FEMINA

(Finite Element Method for thermal, flow, stress and residence time distribution analysis)

Part I -1

User manual



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The examples are in files (postfix GEO) which are part of FEMINA installation. You can run these files either by command F (batch file processing) or M (processing macro). Files F... solve 2D flows, P... solve pipelines and heat exchangers, R... residence time distribution models, S... structural analysis, T... 2D and 3D thermal problems, Z... tomography.

FCAVIUVP	cavity	flow	PSTAS
FCYLPSIN			PSTUB
FDIFCREE			PTRUSS
FPARUVP			PVETEV1
FPCARE			PVETEV2
FQUAD			pvetev3
FSCREE			PYMOC
FSUVP			PYPSILON
FYUVP			ROPTIMA1
ICON1			ROPTIMA2
ICON2			RPAS
PBLAYER			RPASERI
PBMIX			RTDOPT
PCSTR			SBEAM
PCSTRP			SHAK
PFOUL			SHEL2
PCHAND			SHEL3
PICHEV			STERB10
PIHEAT			STRUSS
PIPELIN			TCUBE
PIPEOPT1			THOLE3
PIPEOPT2			TKONZERV
PIPET1			TKURE
PISERIE			TLPIPE
PLICE			TMELT
PLOOJONG			TOKURE
PLOOP			TRHOMB
PLOOP1			TRPIPE
POHMICAS			ZTOMELS0
PPSIGMA			ZTOMELS1
PPUMP1			ZTOMOVE0
PRESPO			ZTOMOVE1
PRESP1			ztomtra0
PRESP2			ZTOMTRA1
PRCHAR			ZTOMTRB0
PSTAG			ZTOMTRB1

List of symbols

a	thermal diffusivity	$[m^2.s^{-1}]$
a_e	aross section	[111.8]
A A	preexponencial factor of protein decomposition reaction	[111] [s ⁻¹]
Λ _N	specific heat capacity	[5]
C _p	native protein concentration	[J.Kg .K]
C _N	denaturated (unfolded) protein concentration	[kg m ⁻³]
C)	protein agglomerate concentration	[kg m ⁻³]
d	tube diameter	[ng.in]
D _e	effective diffusion coefficient (dispersion)	$[m^2,s^{-1}]$
D_N	diffusion coefficient (e.g. native proteins)	$[m^2,s^{-1}]$
D_{D}	diffusion coefficient (e.g. unfolded proteins)	$[m^2.s^{-1}]$
DA	diffusion coefficient (e.g. agglomerates)	$[m^2.s^{-1}]$
E _N	activation energy of protein decomposition	[kJ.kmol ⁻¹]
E	activation energy in Ebert Panchal model of crude oil fouling	[kJ/mol]
f	Fanning friction factor	[-]
g	gravity acceleration	$[m.s^{-2}]$
h	characteristic size of element	[m]
k	heat transfer coefficient	$[W.m^{-2}.K^{-1}]$
k _N ,k _D ,k _A	mass transfer coefficients	$[m.s^{-1}]$
Li	surface coordinate in a triangle	[-]
L _{ij}	length of element i-j	[m]
'n	mass flowrate	$[kg.s^{-1}]$
M _{ii}	mass matrix or heat capacity matrix	[kg]
Ni	base function	[-]
p	pressure	[Pa]
Pé	Peclet number of element	[-]
r	radial coordinate	[m]
R	universal gas constant = $8.314 \cdot 10^{-3}$	[kJ/mol]
t	time	[s]
Δt	time step	[s]
Т	temperature	[C]
T_W	wall temperature	[C]
Te	ambient temperature	[C]
u _x ,u _y	velocity components in Cartesian coordinate system	$[m.s^{-1}]$
u _x ,u _r	velocity components in cylindrical coordinate system	$[m.s^{-1}]$
U	electric potential	[V]
<i>V</i> ׂ	volumetric flowrate	$[m^3.s^{-1}]$
W	test (weighting) function	[-]
x,y,z	Cartesian coordinates	[m]
x,r	cylindrical coordinates	[m]
α	upwind correction coefficient	[-]
α	Ebert Panchal model coefficient	[m ² .K/J]
β	thermal expansion coefficient $(=1/(273.15+T)$ for gases)	[K ⁻¹]
γ	shear rate	$[s^{-1}]$
γ	Ebert Panchal model coefficient	[Pa.m ² .K/J]
λ	thermal conductivity	$[W.m^{-1}.K^{-1}]$
$\lambda_{\rm s}$	structural parameter (thixotropy)	[-]
μ	dynamic viscosity	[Pa.s]
ρ	density	[kg.m ⁻³]
Ψ	stream function	[kg.m ⁻³]
ω	vorticity	[s ⁻¹]

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1. INTRODUCTION

Program FEMINA has been designed for description of continuous systems by mathematical models and first of all for their identification, which means for calculation of optimal parameters of a selected model or for a selection of the most suitable model from several possible alternatives. Examples of continuous flow systems are pipeline networks with valves, pumps, mixed vessels, heat exchangers or individual apparatuses. Such a continuous system can be described in principle by the three different ways:

- 1) *By an algebraic model*, which is a function defining some characteristics of system, e.g. residence time distribution. This kind of information is sufficient, for example, for calculation of a first order chemical reaction running in a nonideal chemical reactor.
- 2) By a lumped parameter model, substituting a real system by a set of basic flow units, more specifically by a set of ideally mixed vessels and piston flow regions. Such a model can be mathematically described by a system of ordinary differential equation for time courses of a traced component in basic flow units. Model parameters are in this case volumes of basic units and flowrates in connecting streams. Models of this kind can be used for calculation of chemical reactions, for detection of dead or stagnant regions, bypass flows and so on. For example lumped parameter models consisting of only few basic units are capable to predict formation of NOxes in burners described by reaction mechanism with approximately 3000 elementary reactions, which is far beyond capabilities of CFD codes.
- 3) *By continuous models*, describing velocities, pressures, temperatures and concentrations in a general point *x*,*y*,*z* and time *t*. These models are usually based upon partial differential equations for momentum heat and mass transfer, completed by semiempirical models of turbulence or distribution of mater in heterogeneous systems. Continuous models, unlike the previous ones, are spatially localised and therefore it is possible to predict local values of key components and to assess the influence of apparatuses geometry upon their spatial distribution.

Algebraic models are most easily evaluated, however, because they are not usually derived from fundamental physical principles, they must be inevitably identified from experiments (either real or numerical). *Lumped parameter models* can be also relatively simply solved by Runge Kutta or by integral transform methods. Even if they reflect the fundamental principle of mass conservation, it is not sufficient for unique model parameters identification and experimentally obtained data must be used again. Transport equations of *continuous models* are solved numerically, usually by the control volume, finite or boundary element methods. Because momentum, mass and energy balances are at least approximately satisfied, only few additional information is required by these models: Experimental or empirical data are usually necessary only for refining boundary conditions (e.g. turbulence intensity at inlet, heat and mass transfer coefficients), parameters of turbulence models and parameters of heuristic models of inter-phase transports. Anyway, experimental verification of numerically obtained solution of continuous models is always desirable, because for example numerical diffusion can distort results considerably and sometimes it is probably better to use simplified 2D model with a fine mesh (and suppressed numerical diffusion) than a complicated 3D model with a rough mesh.

FEMINA makes use all the three mentioned kinds of mathematical models. Algebraic models are represented by user defined functions or tables, lumped parameter models (ordinary differential equations described by a simple language in a similar way as in the previous version of RTD programs) are solved numerically by Runge Kutta methods and continuous models are solved by finite element method (steady/transient electrical, temperature, concentration and flow fields can be calculated in relatively simple one and two dimensional systems, e.g. pipeline networks or rotationally symmetric apparatuses). The main reason, why all the three categories of models are included in FEMINA consists in the possibility to identify parameters of simple models using results of a more complicated one and for example an algebraic model (some empirical relation) can be identified using

either experimental data or by using a lumped parameter model or even continuous finite element model. This is because FEMINA is equipped with optimisation algorithms (modification of mathematical method Marquardt Levenberg and memetic algorithm SOMA, one of the best software for artificial intelligence), enabling calculations of any parameter of an arbitrary model by comparison with reference data, and these reference data can be retrieved directly from experiment or by postprocessing results of a more complicated mathematical model. The reference mathematical model can, but need not be solved by FEMINA, because it is possible to make use results of CFD programs, for example velocity field calculated by Fluent or Cosmos – FEMINA plays in this case only the role of postprocessor. However even this role is not negligible, because optimisation is based upon comparison of model prediction at simulated stimulus-response experiments (responses to tracer injection) and FEMINA is, or will be, equipped with algorithms for simulation of instruments e.g. collimated detectors of γ -radiation.

Functional structure of FEMINA is shown in the following scheme



FEMINA is formed by several independent programs: The main program FEMINA.EXE is first of all pre and postprocessor (preparing RTD models, finite element mesh), graphics interface, it ensures import, export and interactive data processing (especially RTD processing), and also contains optimisation algorithms. Processing of created models for a specified set of parameters is realised in independent programmes called from FEMINA.EXE:



The scheme shows, that the communication between FEMINA.EXE a computational programs is via files, for example the binary file RUNFEM.BIN contains database of FEMINA comprising coordinates of nodal points, parameters of finite elements, material data, text of interpreted files describing models of differential equations, user defined functions and so on. Some programs (e.g. RANNREG.EXE) communicate with FEMINA.EXE by dedicated text files, e.g. RANNREG.DAT, which can be processed by any text editor.

FEMINA is supplied with the complete source code, and therefore can be modified as soon as you have a licence for a Fortran Compiler, for example Microsoft Fortran Power Station for Windows or Compaq Visual Fortran. The whole code is quite long (approximately 50000 lines) and it is not easy to make significant changes, however the source code is invaluable for debugging.

FEMINA is written in Power Station Fortran for Windows (QuickWin), while independent "number crunching" programs are written in standard Fortran 99, operates in MS-DOS mode and are fully portable to any operating system. The same source code can be for example compiled and linked also by Compaq Fortran – generated executable programs are faster in this case (approximately 3-times). All programmes make use of the libraries MINIPF.LIB (Power Station Fortran) or MINICF.LIB (Compaq Fortran), which contain subroutines for frontal methods, mesh generation and graphics (compile and link by a single command *fl32 /MW /4Yb %1 /link minipf.lib*). Documentation of libraries MINIPF, MINICF is supported by program LIST.EXE, producing list of subroutines ZQUICK.TXT and a brief reference manual ZREFER.TXT. Library subroutines are compiled using batch FC.BAT (Power Station Fortran) or QC.BAT (Compaq Fortran), and inserted into libraries by program *LIB minipf.lib novaproc.obj*, resp. *LIB /REMOVE:procedura.obj minipf.lib*. Actual version of program FEMINA, libraries MINIPF.LIB, MINICF.LIB and documentation are accessible at the following address

http://www.fsid.cvut.cz/~zitny/index.htm

as a file FEMINA.ZIP.

Installation of FEMINA is simple. All executable and working files must be inserted to the working directory, for example FEMINA, and files *.mdt, *.bmp, *.cmd (predefined models, pictures and configuration file) should be located in the subdirectory of working directory FILES:

/femina/	femina.exe, runfem.exe, runbox.exe,
/femina/FILES/	\$femina.cmd,\$femwin.cfg,\$pumps.bmp,, S00.mdt,

Some problems appear if your display driver (in Windows 95,98, or XP) is set to the true colour mode (32 bits) -<u>colour quality should be decreased to 16 bits</u>, and recommended resolution is 1024 x 768 pixels. In case of notebooks which are not fully IBM compatible the default size and position of created windows should be adjusted by using the command SETWIN executed from FEMINA anytimes during a session. There are three levels of the configurator: Easy, Basic and eXpert – it is usually sufficient to use the Easy option (it is really easy, write SETWIN into the command line of FEMINA and follows instructions). The SETWIN command modifies the configuration file \$FEMWIN.CFG in the directory *femina/files* and therefore it is sufficient to perform the windows setting only once.

The following chapters present selected applications (chapter 2 is something like a introductory guide about FEMINA), the chapter 3 lists and shortly describes FEMINA commands (quick reference). Chapter 4, theoretical fundamentals, describes methods for solution of partial differential transport equations, RTD analysis, response processing methods and optimisation algorithms used by FEMINA.