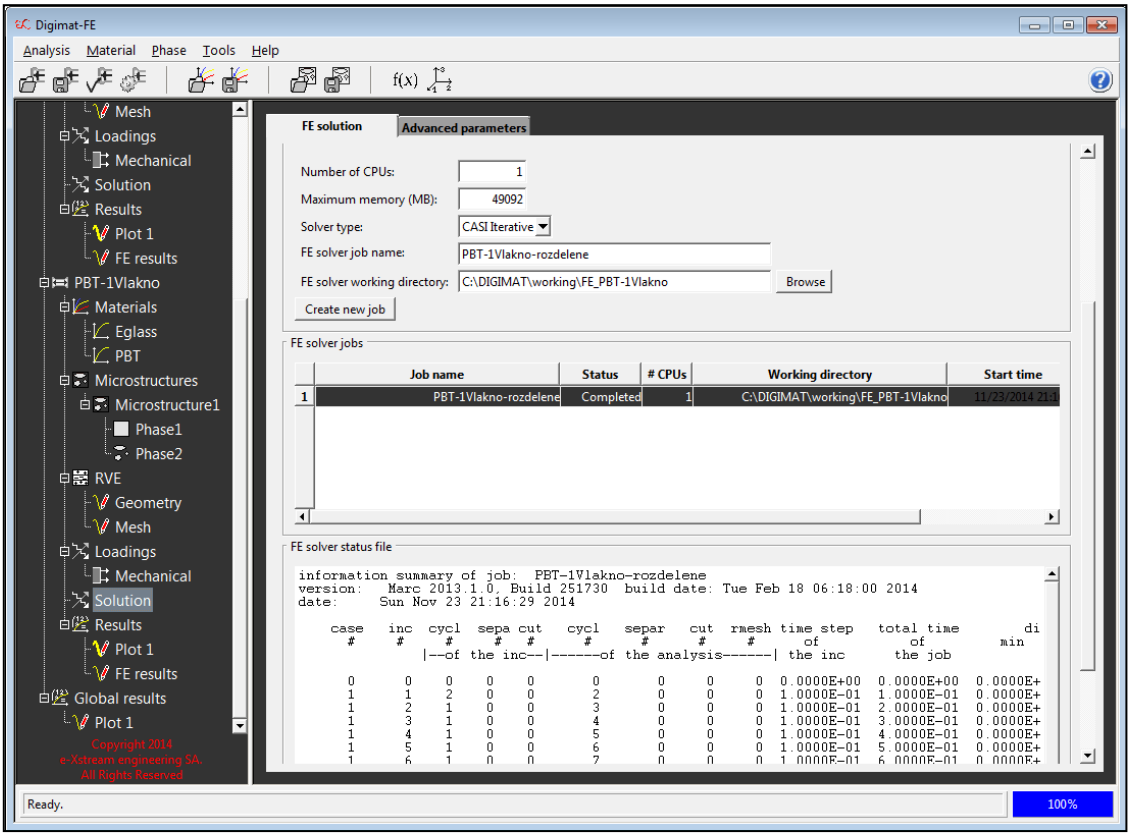
Typ elementů bez nutnosti napojení na externí software

Síť je vygenerována v Digimatu

Definování zatížení a typy analýz

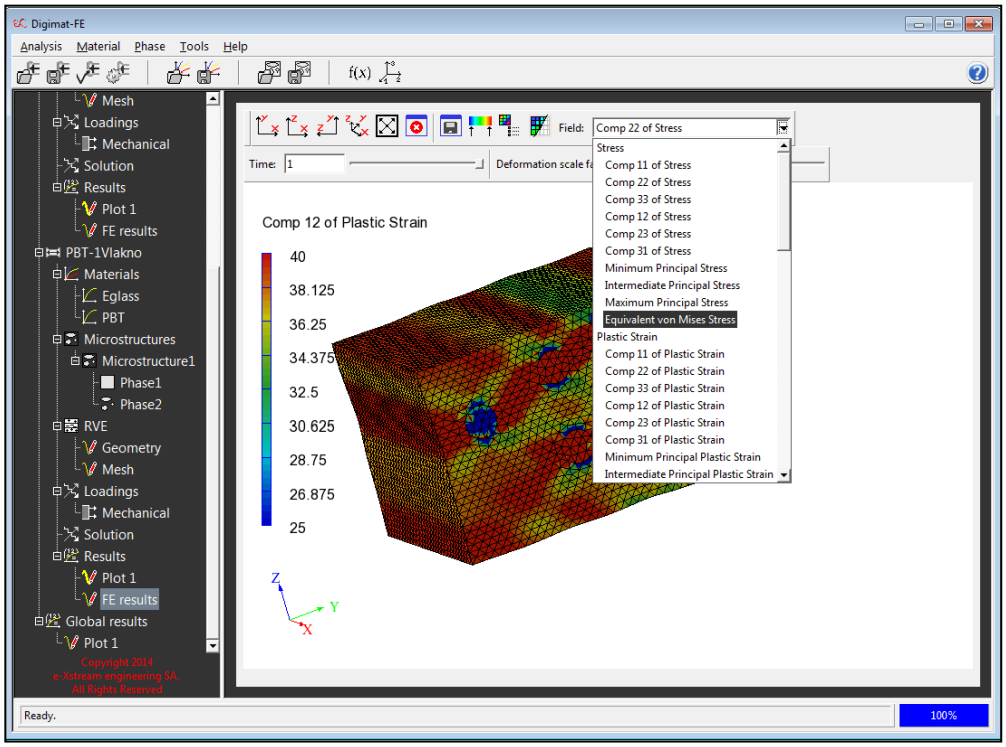


Výpočet

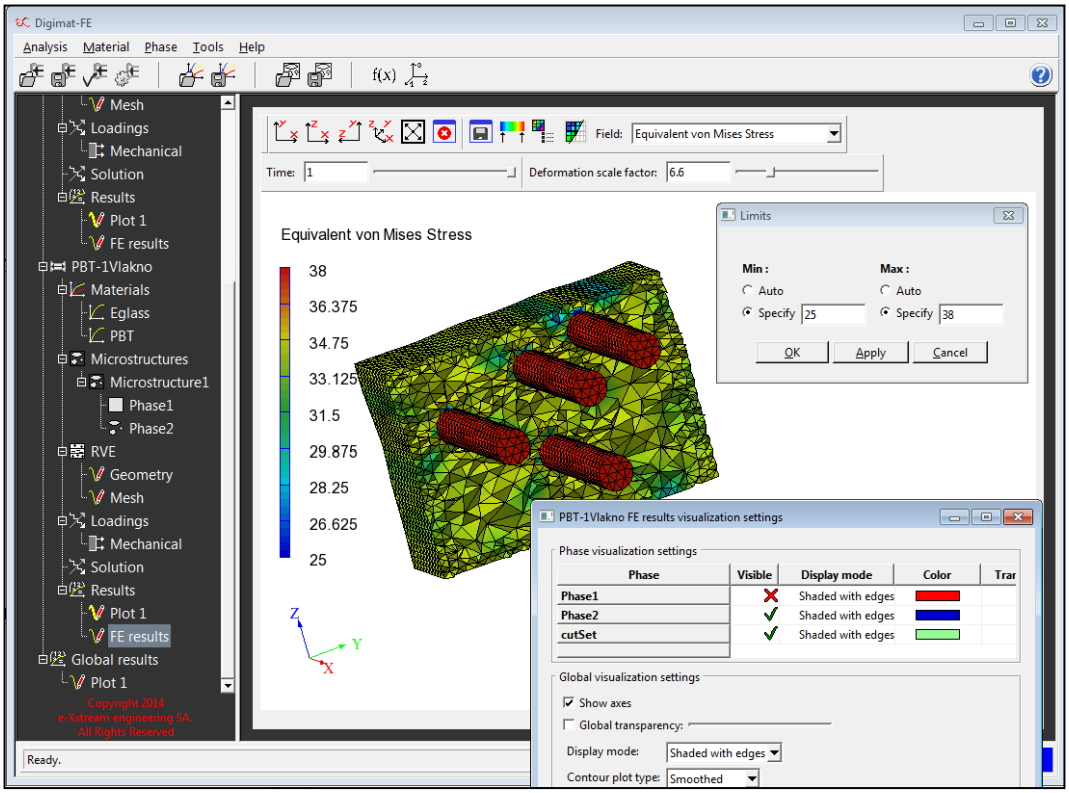


Uživatel zadá jen typ řešiče, počet jader a velikost výpočetního kroku… Analýza je následně automaticky spuštěna (na jádře software Marc)

Vyhodnocení výsledků

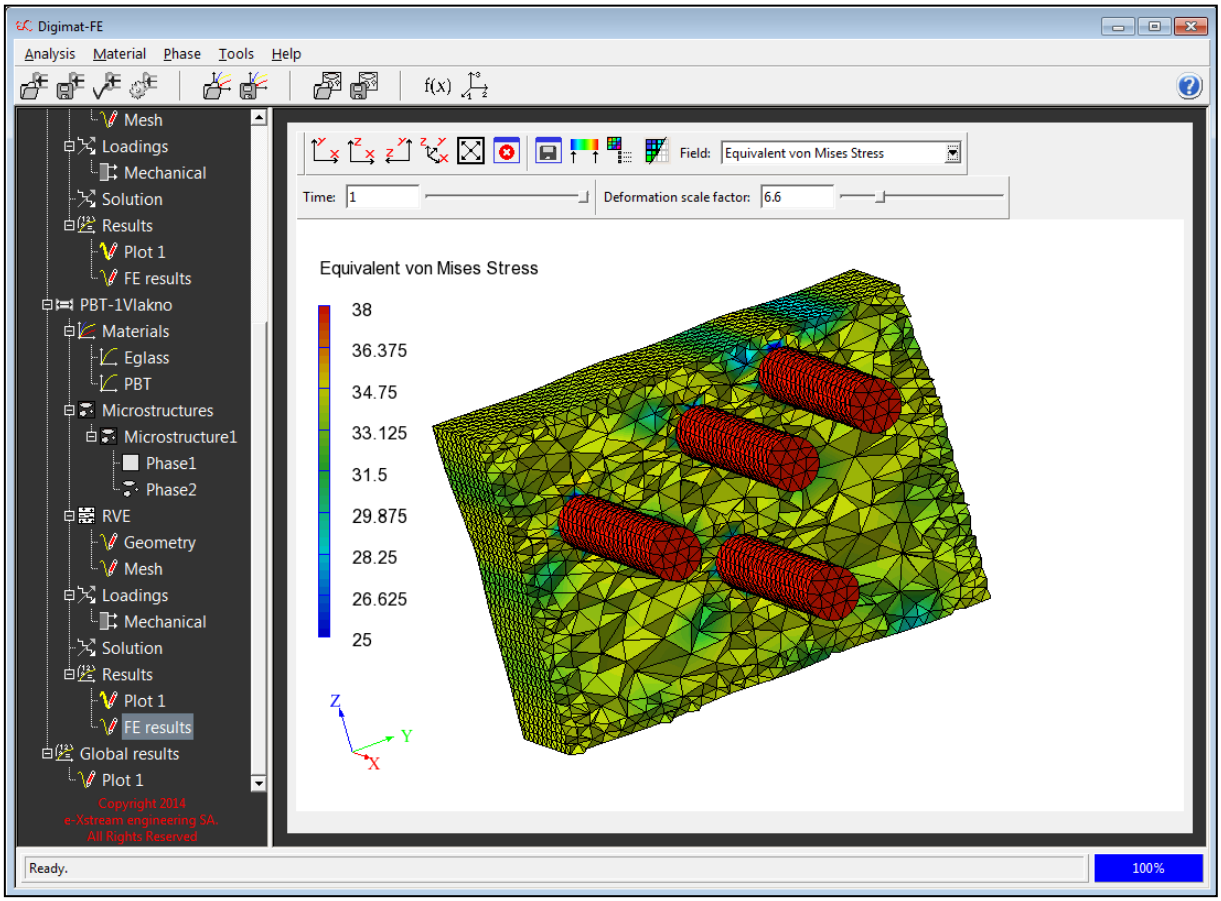


Po dopočítání analýzy uživatel může vyhodnocovat různé typy výsledků přímo v prostředí Digimatu.



Výsledky lze znázorňovat jak na jednotlivých složkách kompozitu, tak i v kombinaci řezu + složka kompozitu. Lze volit rozsahy zobrazovaných výsledků i např. typ znázornění jednotlivých složek.

Hlavní přínos



Modul FE-Solver umožňuje provádět analýzy struktur i uživatelům bez předchozí znalosti strukturálních softwarů. Vhodné i do výuky, kdy studenti budou pracovat s menšími modely – výsledky analýz během doby cvičení (dle velikosti modelu).