Research and Development Center for Bioengineering (BioIRC) and University of Kragujevac

M. Kojic, M. Milosevic, V. Simic, B. Milicevic

PAK-KTM

PROGRAM FOR STRUCTURAL ANALYSIS - KOJIC TRANSPORT MODEL

REQUIREMENTS AND USERS MANUAL

Kragujevac, 2023
SERBIA

CONTENTS

A. REQUIREMENTS

Windows:

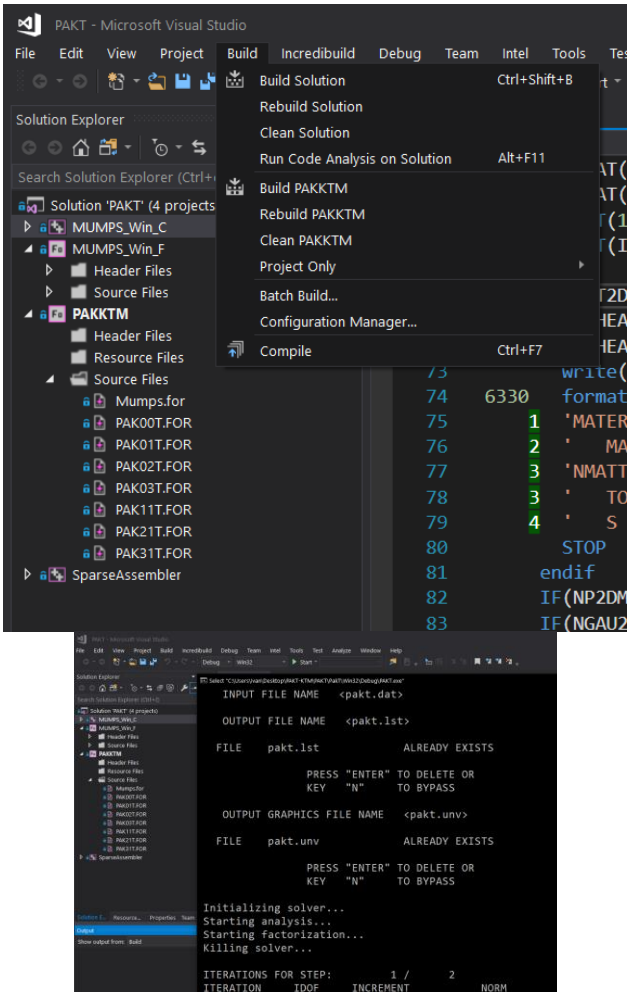
- VisualStudio >=2017
- Intel® oneAPI Base Toolkit
- Intel® Distribution for GDB*
- Intel® oneAPI HPC Toolkit

Linux:

- GNU Fortran (GCC) 4.4.7 20120313
- The C compiler GNU 4.4.7
- MUMPS 5.0.2.

Compile and run PAKKTM on Windows:

Download code from github and open visual studio. As start-up project set PAKKTM and build project. Once the project is succesfully built you can run pakktm by pressing the Start button as shown below.



Once you build the project, you will have the executable file PAKT.exe in one of the following directories, depending on the configuration chosen:

PAKT-KTM\PAKKTM\PakKTM\Win32\Debug (Configuration: Win32 Debug)
PAKT-KTM\PAKKTM\PakKTM \Win32\Release (Configuration: Win32 Release)
PAKT-KTM\PAKKTM\PakKTM \Win64\Debug (Configuration: Win64 Debug)
PAKT-KTM\PAKKTM\PakKTM\Win64\Release (Configuration: Win64 Release)

This is a console application and you can simly run it by clicking on it, or by using the command line. Console app requires only the name of input file (default is **pak.dat**). Type in input file name, and press enter, also press enter two more times to confirm the names of lst and unv files. You can also leave the default input file name, in which case there is no need to type the name in, just press enter until the calculation starts.

LST file is useful for tracking the progress of simulation, it contains messages explaining many of the input flags and parameters, messages about processed time steps, convergence, calculated norms, errors etc. (Example of LST can be downloaded from https://github.com/BogdanM1/PAK-KTM/tree/master/Examples/pak.lst). **UNV** is the output file of our simulation which contains list of nodes, elements and output fields (such as concentration, pressure, etc.) These fields are presented as either nodal or elemental values.

Compile and run PAKKTM on Linux:

Download code from github navigate to **pakktm/build** and run the following commands:

```
cmake ..
make
./pakktm
```

The program will prompt you to type-in the input dat file (default is pak.dat). Type in input file name, and press enter, also press enter two more times to confirm the names of **lst** and **unv** files. You can also leave the default input file name, in which case there is no need to type the name in, just press enter until the calculation starts.

LST file is useful for tracking the progress of simulation, it contains messages explaining many of the input flags and parameters, messages about processed time steps, convergence, calculated norms, errors etc. (Example of LST can be downloaded from https://github.com/BogdanM1/PAK-KTM/tree/master/Examples/pak.lst). **UNV** is the output file of our simulation which contains list of nodes, elements and output fields (such as concentration, pressure, etc.) These fields are presented as either nodal or elemental values.

B. USERS MANUAL (Input file format description)

In this section we will describe the format of the input file (*.dat).

pak.dat

```
C /1/ HEADING CARD (80A1)
C NASLOV
 COMPOSITE SMEARED FINITE ELEMENT MODEL - KOJIC TRANSPORT MODEL (KTM)
C /3/ BASIC DATA FOR THE PROBLEM (I10,9I5)
C NPT,NGET,NMATC,NMATD,NSTAC,NPER,NPRINT,IANIZ,NULAZ,IGRAF,IDARCY,ICONV,IDIFF,IDINF,ISOLVER,IHEAT,ILAMDA,ICOUPLEDCD (I10,17I5)
        11    1    0    1    1    1   -1    0    1    1    1    0    1    0    1    0    0    0    1    0
C ISMEARED,IPARTSME,IPART,IVSOURCE,IRAVCOEF,DRAVCOEF,BVELCAP,I2D3D,IANIZS,MULTITIS,MULTIMOL,NDIMCELL,INDCELLIN,INDLYMPHH,INDLYM
    5    0    0    0    01.000e+000    0    2    0    1    1    1    0    0    0    0    0    0    0    0
C /4/ BASIC DATA FOR THE PROBLEM
C INTEB,INDSC,IFORM,MAXIT,EPSTA,EPSTR,NJRAP,EPSTRL,IDISJCALC,IDISJMESH,IGRAPHS,NPERS,bImmersed,bCalcConc(4I5,2F10.2,6I5)
    0    0    0   30  0.000000  0.050000    2  0.001000    0    0    1    0    0    0
C /5/ DATA FOR RESTART
C IREST,NCZK,NCZR,VREM0,NPTPR (3I5,D15.8,I5)
    1    0    0
C /6/ DATA FOR TIME STEPS (2I5,F10.0)
C   NKDT(I)/DTDT(I)     (I=1,NPER)
        2
1.000e+000
C  CAPILLARY DIAMETERS DIACAPX,DIACAPY,DIACAPZ
1.000e+0001.000e+0001.000e+000
C  DATA ABOUT MATERIAL DATA MATRICES
C  FOR ICONV.EQ.1 -ICMTABLE(MM,I),I=1,6 (10I5) 0-NOT USED 1-CONSTANT, 2-FUNCTION OF C, 3-ASSOCIATIATION TO NODES
C  IMIGTABLE(I),I=1,10),(VMIGC(I),I=1,10) (10I3,10F10.2)
  0  0  0  0  0  0  0  0  0  01.000e+000
C   FLAGS FOR CHEMOTAXIS INDCHTAX,(INDCHTAXV(I),I=1,10) (11I3)
  0  0  0  0  0  0  0  0  0  0  0
```

Partial input file example (pak.dat)

/1/ HEADING CARD

NOTE	COLUMN	VARIABLE	DESCRIPTION
1-80		NASLOV (80)	Heading for the problem with length of 80 characters

/2/ BASIC DATA FOR THE PROBLEM

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	NPT	Total number of nodal points.
(2)	6-10	NGET	Number of element groups. default set to "1"
(3)	11-15	NMATC	Total number of different materials. default set to "1"
(4)	16-20	NMATD	
(5)	21-25	NPER	Number of constant time step periods.
(6)	26-30	NPRINT	Output printing interval. EQ. 0: results are printed in all time steps
(7)	31-35	IANIZ	Not used in this version of program
(8)	36-40	NULAZ	Kind of printout of input data EQ. 1; card image, input data read and generated, are printed EQ. 2; card image printed EQ. 3; input data read and generated are printed
(9)	41-45	IGRAF	Indicator for graphics file. EQ. 0; not formed EQ. 1; formed
(10)	46-50	IDARCY	Flag for Darcy flow calculation, EQ.0, case not used in this code, reset to 1, EQ. 1, Darcy flow calculation, EQ.-1, equivalent Darcy coefficient, EQ.-2, equivalent diffusion coeff. Calculation
(11)	51-55	ICONV	Indicator for convection EQ. 0; No convection EQ. 1; convection type problem
(12)	56-60	IDIFF	Indicator for diffusion EQ. 0; No diffusion EQ. 1; diffusion type problem
(13)	61-65	IDNIF	Inertial Fluid Forces EQ. 0; No inertial fluid forces EQ. 1; Inertial fluid forces
(14)	66-70	ISOLVER	Flag for solver type EQ. 0; Skyline EQ. 1; MUMPS
(15)	71-75	IHEAT	Flag for heat type problems EQ. 0; No heat EQ. 1; Heat type problem
(16)	76-80	ILAMBDA	Lagrange multipliers for mixed formulation EQ. 0; No EQ. 1; Yes

Notes:

(1) NP is total number of nodal points in structure. Node numbering is from 1 to NP, free node numbering is not supported.
(2) One element group can be used in this version of PAKT program.
(3) NMATT is total number of different material sets used in FE model. Number of cards /9/ is equal to NMATT. Each material set has its sequence number defined in sequence of reading cards /9/.
(4) For NSTAC.EQ.0 problem is steady, linear or nonlinear, and solved in one time step. For NSTAC.EQ.1 problem is transient. Linear problem is solved by using time incrementation procedure, without iterations in time step; or, incremental-iterative procedure for nonlinear case is employed.
(5) In case of NSTAC.EQ.1, NPER.GE.1 is total number of time periods with constant time step for each period. NPER.EQ.0 for steady-state problems.
(6) NPRINT is parameter used for printout of data control. For NPRINT.EQ.0 data (nodal temperatures) are printed for all time steps. For NPRINT=K nodal temperatures are printed for steps 1, 1+m*K, m=1,2,..., and last time step.

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	ISMEARED	Flag for smeared capillary model EQ. 0; No smeared is used EQ. 1; Diffusion only, uniform concentration in capillaries EQ. 2; Convection only in capillaries EQ. 3; Diffusion only in capillaries (with or without convection) EQ. 4; Convection (ICONV= 1 or 0) EQ. 5; Diffusion coupled with tissue
(2)	6-10	IPARTSME	Flag for partition of capillary wall (ISMEARED =1)
(3)	11-15	IPART	Flag for partitioning in continuum
(4)	16-20	IVSOURCE	Flag for volumetric source
(5)	21-25	IRAVCOEF	Flag for surface-volume ratio EQ. 0; Use equation for straight pipe EQ. 1; Diffusion only, uniform concentration in capillaries
(6)	26-30	DRAVCOEF	Output printing interval. EQ. 0: results are printed in all time steps
(7)	31-35	BVELCAP	Not used in this version of program
(8)	36-40	I2D3D	Flag for 2D-3D problem (0-reset to 2) EQ. 2-2D problem EQ. 3-3D problem
(9)	41-45	IANIZS	Flag for anisotropy for ISMEARED.GE.2
(10)	46-50	INDION	Flag for ionic transport, EQ.0, NO, EQ. 1, YES
(11)	51-55	INDELECTR	Flag for modeling electric field, EQ.0, NO, EQ. 1, Coupled with diffusion

			EQ. 2, Electric field only
(12)	56-60	IVITTORIO	Vittorio tumor growth model EQ.0, NO, EQ.1, YES
(13)	61-65	IMMUNE	Immune cells flag EQ. 0; No immune cells EQ. 1; Immune cells model

/3/ BASIC DATA FOR THE PROBLEM

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	INTEB	Time integration method used EQ. 0; default set to "1" EQ. 1; Euler backward integration ($\alpha = 1$)
(2)	6-10	INDSC	Print of results at prescribed nodes EQ. 0; at all nodes EQ. 1; at selected nodes
	11-15	IFORM	Print of results in prescribed format EQ. 0; print in format D13.5 EQ. 1; print in format F10.3
	16-20	MAXIT	Maximum number of iterations EQ. 0; default set to "15"
	21-30	EPSTA	Absolute accuracy at iterations
(4)	31-40	EPSTR	Relative accuracy at iterations EQ. 0; default set to "1. E-3"
	41-45	NJRAP	Iteration method employed EQ. 0; default set to "1" EQ. 1; modified Newton EQ. 2; full Newton
(5)	46-50	IDISJCALC	Flag for joint calculation for pressure and concentration

Notes:

(1) Euler backward integration method with α=1 is only supported in current version of program PAKT, default value is INTEB=1.

(2) For INDSC=0 node temperatures are printed for all nodes. In case of INCSC=1 nodal temperatures are printed at selected nodes; defined in card /14/- by node and increment for automatic node generation.

(3) Maximum number at equilibrium iteration in time step; for MAXT.EQ.0 default value is MAXIT=15.

(4) EPSTA is absolute accuracy at iterations for increment of nodal temperature for i-th iteration

$$\left|\Delta T_K^{(i)}\right| \leq \text{EPSTA} \ , \quad K = 1,2,..., NP$$

where $\Delta T_K^{(i)}$ is increment of nodal temperature at node K for i-th iteration.

EPSTR is relative accuracy at iteration defined by using norm of nodal temperature increment

$$\left\|\Delta \mathbf{T}^{(i)}\right\| = \sqrt{\sum \left(\Delta T_K^{(i)}\right)^2}$$

Convergence criterion is ratio

$$\frac{\left\|\Delta \mathbf{T}^{(i)}\right\|}{\left\|\Delta \mathbf{T}^{(1)}\right\|} \leq \text{EPSTR}$$

where $\left\|\Delta \mathbf{T}^{(1)}\right\|$ is norm of nodal temperature increment at first iteration.

If EPSTA.GT.0 and EPSTR.GT.0 iterations continue, and stop when both criteria are satisfied.

/4/ DATA FOR RESTART (3I5,D15.8)

NOTE	COLUMN	VARIABLE	DESCRIPTION
	1-5	IREST	Indicators for job execution EQ. 0; check of input data EQ. 1; job execution EQ. 2; restart
(1)	6-10	NCZK	Number of last steps to be written on file EQ. 0; write all steps
(1)	11-15	NCZR	Number of steps to be read from file at restart.
	16-30	VREMO	Time of start for job execution
	31-35	NPTPR	Number of nodal points before file execution

Note:

(1) Indicator NCZK defines number of last steps during job execution (IREST.EQ.1) that are to be written on file named ZITEMP. Then, during restart run (IREST.EQ.2) NCZR number of steps is read from file ZITEMP; since ZITEMP file is sequential, it must be NCZR=NCZK.

/5/ DATA FOR TIME STEPS

If NPER.EQ.0 is card /3/ skip this group of cards a) and b).

a) Number of time steps card

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	NKDT(1)	Number of time steps in first solution period
	6-10	NKDT(2)	Number of time steps in the second solution period
	.	. .	
	.	. .	
	.	. .	
		NKDT(NPER)	Number of time steps in NPER-th solution period

b) Card of time increment per step in solution period

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-10	DTDT(1)	Time increment for first solution period
		DTDT(2)	Time increment for the second solution period
	.	. .	
	.	. .	
	.	. .	
		DTDT(NPER)	Time increment for NPER-th solution period

Note:
(1) Number of solution periods NPER on card /3/

/6/ DATA ABOUT MATERIAL DATA MATRICES

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-15	DIACAPX, DIACAPY, DIACAPZ	Capillary diameters for X, Y and Z direction.
(2)	16-45	IMIGTABLE	Flags for cell migration velocities EQ.0: Not used EQ.1: Constant for all nodes EQ.2: Time function used EQ.3: Set nodal values LT.0: Molecule gradient driven
(3)	46-75	INDCHTAX	Flags for cell usage of chemotaxis EQ.0: Not used
(4)	76-80	MOLNUM	Molecule number
(5)	81-90	K1,K2,K3	Flags for diffusion tensor (K1- pipe domain, K2-extracellular, K3-capillary domain)
(6)	91-130	DPIPE, DEXT, DCAPX, DCAPY	Diffusion coefficients for: pipe domain extracellular domain capillary domain in X and Y direction
(7)	131-160	KV(I)	Flags for diffusion coefficients for cell groups I=1,10 (Maximum number of cell groups- 10)
(8)	161-190	IPARTC	Flags for partitioning coefficients for pipe, capillary, and cell groups
(9)	191-230	PARTC	Partitioning coefficients for pipe, capillary and cell groups
(10)	231-260	IACTIVEC	Flags for active transport coefficients for cell groups
(11)	261-270	ACTIVEC	Active transport coefficients- Inlet/ outlet
(12)	271-300	ISOURCEC	Flags for source terms for cell groups
(13)	301-310	SOURCEC	Source term values for cell groups
(14)	311-340	IADHISEC	Flags for adhesion terms for pipe, capillary, and cell groups
(15)	341-350	ADHISEC	Adhesion coefficients for pipe, capillary, and cell groups
(16)	351-380	IDEADHISEC	Flags for deadhesion terms for pipe, capillary, and cell groups
(17)	381-390	DEADHISEC	Deadhesion coefficients for pipe, capillary, and cell groups
(18)	391-426	IWALLPIPEC, IWALLCAPC, IWALLCELLC	Flags for wall diffusion coefficient in pipe, capillary, and cell domains
(19)	427-436	DWALLPIPEC, DWALLCAPC, DWALLCELLC	The wall diffusion coefficient in pipe, capillary, and cell domains
(20)	437-466	ICRITICALV	Flags for cells critical value: healthy, cancer, necrotic, and immune

(21)	467-476	CRITICALV	Cells critical values: healthy, cancer, necrotic, and immune
(22)	477-486	WEIGHTMOLV	Molecular weights values

/7/ DATA FOR NODAL POINT DATA

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	N	Nodal point number
	9-10	IDTLOC (N)	Prescribed values indicator at node N EQ. 1; Prescribed concentration, pressure or heat is EQ. -1; Prescribed velocity EQ. -2; Restrained flux
	11-20	CORD(N,1)	X - coordinate
	21-30	CORD(N,2)	Y - coordinate
	31-40	CORD(N,3)	Z - coordinate
(2)	41-53	VOLFRACTV(N)	Volumetric fraction of capillaries in nodal points
(3)	54-66	DIAMSMEV(N)	Diameter of capillaries in nodal points
(4)	67-79	THICKSMEV(N)	Wall thickness of capillaries in nodal points
(5)	67-79	VOLSME	Nodal volume
(6)	67-79	WALLAREAC	Wall area coefficient
(7)	67-79	RVEE	Wall area coefficient
(8)	67-79	PIPEDIAE	Pipe diameter

/8/ ELEMENT GROUP DATA

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	NETIP	Element type EQ. 1; ISOPARAMETRIC 1D EQ. 2; ISOPARAMETRIC 2D EQ. 3; ISOPARAMETRIC 3D
	6-10	NET	Number of elements in the group
	11-15	INDAX	Indicator for axisymmetric elements EQ. 0; 2D in plane EQ. 1; axisymmetric in plane xy; y is axis of symmetry
	16-20	IZIP	Indicator for volumetric source or sink EQ. 0; There is no volumetric source EQ. 1; Volumetric source is function of time EQ. 2; Volumetric source is function of temperature
	21-25	INDIFUSE	Indicator for diffusion inside element group
	26-30	IPIPEE	Indicator for pipe group inside element group

/8-1/ DATA FOR 1D ELEMENT GROUP

a) Card with data about 1D element

NOTE	COLUMN	VARIABLE	DESCRIPTION
(2)	1-5	NMAT1D	Total number of materials for 1D element
	6-10	MAT1D	Not used in this version of program
	11-15	NP1DMX	Maximum number of nodal points per element EQ. 0; two nodes per element
(3)	16-20	IPR1DC	Indicator for printout of coordinates of Gauss points EQ. 0; not printed EQ. 1; printed in all elements EQ. 2; printed in prescribed elements
(4)	21-25	IPTG1	Indicator for printout of temperatures at Gauss points EQ. 0; not printed EQ. 1; printed in all elements EQ. 2; printed in prescribed elements
	26-30	NGAU1X	Number of Gauss points in direction r
(5)	31-35	ICONECTIV	Flag for connectivity (fictitious) of 1D elements EQ. 0; not used EQ. 1; Used for connection 1D-continuum
(6)	36-40	IWALLD	Flag for wall use of diffusivity
(7)	41-45	IPARABOLIC	Flag for velocity profile EQ. 0; Non parabolic EQ. 1; Parabolic profile
(8)	46-50	IDEFORM	Flag for pipe wall deformation

b) Data for each element in group (9I5)

NOTE	COLUMN	VARIABLE	DESCRIPTION
	1-5	NN	Element number
	6-10	NEL(NN,1)	First node of element NN
	11-15	NEL(NN,2)	Second node
(5)	26-30	NMAT	Material set number for element NN
	31-35	NQQ	Internal heat generation function number
(6)	36-40	KORE	Step for generation data about elements
(6)	41-45	NBEG	Number of elements which will be generated
(7)	46-50	IPRCO	Indicator of printing of coordinates at Gauss points EQ. 0; not printed EQ. 1; printed
(8)	51-55	IPGS	Indicator of printing temperatures at Gauss points EQ. 0; not printed EQ. 1; printed

/8-2/ DATA FOR 2D ELEMENT GROUP

a) Card with data about 2D element

NOTE	COLUMN	VARIABLE	DESCRIPTION
(2)	1-5	NMAT2D	Total number of materials for 2D element
	6-10	MAT2D	Not used in this version of program
	11-15	NP2DMX	Maximum number of nodal points per element EQ. 0; four nodes per element
(3)	16-20	IPR2DC	Indicator for printout of coordinates of Gauss points EQ. 0; not printed EQ. 1; printed for all elements EQ. 2; printed for prescribed elements
(4)	21-25	IPTG2	Indicator for printout of temperatures at Gauss points EQ. 0; not printed EQ. 1; printed for all elements EQ. 2; printed for prescribed elements
	26-30	NGAU2X	Number of Gauss points in direction r EQ. 0; NGAUSX=2
	31-35	NGAU2Y	Number of Gauss points in direction s EQ. 0; NGAUSY=2
(5)	36-40	NTHIC	Indicator of thickness EQ. 0; thicknesses are constant EQ. 1; thicknesses are variable
(5)	41-50	THIC	Thickness EQ. 0.0; thickness of all elements is equal to 1.0

b) Data for each element in group (11I5,F10.0)

NOTE	COLUMN	VARIABLE	DESCRIPTION
	1-5	NN	Element number
(6)	6-10	NEL(NN,1)	First node of element NN
	11-15	NEL(NN,2)	Second node
	16-20	NEL(NN,3)	Third node
	21-25	NEL(NN,4)	Fourth node
(7)	26-30	NMAT	Material sequence number for element NN
	31-35	NQQ	Internal heat generation function number
(8)	36-40	KORE	Step for generation data about elements
(8)	41-45	NBEG	Number of elements which will be generated
(9)	46-50	IPRCO	Indicator of printing of coordinates at Gauss points EQ. 0; not printed EQ. 1; printed
(10)	51-55	IPGS	Indicator of printing temperatures at Gauss points EQ. 0; not printed EQ. 1; printed
(11)	56-65	THI	Element thickness

/8-3/ DATA FOR 3D ELEMENT GROUP (8I5)

a) Card with data about 3D element

NOTE	COLUMN	VARIABLE	DESCRIPTION
(2)	1-5	NMAT3D	Total number of materials for 3D elements
(2)	6-10	MAT3D	Not used in this version of program
(3)	11-15	NP3DMX	Maximum number of nodal points per element. If NP3DMX.EQ.0, eight node 3D element is used.
(4)	16-20	IPR3DC	Indicator for printout of coordinates of Gauss points EQ. 0; not printed EQ. 1; printed for all steps EQ. 2; printed for prescribed steps
(5)	21-25	IPRTG3	Indicator for printout of temperatures at Gauss points EQ. 0; not printed EQ. 1; printed for all elements EQ. 2; printed for prescribed elements
	26-30	NGAUSX	Number of Gauss points in direction ξ EQ. 0; NGAUSX=2
	31-35	NGAUSY	Number of Gauss points in direction η EQ. 0; NGAUSY=2
	36-40	NGAUSZ	Number of Gauss points in direction ζ EQ. 0; NGAUSZ=2

b) Data for each element in group

NOTE	COLUMN	VARIABLE	DESCRIPTION
	1-5	NN	Element number
	6-10	NEL(NN,1)	First node of element NN
	11-15	NEL(NN,2)	Second node
	.	. .	
	.	. .	
	.	. .	
	41-45	NEL(NN,8)	Eight node
(6)	46-50	NMAT	Material set number for element NN
	51-55	NQQ	Internal heat generation function number
(7)	56-60	KORE	Step for generation data about elements
(7)	61-65	NBEG	Number of elements which will be generated
(8)	66-70	IPRCO	Indicator of printing of coordinates at Gauss points EQ. 0; not printed EQ. 1; printed
(9)	71-75	IPGS	Indicator of printing temperatures at Gauss points EQ. 0; not printed EQ. 1; printed

/9/ DATA ABOUT CAPILLARIES AND CELLS

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	MODCELL	Flag for the type of cell model EQ. 1; 2D axial model EQ. 2; 2D circular model EQ. 3; 3D model
(2)	6-10	NCAPILARY	Number of capillaries (in the case of the wall model used IWALL.EQ.1 this parameter is the number of collagen sleeves)
(3)	11-15	NCELL	Number of cells in the model
(4)	16-20	INTRACELL	Flag for modeling of the cells interior EQ. 0; Not used (no mesh inside any of the cells) EQ. 1; Modeling the cells interior
(5)	21-25	NPMAXCAP	Maximum number of nodes for any capillary
(6)	26-30	NPMAXCELL	Maximum number of nodes for any of the cell membranes
(7)	31-35	ICELL2D3D	Flag for the 2D or 3D cell EQ. 2; 2D cell model EQ. 3; 3D cell model
(8)	36-40	IWALL	Flag for modeling the wall EQ. 0-No wall model EQ. 1-Wall model
(9)	41-45	NZADW	Number of nodes with a prescribed concentration (applicable when IWALL.EQ.1)
(10)	46-50	HMODEL	Model thickness
(11)	51-55	NZADO	Number of nodes with a prescribed outlet concentration
(12)	56-60	NEURONS	Number of large neurons in a detailed model
(13)	61-65	NPMAXNEU	Immune cells flag EQ. 0; No immune cells EQ. 1; Immune cells model

/10/ DATA ABOUT TIME FUNCTIONS

This group of cards is input only if IDT(N) = –1 in card /7/

NOTE	COLUMN	VARIABLE	DESCRIPTION
	1-5	NTABFT	Number of different time functions EQ. 1; time functions are constant EQ. 0; there are no time functions
	6-10	MAXTFT	Maximum number of points for defintion of time functions EQ. 1; time functions are constant

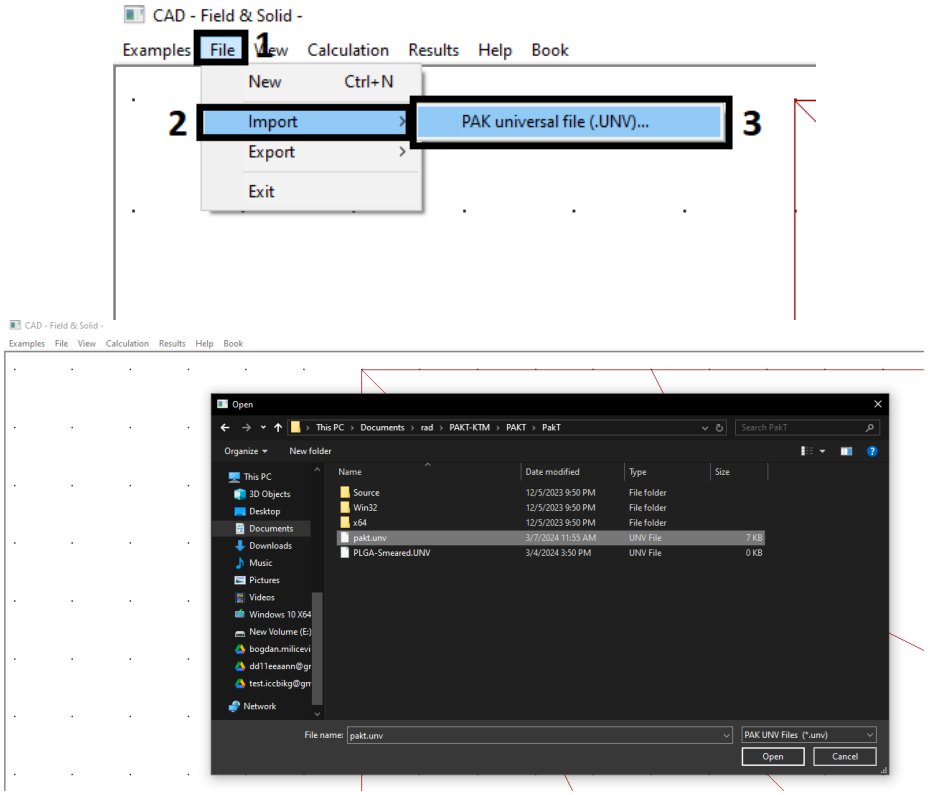
/11/ DATA ABOUT PRESCRIBED VALUES

NOTE	COLUMN	VARIABLE	DESCRIPTION
(1)	1-5	NODE	ID of the prescribed node
(2)	6-10	IDOF	Degree of freedom
(3)	11-15	FAK	Proportionality factor
(4)	16-20	KORC	Prescribed value
(5)	21-25	NPOC	Number of total initial prescribed temperatures EQ. 0; Stationary linear state EQ. 1; Equal initial temperatures EQ. 2; All initial temperatures are different
(6)	26-30	NQP	Number of total different functions of area fluxes EQ. 0; No fluxes on body area
(7)	31-35	MAXTQP	Maximum number of points for defining flux function EQ. 0; No fluxes on the body area EQ. 1; Constant fluxes during time steps GT. 1; Fluxes are variable during time steps
(8)	36-40	NHP	Number of total different functions for the coefficient of heat transfer EQ. 0; No convection of body surface
(9)	41-45	MAXTHP	Maximum number of points for defining the heat transfer function EQ. 0; No convection on the body area EQ. 1; Heat transfer coefficient not temperature dependent EQ. 2; Heat transfer coefficient function of temperature
(10)	46-50	NTOK	Number of different values for environment temperature EQ. 0; No convection on the body surface
(11)	51-55	MAXTOK	Maximum number of values for environmental temperature defined EQ. 0; No convection on the surface EQ. 1; Temperatures are constant within time EQ. 2; Temperatures are variable within time
(12)	56-60	NQE	Number of volumetric heat sources (sinks)
(13)	61-65	MAXTQE	The maximum number of values for the sources function defined EQ. 0; There are no volumetric heat sources EQ. 1; Volumetric heat source functions are linear EQ. 2; Volumetric heat source functions are nonlinear
(14)	66-70	NHR	Number of different values for emissivity coefficient
(15)	71-75	MAXTHR	Number of values for emissivity coefficient EQ. 0; There is not radiation on surface

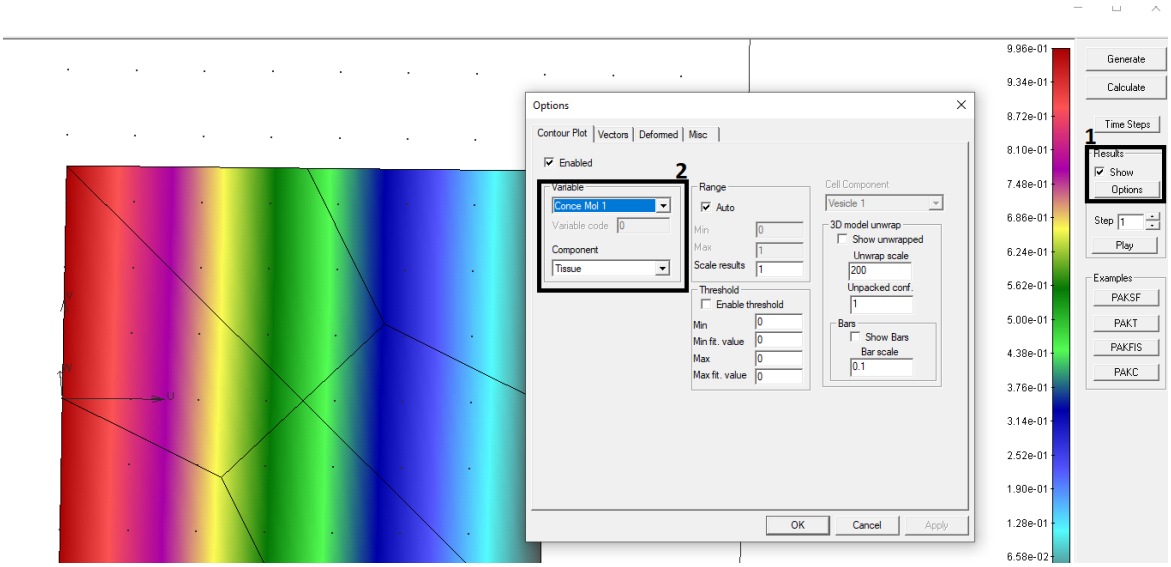
	EQ. 1; Emissivity coefficients are not temperature-dependent EQ. 2; Emissivity coefficients are function of temperature

C. RESULTS VISUALIZATION

UNV file can be loaded into our pre- and post-processing software **CAD-Solid-Field** (https://github.com/miljanmilos/CAD-Solid-Field). Once the UNV is loaded, *CAD-Solid-Field* can be used to visualize the model along with physical fields. First go to "File" then "Import" and then select UNV file that you want to visualize. Within "Results" section press the "Options" button and in pop-up window select the field which you want to visualize as shown in images below.



Importing UNV file



Visualizing the results

UNV file format:

This file starts with:

-1

15

After these lines list of nodes with their coordinates is shown, for example:

```
     1        0        0        8  0.00000E+00  0.20000E+01  0.00000E+00
     2        0        0        8  0.00000E+00 -0.20000E+01  0.00000E+00
       …
```

Then after the lines containing:

-1

-1

71

list of elements is shown. Each element consists of a list of nodes in a previous list. For example

```
     1       27       44        1        1        8        4
     1        5       10        7
     2       27       44        1        1        8        4
     2        6       10        5
       …
```

first element contains nodes 1,5,10 and 7. Second element contains nodes 2,6,10 and 5. Then after the lines containing:

-1

-1

55

physical fields are shown in form of either nodal values or elemental values.