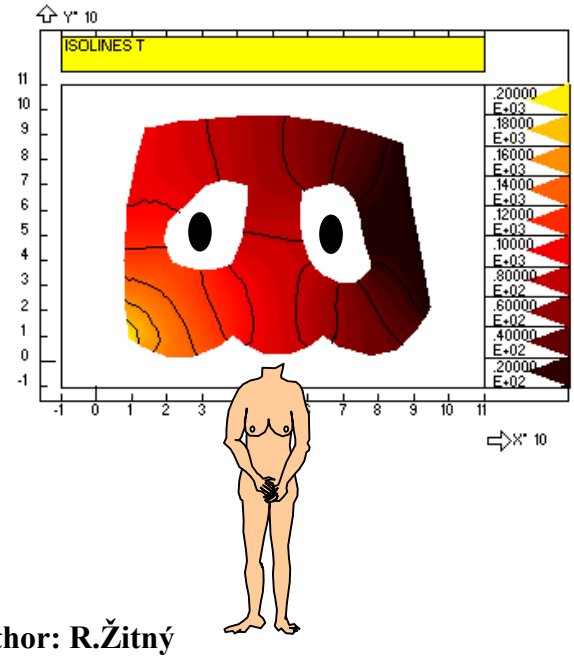
FEMINA

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

Part II.

Theoretical manual



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CONTENT

List of symbols

a	thermal diffusivity	$[m^2.s^{-1}]$
a_e	thermal dispersion	$[m^2.s^{-1}]$
A	cross section	$[m^2]$
A_N	preexponencial factor of protein decomposition reaction	$[s^{-1}]$
c_p	specific heat capacity	$[J.kg^{-1}.K^{-1}]$
c_N	native protein concentration	$[kg.m^{-3}]$
c_D	denaturated (unfolded) protein concentration	$[kg.m^{-3}]$
c_A	protein agglomerate concentration	$[kg.m^{-3}]$
d	tube diameter	[m]
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)	$[m^2.s^{-1}]$
D_A	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	$[m.s^{-1}]$
L_i	surface coordinate in a triangle	[-]
L_{ij}	length of element i-j	[m]
$\dot{m}$	mass flowrate	$[kg.s^{-1}]$
M_{ij}	mass matrix or heat capacity matrix	[kg]
N_i	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]
T	temperature	[C]
T_W	wall temperature	[C]
T_e	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]
$\dot{V}$	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	$[W.m^{-1}.K^{-1}]$
λ_s	structural parameter (thixotropy)	[-]
μ	dynamic viscosity	[Pa.s]
ρ	density	$[kg.m^{-3}]$
ψ	stream function	$[kg.m^{-3}]$
ω	vorticity	$[s^{-1}]$

References

4. Aris R.: Notes on the diffusion type model for longitudinal mixing in flow. Proc.Roy.Soc., A 245, (1958) pp.268
5. Bazeley G.P., Cheung Y.K., Irons B.M., Zienkiewicz O.C.: Triangular elements in bending – conforming and nonconforming solutions, Proc.Conf.Matrix method in Struct.Mech., Air Force Inst. of Tech., Wright Patterson A.F.Base, Ohio, Oct. 1965
6. Bell K.: A refined triangular plate bending element, Int.J.Num.Meth.in Eng., Vol.1, (1969), pp.101-122
7. Bird R.B., Stewart W.E., Lightfoot E.N.: Přenosové jevy, Academia Praha 1968
8. Brahim F., Augustin W., Bohnet M.: Numerical simulation of the fouling process. International Journal of Thermal Sciences, Vol.42, pp.323-334, 2003
9. Campion-Renson A., Crochet M.J.: On the stream function-vorticity finite element solutions of Navier-Stokes equations, Int.J.Num.Meth.in Engng, Vol.12, (1978), pp. 1809-1818
10. Churchill S.W.: Friction factor equation spans all fluid-flow regimes. Chem.Eng. 84, No.5, 91 (1977)
11. De Jong P., Bouman S., Van der Linden H.J.: Fouling of heat transfer equipment in relation to the denaturation of beta-lactoglobulin, J.Soc.of Dairy Technol., 45,3 (1992)
12. Ebert W., Panchal C.B.: Analysis of Exxon crude-oil, slip-stream coking data, Engineering Foundation Conference on Fouling mitigation of heat Exchangers, California, 18-23 June 1955
13. Fortran PowerStation Programmer's Guide, Microsoft Corporation 1995
14. Georgiadis M.C., Rotstein G.E., Macchietto S.: Modelling and simulation of shell and tube heat ecahngers under milk fouling. AIChE Journal, Vol.44, No.4, pp.959-971, 1998
15. Gresho P.M.,Sani R.L.: Incompressible Flow and the Finite Element Method, J.Wiley&Sons, Chichester, 2000
16. Lalande M., Rene F., Tissier J.P.: Fouling and its control in heat exchangers in the dairy industry, Biofouling, 1, 131 (1985)
17. Hood P.: Frontal solution program for unsymmetric matrices, Int.Journal for Numerical Methods in Engineering, Vol.10, (1976), pp.379-399
18. Hughes T.J.R., Brooks A.: A multi-dimensional upwind scheme with no crosswind diffusion, In: Finite Element Methods for Convection Dominated Flows, AMD, Vol.34, (1979), pp.19-36
19. Hunt B.: Diffusion in laminar pipe flow, Int.J.Heat and Mass Transfer, Vol.20, (1977), pp.393-401
20. Huyakorn P.S. et al.: A comparison of various mixed-interpolation finite elements in the velocity-pressure formulation of the Navier-Stokes equations, Computer and Fluids, Vol.6, (1978), pp.25-35
21. Kawahara M. et al: Steady and unsteady finite element analysis of incompressible viscous fluid, Int.Journal for Numerical Methods in Engineering, Vol.10, (1976), pp.437-456
22. Křupka V., Schneider P.: Stavba chemických zařízení I, VUT Brno 1986
23. Lewis R.W., Morgan K., Thomas H.R., Seetharamu K.N.: The finite element method in heat transfer analysis, J.Wiley&Sons,Chichester, 1996
24. Levenberg K.: A Metod for the solution of certain non-linear probléme in lest squares, Q. Appl. Math., 2, (1944), pp.164-168
25. Marquardt D.W.: An algorithm for lest -squares estimation of non-linear parameters, J.Soc.Ind.Appl.Math., 11, (1963), pp. 431-441

26. Martin H.: A theoretical approach to predict the performance of chevron-type plate heat exchangers, Chem. Eng. Process, 35 (1996), pp.301-310
27. Polley G.T. et al: Evaluation of laboratory crude oil treshold fouling data for application to refinery pre-heat trains, Appl. Thermal Eng., 22 (2002), pp.777-788
28. Schneider P., Vykutil J.: Stavba chemických zařízení II, VUT Brno 1990
29. Steffe J.F.: Rheological methods in food process engineering, Freeman press, East Lansing, 1996
30. Taylor G.: Dispersion of soluble matter in solvent flowing slowly through a tube. Proc.Roy.Soc., A 219, (1953), pp.186-203
31. Thýn J. et al: Analysis and diagnostics of industrial processes by radiotracers and radioisotope sealed sources, CTU Prague 2000
32. Toyoda I., Fryer P.J.: A computational model for reaction and mass transfer in fouling from whey protein solution, I Fouling mitigation of industrial heat exchange equipment, Begell House, New York, 1997
33. Wang L., Sundén B.: Optimal design of plate heat exchangers with and without pressure drop specification, Appl.Thermal Eng., 23 (2003), pp.295-311
34. Zelinka I.: Umělá inteligence v problémech globální optimalizace, BEN, Praha 2002.
35. Zienkiewicz O.C., TaylorR.L.: The Finite Element Method, 5-th edition, Butterworth Heinemann, Oxford, 2000
36. Zienkiewicz O.C.: Metod konečnych elementov, MIR Moskva, 1975, překlad z The Finite Element Method in Engineering Science, McGraw-Hill, London, 1971.
37. Žitný R., Šesták J., Tsiapouris A., Linke L.: Thermal pressure forming of a starch based materials - A simplified thermodynamic model, 12th IHTC Grenoble 2002
38. Žitný R.: Knihovna VTV podprogramů, část II. MKPF-metoda konečných prvků pro jedno a dvoudimensionální problémy, 16.sdělení, ČVUT FS Praha 1980
39. Žitný R.: Knihovna VTV podprogramů, část IV. MKPF-metoda konečných prvků pro jedno a dvoudimensionální problémy, 17.sdělení, ČVUT FS Praha 1980
40. Žitný R.: MINIPF.LIB, internal report, ČVUT FS Praha, 2002

4. THEORETICAL FUNDAMENTALS

4.1. Fluid flow, transport equations

4.1.1. Fluid flow formulated in terms of stream function

4.1.1.1. Stokes equation for creeping flow (CREE)

Creeping flow, i.e. flow at Re<1, is of only limited use, mostly for modelling flows of very viscous liquids or flows in tiny geometry (nanotechnology). The formulation, based upon the stream function ψ, has the advantage that the continuity equation is exactly satisfied. In the case that viscosity is constant the problem is linear and velocity field can be solved in only one step – this solution can be used as an initial estimate of velocities for solution of more complicated nonlinear problems. So far only the simplest method CREE based upon cubic polynomial approximation of stream function in triangular elements is implemented. In this case the second derivatives of ψ are continuous only in nodes and not along the whole interface of elements.

The method is based upon principle of minimum dissipated energy, stating that the actual flow field should produce minimum heat by viscous friction (and satisfy of course constraint of incompressibility). The dissipated power can be expressed in a symbolic form as a function of velocity

$$F(\vec{u}) = 2\iint_{\Omega} \mu \vec{\vec{\Delta}} : \vec{\vec{\Delta}} d\Omega = \frac{1}{2}\iint_{\Omega} \mu(\nabla\vec{u} + (\nabla\vec{u})^T) : (\nabla\vec{u} + (\nabla\vec{u})^T) d\Omega \quad , \tag{4.1.1.1-1}$$

and velocity can be expressed in terms of stream function $\vec{\psi} \equiv (\psi_x, \psi_y, \psi_z)$ by using operator *rot*

$$\vec{u} = \nabla \times \vec{\psi} \, . \tag{4.1.1.1-2}$$

What is the advantage of introducing three functions ψ_x, ψ_y, ψ_z instead of three components of velocity? The velocity field described by Eq. (2) satisfies incompressibility constraint for *any* stream function, because

$$\nabla \cdot \vec{u} = \nabla \cdot (\nabla \times \vec{\psi}) = \varepsilon_{kij} \frac{\partial^2 \psi_k}{\partial x_i \partial x_j} = 0 \, . \tag{4.1.1.1-3}$$

It is therefore possible to express the dissipated energy as a function $F(\vec{\psi})$ and to find the functions ψ_x, ψ_y, ψ_z by an *unconstrained* minimisation! This principle can be unfortunately applied only if the inertial terms are negligible, therefore only for creeping flow.

Special case, which is implemented in FEMINA, concerns two-dimensional flows. Here the *x* and *y* components of stream function are identically zero and only one component $\psi_z=\psi$ need to be considered. In the following we shall describe the whole procedure in details, using index notation for cylindrical and Cartesian co-ordinate system separately.

Cylindrical co-ordinate system

We shall consider axially symmetric flow of incompressible liquid in cylindrical coordinate system *r,x* (symmetry axis *x* is horizontal in FEMINA). Velocity components can be expressed in term of stream function[1]

[1] Special attention should be paid to symmetry axis (*r*=0). Radial velocity component u_r is zero, however the axial component u_x must be evaluated as limit, i.e. as a second derivative of stream function in the radial direction *r*.

$$u_x = \frac{1}{r}\frac{\partial \psi}{\partial r} \qquad u_r = -\frac{1}{r}\frac{\partial \psi}{\partial x} \qquad [\psi = \frac{m^3}{s}] \text{ volumetric flowrate} \quad . \tag{4.1.1.1-4}$$

This definition automatically ensures that the continuity equation will be satisfied for any ψ

$$\frac{1}{r}\frac{\partial r u_r}{\partial r} + \frac{\partial u_x}{\partial x} = 0 \,. \tag{4.1.1.1-5}$$

Dissipated energy can be expressed as the following integral, see Bird, page.107

$$F(u_r, u_x) = \iint \mu r \left[2((\frac{\partial u_r}{\partial r})^2 + (\frac{\partial u_x}{\partial x})^2 + (\frac{u_r}{r})^2) + (\frac{\partial u_r}{\partial x} + \frac{\partial u_x}{\partial r})^2 \right] drdx \,, \qquad \text{[W]} \tag{4.1.1.1-6}$$

which after substitution velocity components (4) into Eq.(6) yields functional expression:

$$F(\psi) = \iint \frac{\mu}{r} \left[4((\frac{\partial^2 \psi}{\partial r \partial x})^2 + \frac{1}{r^2}(\frac{\partial \psi}{\partial x})^2 - \frac{1}{r}\frac{\partial^2 \psi}{\partial r \partial x}\frac{\partial \psi}{\partial x}) + (\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r}\frac{\partial \psi}{\partial r})^2 \right] drdz \tag{4.1.1.1-7}$$

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Varying dissipated energy with respect to the stream function and substituting approximation

$$\psi(x,r) = N_j(x,r)\psi_j \,, \qquad \delta\psi(x,r) = N_i(x,r)\delta\psi_i \tag{4.1.1.1-8}$$

we arrive to the system of linear algebraic equations (linear if the viscosity is constant)

$$A_{ij}\psi_j = 0 \tag{4.1.1.1-9}$$

where

$$A_{ij} = \iint \frac{\mu}{r} \left[\begin{array}{l} 4(\frac{\partial^2 N_j}{\partial r \partial x}\frac{\partial^2 N_i}{\partial r \partial x} + \frac{1}{r^2}\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x}) - \frac{2}{r}(\frac{\partial N_j}{\partial x}\frac{\partial^2 N_i}{\partial r \partial x} + \frac{\partial N_i}{\partial x}\frac{\partial^2 N_j}{\partial r \partial x}) + \\ + (\frac{\partial^2 N_j}{\partial x^2} - \frac{\partial^2 N_j}{\partial r^2} + \frac{1}{r}\frac{\partial N_j}{\partial r})(\frac{\partial^2 N_i}{\partial x^2} - \frac{\partial^2 N_i}{\partial r^2} + \frac{1}{r}\frac{\partial N_i}{\partial r}) \end{array} \right] drdx \quad . \tag{4.1.1.1-10}$$

Cartesian co-ordinate system

For planar flows (Cartesian coordinate system *x,y*) the formulation is even simpler

$$u_x = \frac{\partial \psi}{\partial y} \qquad u_y = -\frac{\partial \psi}{\partial x} \qquad [\psi = \frac{m^2}{s}] \text{ volumetric flowrate related to 1 m width of channel,} \tag{4.1.1.1-11}$$

$$A_{ij} = \iint \mu \left[(\frac{\partial^2 N_j}{\partial x^2} - \frac{\partial^2 N_j}{\partial y^2})(\frac{\partial^2 N_i}{\partial x^2} - \frac{\partial^2 N_i}{\partial y^2}) + 4\frac{\partial^2 N_j}{\partial x \partial y}\frac{\partial^2 N_i}{\partial x \partial y} \right] drdz \quad . \tag{4.1.1.1-12}$$

Variable viscosity

Viscosity is the only material parameter in the previous formulation. If it is constant result would be even independent of it. However if the viscosity depends upon temperature or even if it depends upon the calculated velocity field these dependencies must defined as material function (using

FUNDEF or CURDEF). Parameters of this function are temperature (variable TEMP) and second invariant of rate of deformation (variable II), defined in Cartesian coordinate system as

$$II = (\frac{\partial u_x}{\partial x})^2 + (\frac{\partial u_y}{\partial y})^2 + \frac{1}{2}(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x})^2 \qquad (4.1.1.1\text{-}13)$$

and similarly for the cylindrical coordinate system, see Bird page. 107

$$II = (\frac{\partial u_x}{\partial x})^2 + (\frac{\partial u_r}{\partial r})^2 + (\frac{u_r}{r})^2 + \frac{1}{2}(\frac{\partial u_x}{\partial r} + \frac{\partial u_r}{\partial x})^2 \qquad . \qquad (4.1.1.1\text{-}14)$$

Note: The second invariant enables to calculate characteristic shear rate as

$$\dot{\gamma} = \sqrt{2II} \qquad (4.1.1.1\text{-}15)$$

and this expression can be used for definition of apparent viscosity in MPROP.

Implementation

In view of the fact, that second derivatives appear in integrands of (10), resp. (12) at least cubic polynomial ensuring continuity of first derivatives (Bazeley 1965), must by applied. Local matrix A_{ij} of a triangular element has dimension 9 x 9, which corresponds to 3 nodes and to the vector of nodal parameters $\{\psi_1\ \psi_{1,x}\ \psi_{1,y}\ \psi_2\ \psi_{2,x}\ \psi_{2,y}\ \psi_3\ \psi_{3,x}\ \psi_{3,y}\}$.

Results and postprocessing

Post-processing of calculated nodal parameters $\{\psi_i\ \psi_{i,x}\ \psi_{i,y}\}$ results in

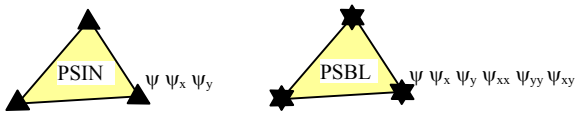
- velocities u_x, u_y
- distribution of dissipated energy in individual elements according Eq. (7)
- total dissipated power F

$$F_e = \iint_{\Omega_e} \frac{\mu}{r} \left[\begin{array}{l} 4(\frac{\partial^2 N_i}{\partial r \partial x}\frac{\partial^2 N_j}{\partial r \partial x} + \frac{1}{r^2}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} - \frac{1}{r}\frac{\partial^2 N_i}{\partial r \partial x}\frac{\partial N_j}{\partial x}) + \\ + (\frac{\partial^2 N_i}{\partial x^2} - \frac{\partial^2 N_i}{\partial r^2} + \frac{1}{r}\frac{\partial N_i}{\partial r})(\frac{\partial^2 N_j}{\partial x^2} - \frac{\partial^2 N_j}{\partial r^2} + \frac{1}{r}\frac{\partial N_j}{\partial r}) \end{array} \right] dr dz \psi_i \psi_j \qquad (4.1.1.1\text{-}16)$$

$$F = \sum_e F_e \qquad [\mathrm{W}]$$

- distribution of the second invariant of the rate of deformation at individual elements according to Eqs. (13-14).

4.1.1.2.Navier Stokes equations formulated by using stream function (PSIN)



This variant is a direct extension of the previous case, again only single equation for the stream function ψ is solved, and the same base functions are used. Therefore the same restrictions follow from the fact, that the very smooth base functions (cubic/quintic polynomials) ensure very smooth solution, nevertheless problems appear when a flow field with discontinuities of viscosity are to be solved. Another drawback: This approach is not suitable for the cases with distribution of flow into several streams.

The method is derived from Navier Stokes equations and takes into account convective and buoyant terms:

Navier Stokes: $\rho\frac{D\vec{u}}{Dt} = -\nabla p + \mu\nabla^2\vec{u} + \vec{f}$ Continuity: $\nabla\cdot\vec{u} = 0$ (4.1.1.2-1)

Vorticity: $\vec{\omega} = -\nabla\times\vec{u}$, $\rho\frac{D\omega_z}{Dt} = \mu\nabla^2\omega_z + Q$ Stream function: $\omega_z = \nabla^2\psi$ (4.1.1.2-2)

Final biharmonic equation for stream function: $\rho\frac{D}{Dt}\nabla^2\psi = \mu\nabla^4\psi + Q$. (4.1.1.2-3)

Resulting system of ordinary differential equations for nodal parameters ψ is obtained by Galerkin's method of weighted residuals with symmetric weights – no upwind technique is applied and therefore it is necessary to use a very fine grid, so that the element Reynolds number restriction $Re_h<1$ would be satisfied. In the following we describe the whole procedure in details, using component instead of symbolic notation for the Cartesian and for the cylindrical co-ordinate system separately.

Cartesian co-ordinate system

Navier Stokes equations for incompressible Newtonian liquid have the following form written in terms of primitive variables (velocities – pressure), see Bird pp.101

$$\rho\left(\frac{\partial u_x}{\partial t} + u_x\frac{\partial u_x}{\partial x} + u_y\frac{\partial u_x}{\partial y}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2}\right) + \rho g_x(1-\beta T) \qquad [\frac{N}{m^3}]\ \text{vol.force} \quad (4.1.1.2\text{-}4)$$

$$\rho\left(\frac{\partial u_y}{\partial t} + u_x\frac{\partial u_y}{\partial x} + u_y\frac{\partial u_y}{\partial y}\right) = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2}\right) + \rho g_y(1-\beta T)\,. \quad (4.1.1.2\text{-}5)$$

These equations follow from the original equations of momentum balances (a conservative form) by using continuity equation for incompressible liquid,

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0\,. \quad (4.1.1.2\text{-}6)$$

Pressure *p* can be eliminated from the Navier Stokes equations so, that we differentiate the momentum balance in the direction *x* with respect to *y*, the second balance equation with respect to *x* and subtract it from the first. Thus we arrive to the transport equation for vorticity

$$\omega = \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} \qquad [\frac{1}{s}] \qquad \text{number of rotations of vortex per second} \tag{4.1.1.2-7}$$

$$\rho(\frac{\partial \omega}{\partial t} + u_x \frac{\partial \omega}{\partial x} + u_y \frac{\partial \omega}{\partial y}) = \mu(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}) + \rho\beta(g_y \frac{\partial T}{\partial x} - g_x \frac{\partial T}{\partial y}) \quad . \qquad [\frac{N}{m^4}] \tag{4.1.1.2-8}$$

Weighted residual method can be applied to the vorticity equation using a test function $W(x,y)$

$$\iint_\Omega W\left[\rho(\frac{\partial \omega}{\partial t} + u_x \frac{\partial \omega}{\partial x} + u_y \frac{\partial \omega}{\partial y}) - \mu(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}) + \rho\beta(g_x \frac{\partial T}{\partial y} - g_y \frac{\partial T}{\partial x})\right] dxdy = 0\,, \tag{4.1.1.2-9}$$

and derivatives of vorticity can be transferred to the test function W by using Green theorem twice

$$\begin{aligned}\iint_\Omega \rho\left[W\frac{\partial \omega}{\partial t} - \omega(u_x \frac{\partial W}{\partial x} + u_y \frac{\partial W}{\partial y}) - \frac{\mu}{\rho}\omega(\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2}) + \beta W(g_x \frac{\partial T}{\partial y} - g_y \frac{\partial T}{\partial x})\right] dxdy + \\ + \int_{\Gamma=\Gamma_\omega+\Gamma_w+\Gamma_0}\left[\rho W\omega(u_x n_x + u_y n_y) + \mu[(\omega\frac{\partial W}{\partial x} - W\frac{\partial \omega}{\partial x})n_x + (\omega\frac{\partial W}{\partial y} - W\frac{\partial \omega}{\partial y})n_y]\right] d\Gamma = 0\end{aligned} \tag{4.1.1.2-10}$$

Now we shall try to simplify the boundary integral. Boundary of region Γ consists in the part Γ_ω where vorticity is known (axis, inlet), wall Γ_w and outlet Γ_0. The first term in the boundary integral ($W\omega u_n$) disappears at wall Γ_w (u=0) and at the part of boundary Γ_ω, where vorticity is prescribed as a strong boundary condition (W=0). Neglecting this term, the Eq.(10) reduces to

$$\begin{aligned}\iint_\Omega \rho\left[W\frac{\partial \omega}{\partial t} - \omega(u_x \frac{\partial W}{\partial x} + u_y \frac{\partial W}{\partial y}) - \frac{\mu}{\rho}\omega(\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2}) + \beta W(g_x \frac{\partial T}{\partial y} - g_y \frac{\partial T}{\partial x})\right] dxdy + \\ + \int_{\Gamma=\Gamma_\omega+\Gamma_w+\Gamma_0} \mu(\omega\frac{\partial W}{\partial n} - W\frac{\partial \omega}{\partial n}) d\Gamma = 0\end{aligned} \tag{4.1.1.2-11}$$

Vorticity ω and velocity components can be expressed in term of stream function ψ from definition

$$u_x = \frac{\partial \psi}{\partial y}\,, \qquad u_y = -\frac{\partial \psi}{\partial x}\,, \qquad \omega = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\,. \tag{4.1.1.2-12}$$

The stream function ψ can be approximated by base functions having integratable squares of second derivatives (cubic polynomial in triangles are used)

$$\psi(x,y) = N_j(x,y)\psi_j\,. \tag{4.1.1.2-13}$$

It should be noted, that the coefficients ψ_j in approximation (13) are not only nodal values of stream function but also first or even second derivatives of ψ, which are necessary for ensuring continuity of first derivatives at element interfaces. When using cubic polynomials N_j in triangles the continuity can be satisfied only at nodes and not along the whole sides (Bazeley 1965, 9 DOF ψ $\psi_{,x}$ $\psi_{,y}$). The polynomials of at least 5th order are to be used if the first derivatives are to be continuous everywhere (Bell 1969, 18 DOF ψ $\psi_{,x}$ $\psi_{,y}$ $\psi_{,xx}$ $\psi_{,xy}$ $\psi_{,yy}$).

Identifying base and test functions $W(x,y) = N_i(x,y)$, it means by using Galerkin method, the Eqs.(11) reduces to the system of ordinary differential equations for nodal parameters ψ_j

$$M_{ij}\frac{\partial \psi_j}{\partial t} + A_{ij}\psi_j = b_i \,. \qquad (4.1.1.2\text{-}14)$$

Mass matrix M is expressed by integrals

$$M_{ij} = \iint_\Omega \rho\left(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\right)d\Omega - \int_\Gamma \rho N_i \frac{\partial N_j}{\partial n}\,d\Gamma \quad , \qquad (4.1.1.2\text{-}15)$$

and matrix of convective and diffusion terms A depends upon velocities u_x, u_y, which are to be evaluated from previous iteration

$$A_{ij} = \iint_\Omega \left(\frac{\partial^2 N_j}{\partial x^2} + \frac{\partial^2 N_j}{\partial y^2}\right)\left[\rho\left(u_x\frac{\partial N_i}{\partial x} + u_y\frac{\partial N_i}{\partial y}\right) + \mu\left(\frac{\partial^2 N_i}{\partial x^2} + \frac{\partial^2 N_i}{\partial y^2}\right)\right]d\Omega +$$
$$- \int_\Gamma \mu\left[\left(\frac{\partial^2 N_j}{\partial x^2} + \frac{\partial^2 N_j}{\partial y^2}\right)\left(n_x\frac{\partial N_i}{\partial x} + n_y\frac{\partial N_i}{\partial y}\right) - N_i\left(\frac{\partial^3 N_j}{\partial x^3}n_x + \frac{\partial^3 N_j}{\partial x\partial y^2}n_x + \frac{\partial^3 N_j}{\partial x^2\partial y}n_y + \frac{\partial^3 N_j}{\partial y^3}n_y\right)\right]d\Gamma \qquad (4.1.1.2\text{-}16)$$

Boundary integral along Γ is completely omitted in FEMINA; which means that only strong and natural boundary conditions are respected. This is correct at inlet, at axis where n_y=0 and vorticity is zero, but problem represent part of boundary with unknown derivatives of stream function (unknown velocities u_x, u_y at outlet) and also a surface of body inserted into the stream of liquid with zero derivatives but unknown value of stream function.

Right hand side vector b_i represents a source term - buoyancy

$$b_i = \iint_\Omega \rho\beta N_i\left(g_x\frac{\partial T}{\partial y} - g_y\frac{\partial T}{\partial x}\right)d\Omega \quad . \qquad (4.1.1.2\text{-}17)$$

Approximating temperature field by linear base functions H the right hand side vector can be expressed as a product of matrix B and vector of nodal temperatures

$$b_i = \left[\iint_\Omega \rho\beta N_i\left(g_x\frac{\partial H_j}{\partial y} - g_y\frac{\partial H_j}{\partial x}\right)d\Omega\right]T_j = B_{ij}T_j \,. \qquad (4.1.1.2\text{-}18)$$

Cylindrical coordinate system

The whole procedure can be in principle repeated even for the cylindrical coordinate system, see Bird pp.102, momentum balance look like this

$$\rho\left(\frac{\partial u_x}{\partial t} + u_x\frac{\partial u_x}{\partial x} + u_r\frac{\partial u_x}{\partial r}\right) = -\frac{\partial p}{\partial x} + \mu\left[\frac{\partial^2 u_x}{\partial x^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_x}{\partial r}\right)\right] + \rho g_x(1-\beta T) \qquad (4.1.1.2\text{-}19)$$

$$\rho\left(\frac{\partial u_r}{\partial t} + u_x\frac{\partial u_r}{\partial x} + u_r\frac{\partial u_r}{\partial r}\right) = -\frac{\partial p}{\partial r} + \mu\left[\frac{\partial^2 u_r}{\partial x^2} + \frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial r u_r}{\partial r}\right)\right] + \rho g_r(1-\beta T) \quad . \qquad (4.1.1.2\text{-}20)$$

Continuity equation in cylindrical system

$$\frac{\partial u_x}{\partial x}+\frac{1}{r}\frac{\partial r u_r}{\partial r}=0\,,\qquad \text{resp.}\qquad \frac{\partial u_x}{\partial x}+\frac{\partial u_r}{\partial r}+\frac{u_r}{r}=0\quad . \tag{4.1.1.2-21}$$

Vorticity equation

$$\omega=\frac{\partial u_x}{\partial r}-\frac{\partial u_r}{\partial x}\qquad . \tag{4.1.1.2-22}$$

$$\rho(\frac{\partial \omega}{\partial t}+u_x\frac{\partial \omega}{\partial x}+u_r\frac{\partial \omega}{\partial r}-\frac{\omega u_r}{r})=\mu(\frac{\partial^2\omega}{\partial x^2}+\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial r\omega}{\partial r}))+\rho\beta(g_r\frac{\partial T}{\partial x}-g_x\frac{\partial T}{\partial r})\ . \tag{4.1.1.2-23}$$

Weighted residual method, after application of Green's theorem to the vorticity equation and neglecting all boundary integrals, gives

$$\iint_\Omega\left[\rho W\frac{\partial \omega}{\partial t}-\rho\omega(u_x\frac{\partial W}{\partial x}+u_r\frac{\partial W}{\partial r})-\mu\omega(\frac{\partial^2 W}{\partial x^2}+r\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial W}{\partial r}))-\rho W\beta(g_r\frac{\partial T}{\partial x}-g_x\frac{\partial T}{\partial r})\right]d\Omega=0\,. \tag{24}$$

Vorticity will be expressed in terms of stream function

$$u_x=\frac{1}{r}\frac{\partial \psi}{\partial r}\qquad u_r=-\frac{1}{r}\frac{\partial \psi}{\partial x}\qquad\qquad \omega=\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial \psi}{\partial r})+\frac{1}{r}\frac{\partial^2\psi}{\partial x^2}\qquad . \tag{4.1.1.2-25}$$

Galerkin method with test functions $W=N_i$ yields again the system of ordinary differential equations (14) with mass matrix

$$M_{ij}=\iint_\Omega\frac{\rho}{r}(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r})d\Omega\qquad , \tag{4.1.1.2-26}$$

and matrix of convective and diffusion term

$$\begin{aligned}A_{ij}&=\iint_\Omega(\frac{1}{r}\frac{\partial^2 N_j}{\partial x^2}+\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial N_j}{\partial r}))[\rho(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})+\mu(\frac{\partial^2 N_i}{\partial x^2}+r\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial N_i}{\partial r}))]d\Omega=\\&=\iint_\Omega(\frac{1}{r}\frac{\partial^2 N_j}{\partial x^2}+\frac{1}{r}\frac{\partial^2 N_j}{\partial r^2}-\frac{1}{r^2}\frac{\partial N_j}{\partial r})[\rho(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})+\mu(\frac{\partial^2 N_i}{\partial x^2}+\frac{\partial^2 N_u}{\partial r^2}-\frac{1}{r}\frac{\partial N_i}{\partial r})]d\Omega\end{aligned}\ . \tag{4.1.1.2-27}$$

Vector b_i remains without changes.

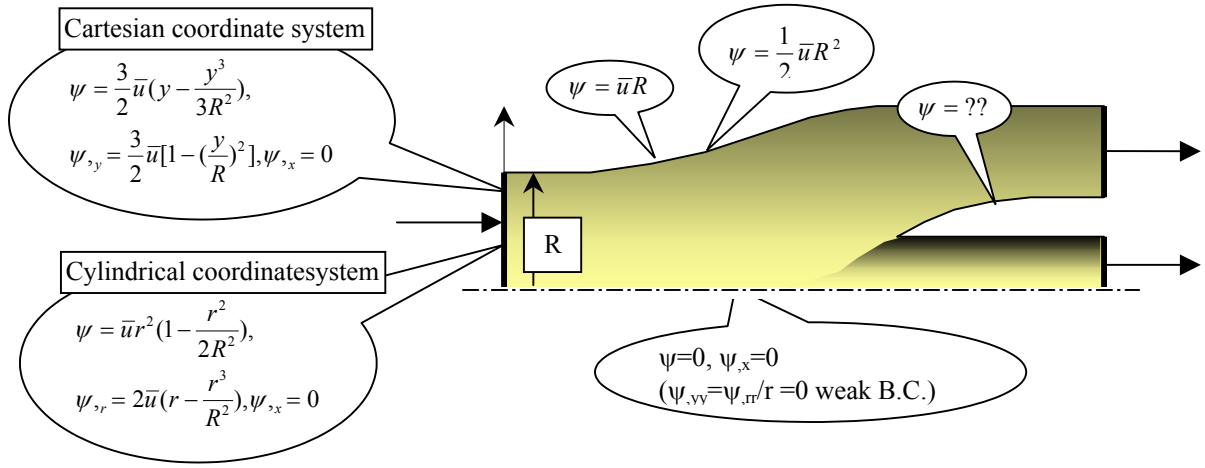
Time discretisation

System of differential equations (14) is solved by implicit Euler's method, giving the following system of algebraic equations for each time step

$$(M_{ij}+\Delta t A_{ij})\psi_j=M_{ij}\psi_j^0+\Delta t B_{ij}T_j\qquad . \tag{4.1.1.2-28}$$

Boundary conditions

Strong boundary conditions are represented by values and first derivatives of stream function ψ. These values are specified at wall and at inlet



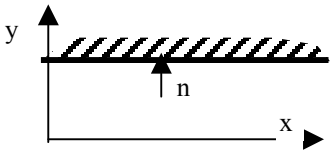
Calculation of pressure

Pressure distribution can be calculated ex post from the velocity field. Pressure is solution of Poisson's equation which follows from N-S equations (in this formulation viscous terms are eliminated by continuity constrains):

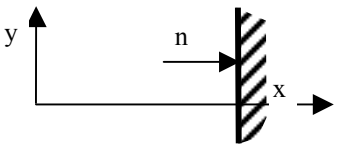
$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + 2\rho[(\frac{\partial^2 \psi}{\partial x \partial y})^2 - \frac{\partial^2 \psi}{\partial x^2}\frac{\partial^2 \psi}{\partial y^2}] + \rho\beta(g_x \frac{\partial T}{\partial x} + g_y \frac{\partial T}{\partial y}) = 0 \quad . \qquad (4.1.1.2\text{-}29)$$

Boundary conditions for pressure at wall follow also from N-S equations

$$\frac{\partial p}{\partial y}|_w = \mu\frac{\partial^2 u_y}{\partial y^2} + \rho g_y(1-\beta T) = -\mu\frac{\partial}{\partial x}\frac{\partial u_x}{\partial y} + \rho g_y(1-\beta T) =$$
$$= -\mu\frac{\partial^3 \psi}{\partial x \partial y^2} + \rho g_y(1-\beta T) = -\mu\frac{\partial \omega}{\partial x} + \rho g_y(1-\beta T) \qquad (4.1.1.2\text{-}30)$$



$$\frac{\partial p}{\partial x}|_w = \mu\frac{\partial^2 u_x}{\partial x^2} + \rho g_x(1-\beta T) = -\mu\frac{\partial}{\partial y}\frac{\partial u_y}{\partial x} + \rho g_x(1-\beta T) =$$
$$= -\mu\frac{\partial^3 \psi}{\partial y \partial x^2} + \rho g_x(1-\beta T) = -\mu\frac{\partial \omega}{\partial y} + \rho g_x(1-\beta T) \qquad (4.1.1.2\text{-}31)$$



Equations (27-28) express the fact, that the normal derivative of pressure is determined by shear rate along the wall and by the gravity forces.

Poisson's Eq. (26) can be solved by Galerkin method, using linear base functions *H*:

$$\{\int_\Omega (\frac{\partial H_i}{\partial x}\frac{\partial H_j}{\partial x}+\frac{\partial H_i}{\partial y}\frac{\partial H_j}{\partial y})d\Omega-\int_\Gamma H_i(\frac{\partial H_j}{\partial x}n_x+\frac{\partial H_j}{\partial y}n_y)d\Gamma\}p_j=$$
$$=\int_\Omega H_i\{2\rho[(\frac{\partial^2 N_j}{\partial x\partial y}\psi_j)^2-\frac{\partial^2 N_j}{\partial x^2}\frac{\partial^2 N_k}{\partial y^2}\psi_j\psi_k]+\rho\beta(g_x\frac{\partial H_j}{\partial x}+g_y\frac{\partial H_j}{\partial y})T_j\}d\Omega \quad . \qquad (4.1.1.2\text{-}32)$$

The same procedure can be applied for cylindrical co-ordinate system. Conclusions are similar, Poisson's equation for pressure looks like this:

$$\frac{\partial^2 p}{\partial x^2}+\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial p}{\partial r})+2\rho[\frac{\partial u_x}{\partial r}\frac{\partial u_r}{\partial x}-\frac{\partial u_x}{\partial x}\frac{\partial u_r}{\partial r}+(\frac{u_r}{r})^2]+\rho\beta(g_x\frac{\partial T}{\partial x}+g_r\frac{1}{r}\frac{\partial rT}{\partial r})=$$
$$=\frac{\partial^2 p}{\partial x^2}+\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial p}{\partial r})+ \qquad (4.1.1.2\text{-}33)$$
$$+\frac{2\rho}{r^2}[(\frac{\partial^2\psi}{\partial r\partial x}-\frac{1}{r}\frac{\partial\psi}{\partial x})^2+\frac{1}{r}\frac{\partial^2\psi}{\partial r\partial x}\frac{\partial\psi}{\partial x}+\frac{\partial^2\psi}{\partial x^2}(\frac{1}{r}\frac{\partial\psi}{\partial r}-\frac{\partial^2\psi}{\partial r^2})]+\rho\beta(g_x\frac{\partial T}{\partial x}+g_r\frac{1}{r}\frac{\partial rT}{\partial r})=0$$

Applying Galerkin's method to the Eq. (33) results in the following system of algebraic equations for nodal pressures p_j

$$\{\int_\Omega r(\frac{\partial H_i}{\partial x}\frac{\partial H_j}{\partial x}+\frac{\partial H_i}{\partial r}\frac{\partial H_j}{\partial r})d\Omega-\int_\Gamma rH_i(\frac{\partial H_j}{\partial x}n_x+\frac{\partial H_j}{\partial r}n_r)d\Gamma\}p_j=$$
$$=\int_\Omega H_i\{\frac{2\rho}{r^2}[(\frac{\partial^2 N_j}{\partial x\partial r}\psi_j-\frac{1}{r}\frac{\partial N_j}{\partial x}\psi_j)^2+(\frac{1}{r}\frac{\partial^2 N_j}{\partial x\partial r}\frac{\partial N_k}{\partial x}+(\frac{1}{r}\frac{\partial N_j}{\partial r}-\frac{\partial^2 N_j}{\partial r^2})\frac{\partial^2 N_k}{\partial x^2})\psi_j\psi_k]+ \qquad (4.1.1.2\text{-}34)$$
$$+\rho\beta(g_x\frac{\partial H_j}{\partial x}+g_y\frac{\partial H_j}{\partial y})T_j\}d\Omega$$

Implementation:

Element matrices M_{ij} A_{ij} in the version PSIN have dimension 9 x 9, which corresponds to 3 nodes with nodal parameters $\{\psi_1\ \psi_{1,x}\ \psi_{1,y}\ \psi_2\ \psi_{2,x}\ \psi_{2,y}\ \psi_3\ \psi_{3,x}\ \psi_{3,y}\}$. Matrix B_{ij} has dimension 9 x 3, which corresponds to linear approximation of temperatures in triangular element.

Variant PSBL (not implemented yet) makes use of Bell's polynomials of the 5th order with 18 degrees of freedom in triangular element $\{\psi_1\ \psi_{1,x}\ \psi_{1,y}\ \psi_{1,xx}\ \psi_{1,yy}\ \psi_{1,xy}\ \psi_2\ \psi_{2,x}\ \psi_{2,y}\ \psi_{2,xx}\ \psi_{2,yy}\ \psi_{2,xy}\ \psi_3\ \psi_{3,x}\ \psi_{3,y}\ \psi_{3,xx}\ \psi_{3,yy}\ \psi_{3,xy}\}$.

Results and post-processing

Using nodal parameters $\{\psi_1\ \psi_{1,x}\ \psi_{1,y}\ \psi_2\ \psi_{2,x}\ \psi_{2,y}\ \psi_3\ \psi_{3,x}\ \psi_{3,y}\}$, resp. $\{\psi_1\ \psi_{1,x}\ \psi_{1,y}\ \psi_{1,xx}\ \psi_{1,yy}\ \psi_{1,xy}\ \psi_2\ \psi_{2,x}\ \psi_{2,y}\ \psi_{2,xx}\ \psi_{2,yy}\ \psi_{2,xy}\ \psi_3\ \psi_{3,x}\ \psi_{3,y}\ \psi_{3,xx}\ \psi_{3,yy}\ \psi_{3,xy}\}$

- velocities
- pressures

are calculated in each time step and these results (ψ and derivative, velocities u_x, u_y and pressure p) are recorded in file *.OUT.

4.1.1.3.Navier Stokes equations – stream function and vorticity (Campion Renson)

Even in this chapter the stream function ψ will be used instead of velocities u_x u_y. However, the single differential equation of the fourth order (biharmonic equation) for the stream function ψ will be decomposed into two equations of only the second order: Poisson's equation for stream function and transport equation of vorticity. Fundamental problem is in the fact that the equation for stream function has too many boundary conditions at wall (values *and* derivatives), while the vorticity equation too few (none at wall). A trick how to resolve the problem has been suggested by Campion-Renson and consists in the following: There is a space of base functions for the stream function ψ with corresponding weights (W_ψ) and a space of vorticity functions with corresponding weights (W_ω). By the word corresponding we have in mind properties of weight functions determined by boundary conditions, it means that for example the weight functions W_ψ should be zero and their first derivatives should be also zero at wall, because both the values and derivatives of ψ are zero. On the other hand no constraint is applied to the weight function W_ω, because vorticity at wall is not known in advance and must be calculated. And now the trick: Weight functions W_ψ are applied in the weak form of vorticity equation, while the functions W_ω in Poisson's equation of stream function! The whole procedure can be demonstrated using symbolic form of transport equation for vorticity and Poisson's equation for the stream function (we consider only 2D case where ω and ψ are *z*-components of vorticity and stream function vectors):

$$\text{Vorticity: } \rho\frac{D\omega}{Dt} = \mu\nabla^2\omega + Q \qquad \text{Stream function: } \omega = \nabla^2\psi \qquad \text{(4.1.1.3-1,2)}$$

Weighted residual method, applying weights W_ψ to vorticity equation (1) and weights W_ω to Eq.(2), gives after little manipulation (Green's theorem) weak formulation

$$\iint_\Omega (W_\psi \rho\frac{D\omega}{Dt} + \mu\nabla W_\psi \cdot \nabla\omega)d\Omega = \int_\Gamma \mu W_\psi \vec{n}\cdot\nabla\omega d\Gamma + \iint_\Omega W_\psi Q d\Omega \qquad \text{(4.1.1.3-3)}$$

and

$$\iint_\Omega \nabla W_\omega \cdot \nabla\psi d\Omega = \int_\Gamma W_\omega \vec{n}\cdot\nabla\psi d\Gamma - \iint_\Omega W_\omega \omega d\Omega\,. \qquad \text{(4.1.1.3-4)}$$

Boundary integral along wall in Eq.(3) is zero because W_ψ is zero, and the integral in (4) is also zero because gradient ψ is zero at wall. Both integrals disappear at inlet and at axis because at this part of boundary both W_ψ and W_ω are zero (strong boundary conditions). At outlet natural boundary conditions hold, corresponding to fully developed flow (zero tangential velocity).

A broad range of base functions can be used, for example simple linear polynomials for both stream function and vorticity, because equations are of only second order. In this case it is also easy to implement *upwind* by using Galerkin Petrov method with asymmetric weights (the same form of weights could be in principle used for both equations, however the asymmetric form is approved only in the transport equation for vorticity). The upwind improves stability of solution at higher Reynolds number, when inertial forces prevail at a prize of decreased accuracy due to numerical viscosity.

In the following we describe the Campion Renson method in more details, for Cartesian and cylindrical co-ordinate system separately.

Cartesian co-ordinate system

Problem formulation is the same as that in the previous chapter. By eliminating pressure from the Navier Stokes equations the following equation for vorticity transport is obtained

$$\omega = \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} \qquad (4.1.1.3\text{-}5)$$

$$\rho(\frac{\partial \omega}{\partial t} + u_x \frac{\partial \omega}{\partial x} + u_y \frac{\partial \omega}{\partial y}) = \mu(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}) + \rho\beta(g_y \frac{\partial T}{\partial x} - g_x \frac{\partial T}{\partial y}). \qquad (4.1.1.3\text{-}6)$$

Velocities can be expressed in terms of stream function

$$u_x = \frac{\partial \psi}{\partial y}, \qquad u_y = -\frac{\partial \psi}{\partial x}, \qquad (4.1.1.3\text{-}7)$$

and substituting into definition of vorticity (5) we arrive to the Poisson's equation for stream function

$$\omega = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}. \qquad (4.1.1.3\text{-}8)$$

Problem is thus described by two differential equations of the second order, transport equation (6) and Poisson's equation (8). Vorticity, stream function and temperatures can be approximated by the same base functions

$$\omega(x,y) = N_j(x,y)\omega_j, \qquad \psi(x,y) = N_j(x,y)\psi_j, \qquad T(x,y) = N_j(x,y)T_j \quad (4.1.1.3\text{-}9,10,11)$$

Weight functions W_ψ can be designed according to Zienkiewicz, Vol. III. pp.27, with asymmetric part dependent upon the flow direction (upwind)

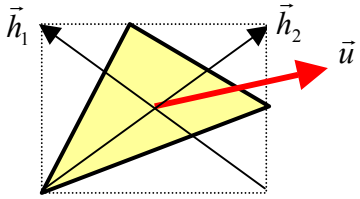
$$W_\psi(x,y) = N_i + \frac{\alpha h}{2|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y}), \qquad (4.1.1.3\text{-}12)$$

where h is a characteristic dimension of element. The optimal value of α depends upon the local Reynolds number of element (Pe is proportional to the element size)

$$\alpha_{opt} = \coth Pe - \frac{1}{Pe}, \qquad Pe = \frac{|u| h\rho}{2\mu}. \qquad (4.1.1.3\text{-}13)$$

It is seen from (12-13) that the asymmetric part of the weight function is significant only if local velocity and size of element are large. The characteristic dimension of element h is not quite strictly defined – its value is calculated in FEMINA according to the following Eq.(14)

$$h = \max(\frac{\vec{h}_1 \cdot \vec{u}}{|\vec{u}|}, \frac{\vec{h}_2 \cdot \vec{u}}{|\vec{u}|}) \qquad (4.1.1.3\text{-}14)$$



Weighted residual method consists in multiplying residuum of transport equation (6) by weight function (12), integrating and using Green's theorem to the second order derivatives. As a result we obtain the following system of ordinary differential equations

$$M_{ij}\frac{d\omega_j}{dt} + A_{ij}\omega_j = B_{ij}T_j \qquad , \tag{4.1.1.3-15}$$

where the mass matrix M and the matrix of convective and viscous transfer A are expressed by integrals

$$M_{ij} = \iint_{\Omega} \rho N_i N_j d\Omega \qquad , \tag{4.1.1.3-16}$$

$$A_{ij} = \iint_{\Omega} \left[\rho[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y})](u_x \frac{\partial N_j}{\partial x} + u_y \frac{\partial N_j}{\partial y}) + \mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}) \right] d\Omega \tag{4.1.1.3-17}$$

$$B_{ij} = \iint_{\Omega} \left[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y}) \right] \beta\rho(g_y \frac{\partial N_j}{\partial x} - g_x \frac{\partial N_j}{\partial y}) d\Omega \quad . \tag{4.1.1.3-18}$$

It should be noted, that the boundary integrals disappear in Eq.(17) due to a clever choice of weight functions W_ψ.

The same procedure applied to Poisson equation (8) results in the system of linear algebraic (and not differential) equations

$$D_{ij}\psi_j + C_{ij}\omega_j = 0 \,, \tag{4.1.1.3-19}$$

where

$$C_{ij} = \iint_{\Omega} N_i N_j d\Omega \qquad , \tag{4.1.1.3-20}$$

$$D_{ij} = \iint_{\Omega} (\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}) d\Omega \quad . \tag{4.1.1.3-21}$$

Cylindrical co-ordinate system

The same procedure applied to formulation in cylindrical co-ordinate system gives vorticity equation

$$\rho(\frac{\partial \omega}{\partial t} + u_x \frac{\partial \omega}{\partial x} + u_r \frac{\partial \omega}{\partial r} - \frac{u_r \omega}{r}) = \mu[\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial}{\partial r}(\frac{1}{r}\frac{dr\omega}{dr})] + \rho\beta(g_r \frac{\partial T}{\partial x} - g_x \frac{\partial T}{\partial r}) \qquad , \tag{4.1.1.3-22}$$

weight functions

$$W(x,y) = N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y} - \frac{u_r N_i}{r}) \qquad , \tag{4.1.1.3-23}$$

and corresponding matrix of convective and viscous terms A and matrix of buoyant forces B

$$A_{ij} = \iint_{\Omega} \left[\begin{array}{l} \rho[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_r \frac{\partial N_i}{\partial r} - \frac{u_r N_i}{r})](u_x \frac{\partial N_j}{\partial x} + u_r \frac{\partial N_j}{\partial r} - \frac{u_r N_j}{r}) + \\ + \mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r} + \frac{N_j}{r}\frac{\partial N_i}{\partial r}) \end{array} \right] d\Omega \quad , \qquad (4.1.1.3\text{-}24)$$

$$B_{ij} = \iint_{\Omega} \left[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_r \frac{\partial N_i}{\partial r} - u_r \frac{N_i}{r}) \right] \beta\rho(g_r \frac{\partial N_j}{\partial x} - g_x \frac{\partial N_j}{\partial r}) d\Omega \quad . \qquad (4.1.1.3\text{-}25)$$

Poisson‘s equation for stream function in cylindrical coordinate system is

$$\omega = \frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial \psi}{\partial r}) + \frac{1}{r}\frac{\partial^2 \psi}{\partial x^2} \quad , \qquad (4.1.1.3\text{-}26)$$

and corresponding matrix *D* looks like this

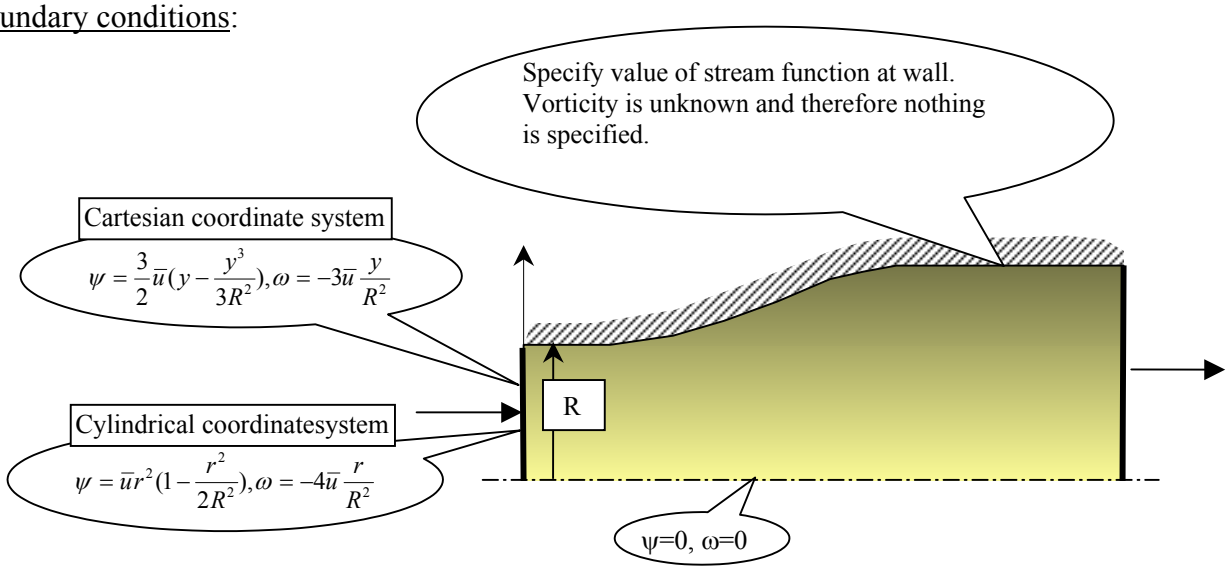
$$D_{ij} = \iint_{\Omega} \frac{1}{r}(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r}) d\Omega \quad . \qquad (4.1.1.3\text{-}27)$$

Time discretisation

Weighted residual method results in the system of ordinary differential equations for vorticity transport (15) completed by the system of algebraic equations (19). Substituting time derivative by time difference we obtain in each time step Δt the following system of algebraic equations for nodal parameters $\{\omega_j\ \psi_j\}$

$$\begin{aligned} (M_{ij} + \Delta t A_{ij})\omega_j &= M_{ij}\omega_j^0 + \Delta t B_{ij} T_j \\ D_{ij}\psi_j + C_{ij}\omega_j &= 0 \end{aligned} \qquad (4.1.1.3\text{-}28)$$

Boundary conditions:



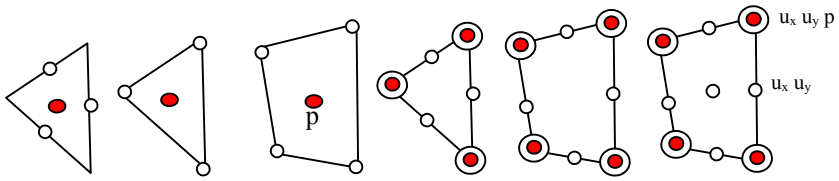
Implementation

The arrangement of coefficients in the element matrix is little bit unusual and follows from the fact that the weight functions W_ψ are applied to the equation of vorticity and vice versa. For arrangement of nodal parameters (ω_1 ψ_1 ω_2 ψ_2 ……..) the corresponding local element matrix has the following structure with change-over rows ($W_{\psi 1}$ $W_{\omega 1}$ $W_{\psi 2}$ $W_{\omega 2}$ …..) – for example the matrix 6 x 6 for triangular element with 3 nodes

$$\begin{bmatrix} C_{11} & D_{11} & C_{12} & D_{12} & C_{13} & D_{13} \\ M_{11}+\Delta tA_{11} & 0 & M_{12}+\Delta tA_{12} & 0 & M_{13}+\Delta tA_{13} & 0 \\ C_{21} & D_{21} & C_{22} & D_{22} & C_{23} & D_{23} \\ M_{21}+\Delta tA_{21} & 0 & M_{22}+\Delta tA_{22} & 0 & M_{23}+\Delta tA_{23} & 0 \\ C_{31} & D_{31} & C_{32} & D_{32} & C_{33} & D_{33} \\ M_{31}+\Delta tA_{31} & 0 & M_{32}+\Delta tA_{32} & 0 & M_{33}+\Delta tA_{33} & 0 \end{bmatrix} \qquad (4.1.1.3\text{-}29)$$

4.1.2. Navier Stokes equation formulated in primitive variables

4.1.2.1. Velocities and pressure (UVP)



A classical method, which is frequently used for solution of Navier Stokes equations operates not with the stream function and vorticity, rather with primitive variables: velocities and pressure. The primary advantage of the stream function oriented methods is therefore lost and continuity equation is not automatically fulfilled. On other hand the methods with primitive variables are easily applied to 3D flows and further on it is possible to apply pressure boundary conditions and therefore to solve problems with several outlets and problems when fluid flows around an obstacle. Simultaneous solution of Navier Stokes transport equations (momentum transport) and continuity equation requires to use hybrid elements with different form of velocity and pressure approximations. Higher degree basis functions must be used for velocities and at least one order degree less polynomials must be used for the approximation of pressure.

Cartesian coordinate system

Let us consider the following formulation describing 2D flow of an incompressible Newtonian liquid

$$\rho(\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y})=-\frac{\partial p}{\partial x}+\mu(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2})+\rho g_x(1-\beta T) \quad , \qquad (4.1.2.1\text{-}1)$$

$$\rho(\frac{\partial u_y}{\partial t}+u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y})=-\frac{\partial p}{\partial y}+\mu(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2})+\rho g_y(1-\beta T) \quad , \qquad (4.1.2.1\text{-}2)$$

and continuity equation

$$\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}=0\,. \qquad (4.1.2.1\text{-}3)$$

Weighted residual method with asymmetric weight functions (Petrov Galerkin), see Zienkiewicz, part III. page 27, will be considered for momentum transport equations

$$u_x(x,y)=N_j(x,y)u_{xj}\,, \qquad u_y(x,y)=N_j(x,y)u_{yj}\,, \qquad p(x,y)=H_j(x,y)p_j\,, \qquad (4.1.2.1\text{-}4)$$

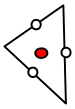
$$W(x,y)=N_i+\frac{\alpha h}{2\,|u|}(u_x\frac{\partial N_i}{\partial x}+u_y\frac{\partial N_i}{\partial y})\,. \qquad (4.1.2.1\text{-}5)$$

Parameter h is an characteristic dimension of element, and optimal value of dimensionless coefficient α is a function of element Reynolds number (Pe)

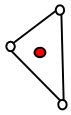
$$\alpha_{opt}=\coth Pe-\frac{1}{Pe}, \qquad Pe=\frac{|u|h\rho}{2\mu}\,. \qquad (4.1.2.1\text{-}6)$$

Optimal value of the coefficient α is $\alpha_{opt} \approx Pe/2$ for very small values of Peclet element number (in this context the Peclet number is the Reynolds number of element), while for very high values of Pe the optimal value of α_{opt} is approaching to one.

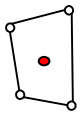
Higher order (quadratic or linear) polynomials $N_j(x,y)$ are used as base (shape) functions for velocities, while a lower order approximation $H_j(x,y)$ is used for pressure (linear or element-wise constant). The reason why it is not possible to use the same base functions for velocities and pressures is stability of solution and for example a simple triangular element with linear approximation of velocities and linear approximation of pressure does not work. A simple explanation is that the second derivatives of velocities ($\nabla^2 u$) and only the first derivatives of pressure (∇p) exist in momentum equations (Navier Stokes equations) and therefore polynomial approximation of velocities should be of one order higher than pressure so that the both terms ($\nabla^2 u$ and ∇p) will be of the same order. There exist many possible combinations of $N_j(x,y)$, $H_j(x,y)$ and only some of them are implemented in FEMINA:



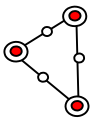
Triangular element P1P0 with midside nodes for velocities and a constant pressure in internal node. This element is incompatible because velocities (and of course pressure) are not continuous, however it usually works. Element is of the first order of accuracy.



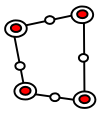
This triangular element P1P0 usually does *not* work due to overconstraints. For example in a regular rectangular mesh N x N the number of elements $2N^2$ is twice the number of velocity nodes N^2 and because equation of continuity should hold in each element ($2N^2$ constraints) there are no free DOF which could be used for approximation of momentum equations (there are $2N^2$ of internal „pressure“ nodes and the same number of velocities).



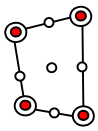
The situation is slightly better in the following element Q1P0 (bilinear velocities, constant pressure), with $2N^2$ velocities and only N^2 pressure constraints. This elements does not meet BB requirement (Babuschka,Brezzi), however is simple and usually works (first order of accuracy).



One of the best elements is P2P1 (quadratic velocities and linear pressure), having a very good ratio of $8N^2$ velocities and N^2 pressures in N x N mesh. Element meets the BB stability requirement and is of the second order of accuracy.



Element Q2(8)Q1 suggested by Hughes, Taylor. This element makes use biquadratic velocities (8-nodes, so called serendipity family) and bilinear pressure. The element is not very good according to our experience.



Similar, but significantly better is the element based upon Lagrangian polynomials with 9-nodes for velocities, and bilinear approximation of pressure. The same ratio of velocity/pressure DOF as in P2P1 triangular element is achieved ($8N^2$ velocities and N^2 pressures).

For all these elements velocities and pressures are described by the following set of ordinary differential equations

$$M_{ij}\frac{\partial u_{xj}}{\partial t} + A_{ij}u_{xj} + P_{ij}^{x}p_j = b_i^x \qquad (4.1.2.1\text{-}7)$$

$$M_{ij}\frac{\partial u_{yj}}{\partial t} + A_{ij}u_{yj} + P_{ij}^{y}p_j = b_i^y \quad , \qquad (4.1.2.1\text{-}8)$$

where

$$M_{ij} = \iint_{\Omega} \rho[N_i + \frac{\alpha h}{2\,|u|}(u_x\frac{\partial N_i}{\partial x} + u_y\frac{\partial N_i}{\partial y})]N_j\,d\Omega \cong \iint_{\Omega} \rho N_i N_j\,d\Omega \quad . \qquad (4.1.2.1\text{-}9)$$

Remark: Neglecting asymmetric term in Eq.(9) is only an approximation, however at least distortion of the diagonal term in the mass matrix is zero, because asymmetric part is an odd function.

$$A_{ij} = \iint_{\Omega}\left[\rho[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y})](u_x \frac{\partial N_j}{\partial x} + u_y \frac{\partial N_j}{\partial y}) + \mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}) \right] d\Omega + \\ - \int_{\Gamma} \mu N_i \frac{\partial N_j}{\partial n} d\Gamma \qquad (4.1.2.1\text{-}10)$$

The asymmetric part is ignored in the viscous term – in this case it is substantiated: Curve integral is zero at wall (N_i=0), at a symmetry axis ($\partial N_j/\partial$n=0), at inlet (N_i=0) and can be nonzero only at outlet as soon as the velocity profile is not fully stabilised. The same holds for curve integrals in the following relations for coefficients of matrix P, corresponding to the pressure gradients in NS equations:

$$P_{ij}^x = \iint_{\Omega}\left[- H_j \frac{\partial N_i}{\partial x} + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y})\frac{\partial H_j}{\partial x} \right] d\Omega + \int_{\Gamma} H_j N_i n_x d\Gamma \qquad (4.1.2.1\text{-}11)$$

$$P_{ij}^y = \iint_{\Omega}\left[- H_j \frac{\partial N_i}{\partial y} + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y})\frac{\partial H_j}{\partial y} \right] d\Omega + \int_{\Gamma} H_j N_i n_y d\Gamma \quad . \qquad (4.1.2.1\text{-}12)$$

Remark: In this term the Green's theorem has been applied only to the symmetric part of weighting function. The resulting term with first derivatives of H_j is omitted.

$$b_i^x = \iint_{\Omega}\left[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y}) \right] \rho g_x (1 - \beta T) d\Omega \qquad (4.1.2.1\text{-}13)$$

$$b_i^y = \iint_{\Omega}\left[N_i + \frac{\alpha h}{2\,|u|}(u_x \frac{\partial N_i}{\partial x} + u_y \frac{\partial N_i}{\partial y}) \right] \rho g_y (1 - \beta T) d\Omega \quad . \qquad (4.1.2.1\text{-}14)$$

Pressure base function H_i are applied to the continuity equation as weight functions

$$Q_{ij}^x u_{xj} + Q_{ij}^y u_{yj} = 0 \quad , \qquad (4.1.2.1\text{-}15)$$

where

$$Q_{ij}^x = \iint_{\Omega} H_i \frac{\partial N_j}{\partial x} d\Omega, \qquad Q_{ij}^y = \iint_{\Omega} H_i \frac{\partial N_j}{\partial y} d\Omega \quad . \qquad (4.1.2.1\text{-}16)$$

Matrices Q are except for sign identical with the transposed matrices P not taking into account asymmetry terms of test functions (i.e. when α=0).

Cylindrical coordinate system

The same hold in principle for flow description in the cylindrical coordinate system with Navier Stokes equations in the form

$$\rho(\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_r \frac{\partial u_x}{\partial r}) = -\frac{\partial p}{\partial x} + \mu[\frac{\partial^2 u_x}{\partial x^2} + \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u_x}{\partial r})] + \rho g_x (1 - \beta T) \qquad (4.1.2.1\text{-}17)$$

$$\rho(\frac{\partial u_r}{\partial t} + u_x \frac{\partial u_r}{\partial x} + u_r \frac{\partial u_r}{\partial r}) = -\frac{\partial p}{\partial r} + \mu[\frac{\partial^2 u_r}{\partial x^2} + \frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial r u_r}{\partial r})] + \rho g_r (1 - \beta T) \qquad (4.1.2.1\text{-}18)$$

and with the continuity equation

$$\frac{\partial u_x}{\partial x}+\frac{1}{r}\frac{\partial r u_r}{\partial r}=0\,. \tag{4.1.2.1-19}$$

We shall apply weight functions *W(x,r)* to the momentum balances in the *x,r* directions

$$\iint_\Omega W[\rho(\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_r\frac{\partial u_x}{\partial r})-\mu(\frac{\partial^2 u_x}{\partial x^2}+\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u_x}{\partial r}))]d\Omega+\iint_\Omega W\frac{\partial p}{\partial x}d\Omega=\iint_\Omega W\rho g_x(1-\beta T)d\Omega \tag{20}$$

$$\iint_\Omega W[\rho(\frac{\partial u_r}{\partial t}+u_x\frac{\partial u_r}{\partial x}+u_r\frac{\partial u_r}{\partial r})-\mu(\frac{\partial^2 u_r}{\partial x^2}+\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial r u_r}{\partial r}))]d\Omega+\iint_\Omega W\frac{\partial p}{\partial r}d\Omega=\iint_\Omega W\rho g_r(1-\beta T)d\Omega \tag{21}$$

and decrease the second order of derivatives in the viscous term by using Green's theorem

$$\iint_\Omega[W\rho(\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_r\frac{\partial u_x}{\partial r})+\mu(\frac{\partial u_x}{\partial x}\frac{\partial W}{\partial x}+\frac{\partial u_x}{\partial r}\frac{\partial W}{\partial r}-\frac{W}{r}\frac{\partial u_x}{\partial r})]d\Omega+\iint_\Omega W\frac{\partial p}{\partial x}d\Omega=$$
$$=\iint_\Omega W\rho g_x(1-\beta T)d\Omega+\int_\Gamma W(\frac{\partial u_x}{\partial x}n_x+\frac{\partial u_x}{\partial r}n_r)d\Gamma \tag{4.1.2.1-22}$$

$$\iint_\Omega[W\rho(\frac{\partial u_r}{\partial t}+u_x\frac{\partial u_r}{\partial x}+u_r\frac{\partial u_r}{\partial r})+\mu(\frac{\partial u_r}{\partial x}\frac{\partial W}{\partial x}+\frac{\partial u_r}{\partial r}\frac{\partial W}{\partial r}+\frac{u_r}{r}\frac{\partial W}{\partial r})]d\Omega+\iint_\Omega W\frac{\partial p}{\partial r}d\Omega=$$
$$=\iint_\Omega W\rho g_r(1-\beta T)d\Omega+\int_\Gamma W(\frac{\partial u_r}{\partial x}n_x+\frac{1}{r}\frac{\partial r u_r}{\partial r}n_r)d\Gamma \tag{4.1.2.1-23}$$

Substituting weight functions with the asymmetric upwind part

$$W(x,r)=N_i+\frac{\alpha h}{2\,|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r}) \tag{4.1.2.1-24}$$

we arrive to the momentum balances in the *x,r* directions described by the following system of ordinary differential equations

$$M_{ij}\frac{\partial u_{xj}}{\partial t}+A^x_{ij}u_{xj}+P^x_{ij}p_j=b^x_i \tag{4.1.2.1-25}$$

$$M_{ij}\frac{\partial u_{rj}}{\partial t}+A^r_{ij}u_{rj}+P^r_{ij}p_j=b^r_i\,. \tag{4.1.2.1-26}$$

The mass matrix *M* is identical for the both equations

$$M_{ij}=\iint_\Omega\rho[N_i+\frac{\alpha h}{2\,|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})]N_j d\Omega\cong\iint_\Omega\rho N_i N_j d\Omega \tag{4.1.2.1-27}$$

(with the same simplification as in the Cartesian coordinate system),

while the matrix *A* differs slightly in the *x* and *r* direction

$$A_{ij}^{x}=\iint_{\Omega}\left[\rho[N_i+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})](u_x\frac{\partial N_j}{\partial x}+u_r\frac{\partial N_j}{\partial r})+\mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r}-\frac{N_i}{r}\frac{\partial N_j}{\partial r})\right]d\Omega+$$
$$-\int_{\Gamma}\mu N_i(\frac{\partial N_j}{\partial x}n_x+\frac{\partial N_j}{\partial r}n_r)d\Gamma \qquad (4.1.2.1\text{-}28)$$

$$A_{ij}^{r}=\iint_{\Omega}\left[\rho[N_i+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})](u_x\frac{\partial N_j}{\partial x}+u_r\frac{\partial N_j}{\partial r})+\mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r}+\frac{N_j}{r}\frac{\partial N_i}{\partial r})\right]d\Omega+$$
$$-\int_{\Gamma}\mu N_i(\frac{\partial N_j}{\partial x}n_x+\frac{1}{r}\frac{\partial rN_j}{\partial r}n_r)d\Gamma \qquad (4.1.2.1\text{-}29)$$

Matrices P as well as right hand side vectors are the same as in the Cartesian coordinate system

$$P_{ij}^{x}=\iint_{\Omega}\left[-H_j\frac{\partial N_i}{\partial x}+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})\frac{\partial H_j}{\partial x}\right]d\Omega+\int_{\Gamma}H_jN_in_xd\Gamma \qquad (4.1.2.1\text{-}30)$$

$$P_{ij}^{r}=\iint_{\Omega}\left[-H_j\frac{\partial N_i}{\partial r}+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})\frac{\partial H_j}{\partial r}\right]d\Omega+\int_{\Gamma}H_jN_in_rd\Gamma \qquad (4.1.2.1\text{-}31)$$

$$b_i^{x}=\iint_{\Omega}\left[N_i+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})\right]\rho g_x(1-\beta T)d\Omega \qquad (4.1.2.1\text{-}32)$$

$$b_i^{r}=\iint_{\Omega}\left[N_i+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})\right]\rho g_r(1-\beta T)d\Omega \qquad (4.1.2.1\text{-}33)$$

Integral form of the continuity equation is based upon symmetrical weight function H_i

$$Q_{ij}^{x}u_{xj}+Q_{ij}^{r}u_{rj}=0 \qquad (4.1.2.1\text{-}34)$$

where

$$Q_{ij}^{x}=\iint_{\Omega}H_i\frac{\partial N_j}{\partial x}d\Omega,\qquad Q_{ij}^{r}=\iint_{\Omega}H_i\frac{1}{r}\frac{\partial rN_j}{\partial r}d\Omega \qquad (4.1.2.1\text{-}35)$$

Matrices Q are except for a sign identical with the transposed matrices P as soon as the asymmetric part of weight functions is zero (α=0).

Time discretization

Result of MWR is the system of ordinary differential equations (7-8), resp. (25-26), completed by algebraic equations (15), resp. (34). Using implicit Euler's method for substitution differential equations by difference equations we arrive at the system of algebraic equations

$$(M_{ij}+\Delta tA_{ij})u_{xj}+\Delta tP_{ij}^{x}p_j=M_{ij}u_{xj}^{0}+\Delta tb_i^{x} \qquad (4.1.2.1\text{-}36)$$

$$(M_{ij}+\Delta tA_{ij})u_{yj}+\Delta tP_{ij}^{y}p_j=M_{ij}u_{yj}^{0}+\Delta tb_i^{y} \qquad (4.1.2.1\text{-}37)$$

completed by continuity equations (15), resp.(34) in the form

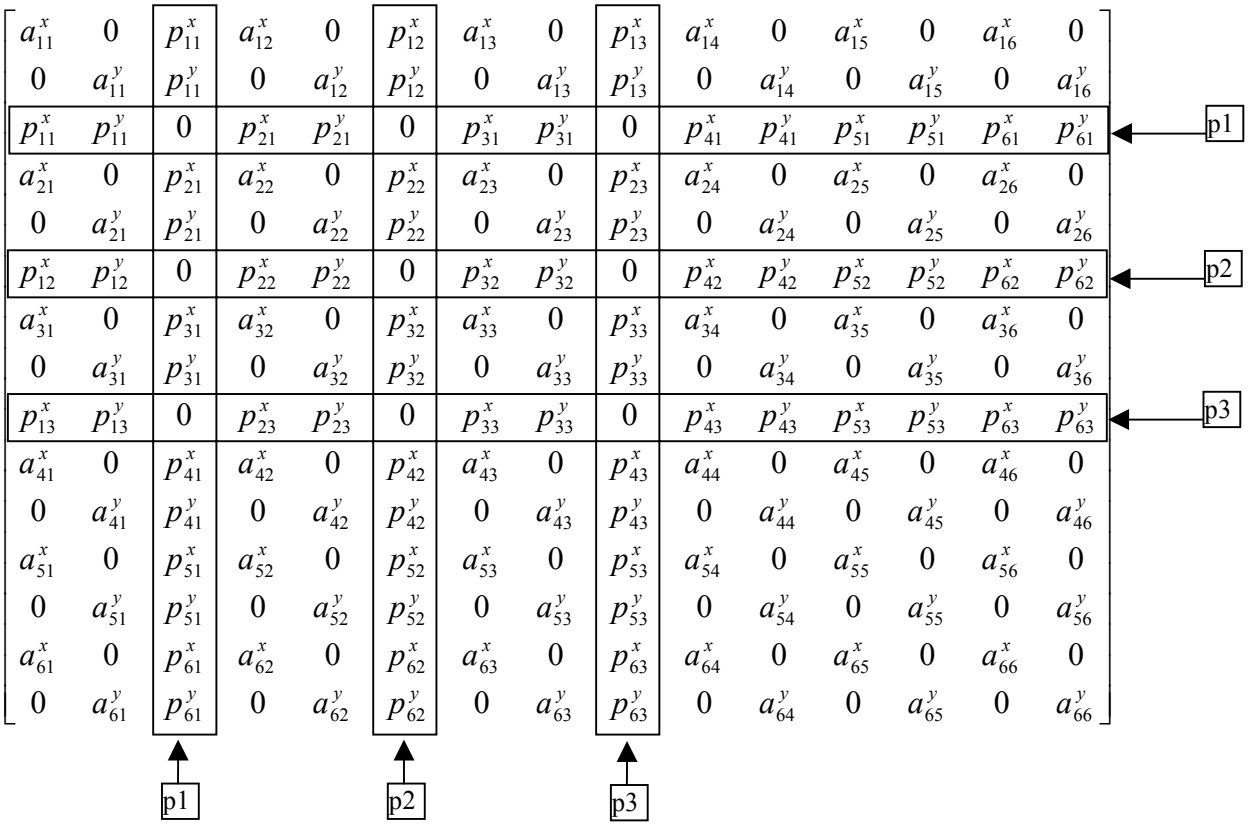
$$\Delta t P^x_{ji} u_{xj} + \Delta t P^y_{ji} u_{yj} = 0 \qquad (4.1.2.1\text{-}38)$$

making use equivalence of matrices P and Q.

Implementation

The UVP method is implemented for several kinds of hybrid elements, triangles with 6 and 4 nodes and quadrilaterals with 5, 8 and 9 nodes:

- Nodal parameter vector for 6 node triangular element has the following structure $\{u_{x1}\ u_{y1}\ p_1\ u_{x2}\ u_{y2}\ p_2\ u_{x3}\ u_{y3}\ p_3\ u_{x4}\ u_{y4}\ u_{x5}\ u_{y5}\ u_{x6}\ u_{y6}\}$, and corresponding element matrix has dimension 15 x 15, see the following figure.



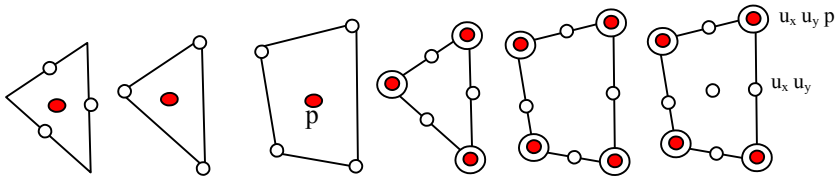
Symbols a_{ij} are elements of matrix A with dimension 6 x 6 (base functions N_j for velocities), and p_{ij} are elements of matrix P (6 x 3), corresponding to 6 base functions N_j and three base functions H_j for pressure:

- Nodal parameter vector for 4 node triangular element (3 nodes velocities, internal node for discontinuous pressure) has the following structure $\{u_{x1}\ u_{y1}\ u_{x2}\ u_{y2}\ u_{x3}\ u_{y3}\ p_4\}$, and corresponding element matrix has dimension 7 x 7.

Results of processing and post-processing

No post-processing is carried out in UVP operation, the only results are nodal velocities and pressures saved in individual time steps into file *.OUT.

4.1.2.2. Velocities and pressure – pseudo-compressibility method (UVPP)



This method, implementation, and also applications are nearly the same as in the standard UVP method described in previous chapter. The only difference is in a modification of continuity equation where a pressure is introduced.

$$\rho\frac{D\vec{u}}{Dt} = -\nabla p + \nabla\cdot\mu\nabla\vec{u} + \rho\vec{g}(1-\beta T)\,, \qquad \nabla\cdot\vec{u} = -\frac{1}{\lambda}\frac{\partial p}{\partial t} \qquad \text{(4.1.2.2-1,2)}$$

The modified continuity equation is related to the continuity equation for compressible fluids

$$\nabla\cdot\vec{u} = -\frac{1}{\rho}\frac{D\rho}{Dt}\,, \qquad \rho = \rho_0 + \frac{p}{c^2}\quad, \qquad \text{(4.1.2.2-3,4)}$$

where ρ is density, which can be approximately related to pressure *p* and speed of sound *c,* giving

$$\nabla\cdot\vec{u} = -\frac{1}{\rho_0 c^2}\frac{Dp}{Dt}\,, \qquad \text{(4.1.2.2-5)}$$

and this equation corresponds to Eq.(2). It is seen that the parameter $\lambda \approx \rho_0 c^2$ is to be very high in liquids, where speed of sound is of the order 10^3 [m/s], density is also 10^3 [kg/m^3], therefore $\lambda \approx 10^9$!

It is not necessary to repeat all steps and details of derivation, because it is very similar to the previous case described in chapter 4.1.2.1. Only explanation of possible benefit: UVPP method should result in a system of equations which are identical with the UVP matrix with the exception of diagonal terms in rows corresponding continuity equations. Zeroes in UVP are replaced by non-zero values (their magnitude depends first of all upon specified value of λ-parameter) and the system matrix should be better conditioned – "more regular" with a positive effect for example upon the influence of round-off errors.

4.1.2.3. Navier Stokes equations penalty method (PENS)

By using rather drastic modification of the continuity equation it is possible to completely eliminate pressure from the Navier Stokes equations. The method is known under the name penalty method and therefore the identifier PENS (PENalty Navier Stokes) is used in FEMINA.

Cartesian coordinate system

Let us consider the following form of Navier Stokes equations for Newtonian liquids

$$\rho(\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y})=-\frac{\partial p}{\partial x}+\mu(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2})+\rho g_x(1-\beta T) \qquad (4.1.2.3\text{-}1)$$

$$\rho(\frac{\partial u_y}{\partial t}+u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y})=-\frac{\partial p}{\partial y}+\mu(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2})+\rho g_y(1-\beta T)\,. \qquad (4.1.2.3\text{-}2)$$

Continuity equation for incompressible liquid is substituted by equation

$$\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}=-\frac{p}{\lambda}, \qquad \lambda[\text{Pa.s}] \text{ has dimension of volumetric viscosity} \qquad (4.1.2.3\text{-}3)$$

where λ is a penalty parameter, which should be so large, that the right hand side, residuum of continuity, is nearly zero for typical values of pressure $p(x,y)$. The minus sign corresponds to the fact, that expansion of volume (positive value of divergence of velocity) implies under-pressure. Correct choice of parameter λ decides, whether solution will be successful or not. Too small value means, that the continuity equation will not be fulfilled, and on the other hand too high value suppresses momentum balances, because in that case all equations are reduced to the continuity requirement and this is not enough to ensure uniqueness of solution (too high value of λ entrains a loss of convergence).

Substituting for pressure p from Eq.(3) into momentum balances (1,2), the following pair of equations for unknown velocity components will be obtained

$$\rho(\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y})=\lambda(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_y}{\partial y\partial x})+\mu(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2})+\rho g_x(1-\beta T) \qquad (4.1.2.3\text{-}4)$$

$$\rho(\frac{\partial u_y}{\partial t}+u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y})=\lambda(\frac{\partial^2 u_x}{\partial x\partial y}+\frac{\partial^2 u_y}{\partial y^2})+\mu(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2})+\rho g_y(1-\beta T)\quad . \qquad (4.1.2.3\text{-}5)$$

Weighted residual method with asymmetric test functions (Petrof Galerkin), see. Zienkiewicz, III. str.27 can be applied to previous equations, giving

$$u_x(x,y)=N_j(x,y)u_{xj}, \qquad u_y(x,y)=N_j(x,y)u_{yj}, \qquad , \qquad (4.1.2.3\text{-}6)$$

$$W(x,y)=N_i+\frac{\alpha h}{2\,|\,u\,|}(u_x\frac{\partial N_i}{\partial x}+u_y\frac{\partial N_i}{\partial y}), \qquad (4.1.2.3\text{-}7)$$

where h is a characteristic dimension of element, and for optimal value of α holds

$$\alpha_{opt} = \coth Pe - \frac{1}{Pe}, \qquad Pe = \frac{|u|h\rho}{2\mu}. \tag{4.1.2.3-8}$$

More or less arbitrary polynomials (linear, quadratic,…) which need not satisfy continuity of derivatives can be used as a basis $N_j(x,y)$ for approximation of velocities.

Momentum balances in directions x,y are represented by system of ordinary differential equations for unknown nodal velocities

$$M_{ij}\frac{\partial u_{xj}}{\partial t} + A_{ij}^{x}u_{xj} + P_{ij}^{x}u_{yj} = b_i^{x} \tag{4.1.2.3-9}$$

$$M_{ij}\frac{\partial u_{yj}}{\partial t} + A_{ij}^{y}u_{yj} + P_{ij}^{y}u_{xj} = b_i^{y} \tag{4.1.2.3-10}$$

where

$$M_{ij} = \iint_{\Omega} \rho N_i N_j d\Omega \tag{4.1.2.3-11}$$

$$A_{ij}^{x} = \iint_{\Omega}\left[\rho[N_i + \frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x} + u_y\frac{\partial N_i}{\partial y})](u_x\frac{\partial N_j}{\partial x} + u_y\frac{\partial N_j}{\partial y}) + (\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x})(\mu+\lambda) + \mu(\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y})\right]d\Omega \tag{4.1.2.3-12}$$

$$A_{ij}^{y} = \iint_{\Omega}\left[\rho[N_i + \frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x} + u_y\frac{\partial N_i}{\partial y})](u_x\frac{\partial N_j}{\partial x} + u_y\frac{\partial N_j}{\partial y}) + (\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y})(\mu+\lambda) + \mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x})\right]d\Omega \tag{4.1.2.3-13}$$

Effect of asymmetric weight functions upon viscous and upon pressure terms has been ignored in preceding integrals. This is a pragmatic simplification, because otherwise the application of Green's theorem would cause appearance of second derivatives in integrands. The same holds for the following matrix P

$$P_{ij}^{x} = P_{ij}^{y} = \frac{\lambda}{2}\iint_{\Omega}\left[\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial x}\right]d\Omega. \tag{4.1.2.3-14}$$

Asymmetric weight function can be preserved in the right hand side vectors, describing contribution of buoyancy

$$b_i^{x} = \iint_{\Omega}\left[N_i + \frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x} + u_y\frac{\partial N_i}{\partial y})\right]\rho g_x(1-\beta T)d\Omega \tag{4.1.2.3-15}$$

$$b_i^{y} = \iint_{\Omega}\left[N_i + \frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x} + u_y\frac{\partial N_i}{\partial y})\right]\rho g_y(1-\beta T)d\Omega \quad . \tag{4.1.2.3-16}$$

Formulation in Cartesian co-ordinate system is now completed.

Cylindrical co-ordinate system

Navier Stokes equations (x is the axis of cylindrical system) look like this

$$\rho(\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_r\frac{\partial u_x}{\partial r})=-\frac{\partial p}{\partial x}+\mu[\frac{\partial^2 u_x}{\partial x^2}+\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u_x}{\partial r})]+\rho g_x(1-\beta T) \qquad (4.1.2.3\text{-}17)$$

$$\rho(\frac{\partial u_r}{\partial t}+u_x\frac{\partial u_r}{\partial x}+u_r\frac{\partial u_r}{\partial r})=-\frac{\partial p}{\partial r}+\mu[\frac{\partial^2 u_r}{\partial x^2}+\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial r u_r}{\partial r})]+\rho g_r(1-\beta T) \qquad (4.1.2.3\text{-}18)$$

and modified continuity equation

$$\frac{\partial u_x}{\partial x}+\frac{1}{r}\frac{\partial r u_r}{\partial r}=-\frac{p}{\lambda}\,. \qquad (4.1.2.3\text{-}19)$$

Matrices *A,P* are described in this case by integrals

$$A_{ij}^x=\iint_\Omega\left[\begin{array}{l}\rho[N_i+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})](u_x\frac{\partial N_j}{\partial x}+u_r\frac{\partial N_j}{\partial r})+\\+(\mu+\lambda)(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x})+\mu(\frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r}-\frac{N_i}{r}\frac{\partial N_j}{\partial r})\end{array}\right]d\Omega \qquad (4.1.2.3\text{-}20)$$

$$A_{ij}^r=\iint_\Omega\left[\begin{array}{l}\rho[N_i+\frac{\alpha h}{2|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})](u_x\frac{\partial N_j}{\partial x}+u_r\frac{\partial N_j}{\partial r})+\\+\mu(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x})+(\mu+\lambda)(\frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r}+\frac{N_j}{r}\frac{\partial N_i}{\partial r})\end{array}\right]d\Omega \qquad (4.1.2.3\text{-}21)$$

$$P_{ij}^x=\lambda\iint_\Omega\left[\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial r}+\frac{1}{r}N_j\frac{\partial N_i}{\partial x}\right]d\Omega \qquad (4.1.2.3\text{-}22)$$

$$P_{ij}^r=\lambda\iint_\Omega\left[\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial r}\right]d\Omega \qquad (4.1.2.3\text{-}23)$$

while the right hand side vectors remain without changes.

Time discretisation

Substituting time derivatives in Eqs.(9-10) by first differences, we arrive to the final system of algebraic equations for nodal velocities in each time step:

$$(M_{ij}+\Delta tA_{ij}^x)u_{xj}+\Delta tP_{ij}^x u_{yj}=M_{ij}u_{xj}^0+\Delta tb_i^x \qquad (4.1.2.3\text{-}24)$$

$$(M_{ij}+\Delta tA_{ij}^y)u_{yj}+\Delta tP_{ij}^y u_{xj}=M_{ij}u_{yj}^0+\Delta tb_i^y\,. \qquad (4.1.2.3\text{-}25)$$

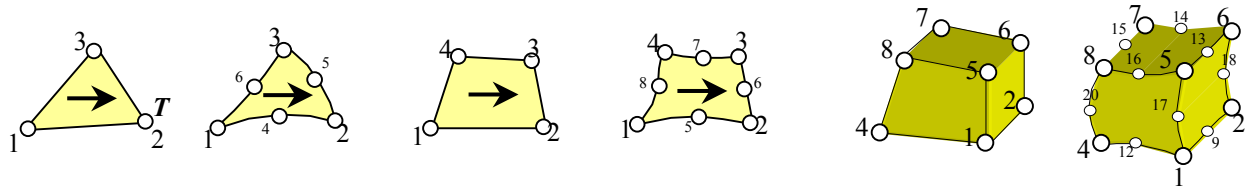
Implementation

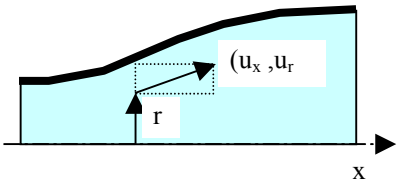
On contrary to previous hybrid elements (combining nodal parameters for velocities and pressure) it is possible to use a broader range of base functions in the penalty method. Therefore the method PENS is implemented for triangles and quadrilateral elements, having arbitrary number of nodes.

Results and postprocessing

There is no postprocessing implemented in the method PENS so far, the only results are velocities saved during solution into file *.OUT in each time step.

4.1.3. Temperature field in a known velocity field with ohmic heating





Transport of heat by convection and conduction with volumetric heat sources is described by the Fourier Kirchhoff equation for temperatures. This equation can be written in cylindrical coordinate system as

$$\rho c_p(\frac{\partial T}{\partial t}+u_x\frac{\partial T}{\partial x}+u_r\frac{\partial T}{\partial r})=\frac{\partial}{\partial x}(\lambda\frac{\partial T}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\lambda r\frac{\partial T}{\partial r})+\kappa[(\frac{\partial U}{\partial x})^2+(\frac{\partial U}{\partial r})^2]+Q-ST\,, \qquad (4.1.3\text{-}1)$$

where the source term is expressed as the sum of electric heat (U is an electric potential) and the term Q, defined by user as a function. The last term ST is a sink defined also as a user function S.

Let us assume that heat is transferred from a part of surface (boundary Γ) as described by the boundary condition of the third kind (T_e is ambient temperature, k is heat transfer coefficient)

$$\lambda\frac{\partial T}{\partial n}=k(T_e-T)\,. \qquad (4.1.3\text{-}2)$$

The Eq.(1) together with the boundary conditions (2) can be reformulated by weighted residual methods, giving weak formulation of the problem

$$\iint_\Omega r\{W[\rho c_p(\frac{\partial T}{\partial t}+u_x\frac{\partial T}{\partial x}+u_r\frac{\partial T}{\partial r})+ST]+\lambda(\frac{\partial T}{\partial x}\frac{\partial W}{\partial x}+\frac{\partial T}{\partial r}\frac{\partial W}{\partial r})\}drdx-\int_\Gamma rWk(T_e-T)d\Gamma=$$
$$=\iint_\Omega rW\{\kappa[(\frac{\partial U}{\partial x})^2+(\frac{\partial U}{\partial r})^2]+Q\}drdx \qquad (4.1.3\text{-}3)$$

.

Temperature T will be approximated by the base functions N_j and asymmetric weighting functions W_i will be designed according to Zienkiewicz

$$W_i(x,y)=N_i+\frac{\alpha h}{2\,|u|}(u_x\frac{\partial N_i}{\partial x}+u_r\frac{\partial N_i}{\partial r})\,, \qquad (4.1.3\text{-}4)$$

where the coefficient $\alpha\in(0,1)$ depends upon the local value of Peclet number $Pe=\dfrac{|u|h\rho c_p}{2\lambda}$.

Thus we arrive to the system of ordinary differential equations for unknown nodal temperatures $T_j(t)$

$$M_{ij}\frac{dT_j}{dt}+A_{ij}T_j=b_i \qquad (4.1.3\text{-}5)$$

where

$$M_{ij}=\iint\rho c_p rN_iN_j d\Omega \qquad \text{(this is only an approximation replacing } W_i \text{ by } N_i) \qquad (4.1.3\text{-}6)$$

$$A_{ij} = \iint_{\Omega} r\{W_i[\rho c_p(u_x \frac{\partial N_j}{\partial x} + u_r \frac{\partial N_j}{\partial r}) + SN_j] + \lambda(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r})]drdx + \int_{\Gamma} rkN_i N_j d\Gamma \quad (4.1.3\text{-}7)$$

$$b_i = \iint_{\Omega} rW_i\{\kappa[(\frac{\partial U}{\partial x})^2 + (\frac{\partial U}{\partial r})^2] + Q\}drdx + \int_{\Gamma} rkT_e N_i d\Gamma \text{ (also an approximation of } W_i \text{ by } N_i). \quad (4.1.3\text{-}8)$$

The ordinary differential equations (5) can be solved by the one step Euler method as

$$(M_{ij} + \theta\Delta t A_{ij})T_j = [M_{ij} - (1-\theta)\Delta t A_{ij}]T_j^0 + \Delta t b_i \quad . \quad (4.1.3\text{-}9)$$

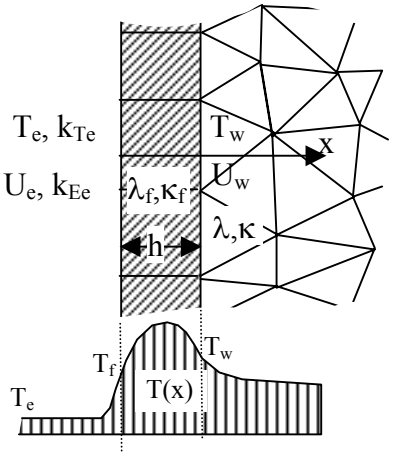
It is obvious, that the formulation in the Cartesian coordinate system is identical, only the multiplication by radius *r* is omitted in integrands. Also the 3D elements are designed in the same way, only with different base functions.

Fouling in 2D and 3D elements

Special arrangement of previously described elements concerns fouling at a boundary, which is described by a modified boundary condition of the third kind (2). It is assumed that the boundary is formed by a thin layer of deposits characterised by a thermal conductivity λ_f and electrical conductivity κ_f (changing thickness of this layer is calculated in a similar way as in the 1D elements PIPE2D and stored as an element parameter). It is assumed that this layer represents not only a passive thermal resistance but also a volumetric heat source caused by ohmic heating. Assuming a constant intensity of electric field (therefore a uniform volumetric heat source), and also uniform thermal properties of layer, the temperature profile across the layer will be a quadratic and the electric potential a linear function.

Neglecting heat accumulation in the layer, the temperature profile is described by equation

$$0 = \lambda_f \frac{\partial^2 T}{\partial x^2} + Q, \qquad Q = \kappa_f(\frac{U_f - U_w}{h})^2 \quad (4.1.3\text{-}10)$$



where U_f is voltage at the backside and U_w at the frontside of layer.

Now it is assumed that on the backside of fouled layer a finite thermal resistance as well as a finite electrical resistance exist, expressed as

$$-\lambda_f \frac{\partial T_f}{\partial x} = k_{Te}(T_e - T_f) \quad (4.1.3\text{-}11)$$

$$(U_e - U_f)k_{Ee} = \frac{\kappa_f}{h}(U_f - U_w), \quad (4.1.3\text{-}12)$$

assuming again a linear profile of electric potential inside the layer. Taking into account boundary conditions at interfaces on the back and the front side of layer, the unknown values of temperature T_f and potential U_f can be eliminated, giving new boundary conditions for the electric field *U*

$$\kappa\frac{\partial U}{\partial n} = \frac{k_{Ee}}{1 + k_{Ee}\frac{h}{\kappa_f}}(U_e - U_w) = \frac{k_{Ee}\kappa_f}{\kappa_f + k_{Ee}h}(U_e - U_w) \quad (4.1.3\text{-}13)$$

and for the temperature field

$$\lambda\frac{\partial T}{\partial n}=\frac{1}{\frac{1}{k_{Te}}+\frac{h}{\lambda_f}}[T_e+\frac{Qh}{\lambda_f}(\frac{\lambda_f}{k_{Te}}+\frac{h}{2})-T_w]=\frac{k_{Te}\lambda_f}{\lambda_f+k_{Te}h}[T_e+\frac{Qh}{\lambda_f}(\frac{\lambda_f}{k_{Te}}+\frac{h}{2})-T_w], \quad (4.1.3\text{-}14)$$

where the volumetric heat source Q is expressed in terms of presumably known voltages

$$Q=\frac{\kappa_f}{h^2(1+\frac{\kappa_f}{hk_{Ee}})^2}(U_e-U_w)^2=\frac{\kappa_f k_{Ee}^2}{(\kappa_f+k_{Ee}h)^2}(U_e-U_w)^2. \quad (4.1.3\text{-}15)$$

Temperature profile inside the layer is described by equation

$$T(x)=T_e+\frac{1}{\lambda_f}[\lambda\frac{\partial T}{\partial x}(\frac{\lambda_f}{k_{Te}}+x)+Q(\frac{h\lambda_f}{k_{Te}}+hx-\frac{x^2}{2})]. \quad (4.1.3\text{-}16)$$

Taken together, fouled layer must by described by its thickness h (element parameter), λ_f , κ_f (material properties) and also the parameters k_{Te}, k_{Ee} (functions), T_e, U_e (RCONST) must be specified.

Model of fouling describes the rate of fouled layer growth by a user function $f(T,\tau,c_N,\ldots)$ in a similar way as for 1D elements (index of this function must be specified as an OPTION parameter)

$$\frac{dh}{dt}=f(T,\tau,...). \quad (4.1.3\text{-}17)$$

Implementation.

Triangular elements with three and six nodes (T3,T6) and quadrilateral elements with four or eight node elements (Q4,Q8) as well as eight and 20 nodes brick elements (B8, B20) are available for 2D and 3D models. Base functions in triangular elements are calculated by subroutine FDFT, isoparametric functions are defined in FDFQ in quadrilaterals, and FDFVL is used for 3D.

Integration is carried out by Gauss method, and different number of integration points can be selected: 1,3,4,6,7,12,16 for elements T3,T6, 1x1, 2x2, 3x3, 4x4 for elements Q4,Q8 and 1x1x1, 2x2x2, 3x3x3, 4x4x4 for elements B8, B20.

Boundary conditions of the third kind are included in the boundary integrals (7-8), calculated simultaneously with surface integrals when processing triangular or quadrilateral elements. The most difficult problem is identification of the element sides forming a part of the boundary Γ. This problem is solved on the basis of information about nodal parameters: The fact that the status of a nodal parameter (IPU) is greater than 20 means that it is a node with prescribed boundary condition of the third kind. In case of elements with nodes at midpoints of sides (T6, Q8) the status of mid-nodes determines whether the corresponding side is, or is not a part of boundary with prescribed boundary conditions of the third kind.[2] More complicated is the case of triangular element T3 having two sides as a part of boundary (this element forms a corner of a region), because then all three nodes of element lie on the boundary and the common node of the two boundary sides must be identified by inspection of the whole connectivity matrix of elements (the node in the corner should not be located in any other element).

As soon as the element sides forming a part of boundary Γ are identified, the curve integrals (7-8) are calculated by Gauss integration of base functions defined by procedure FDCR. Because the heat transfer coefficient k in (7-8) is referenced by a status of nodes and because this status is interpreted as the index of user defined function (function number 21,22,...), the heat transfer coefficient can be a function of temperature, time, concentrations, and other variables.

[2] Negative values IPU indicate strong boundary conditions (directly specified temperatures), values 0 and higher indicate free parameters. Indices greater than 20 define weak boundary conditions of the third kind.

4.1.4. Phase changes

Heat transfer with phase changes can be modelled using previously described method for heat transfer without phase changes when defining temperature dependent specific heat capacity with a sharp peek characterising a sudden enthalpy increase at a phase change temperature. This approach has been described in the introductory example, and therefore it will not be discussed here. We only note that this seemingly simple method is applicable only for a sufficiently smooth phase transition without step enthalpy changes. In this chapter we focus upon description of a sharp transition (melting or freezing) characterised by two parameters: temperature of phase change T_M and the enthalpy of liquid just at this temperature h_M (this value is the sum of enthalpy of fusion and the enthalpy of solid at melting point temperature).

Enthalpy balance for cylindrical coordinate system and incompressible liquids can be written in a general form which is nearly the same as the Eq.(1) in the previous chapter

$$\rho(\frac{\partial h}{\partial t}+u_x\frac{\partial h}{\partial x}+u_r\frac{\partial h}{\partial r})=\frac{\partial}{\partial x}(\lambda\frac{\partial T}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\lambda r\frac{\partial T}{\partial r})+\kappa[(\frac{\partial U}{\partial x})^2+(\frac{\partial U}{\partial r})^2]+Q-ST \quad (4.1.4\text{-}1)$$

The difference is in the fact that there are two unknown variables, specific enthalpy h [J/kg] and temperature T, related by the equation

$$h=\int_0^{T_M}c_p dT+r_{SL}+\int_{T_M}^{T}c_p dT\,. \quad (4.1.4\text{-}2)$$

There are several ways how to solve this system of equations by finite element methods. It is for example possible to approximate temperature and enthalpy as independent functions and to formulate element matrices for two nodal parameters T_j and h_j – this approach can be selected in Femina as the option *Phase changes*=1.

Options *Phase changes*=2,3,4,5 calculate only temperatures from the modified Eq.(1)

$$\rho\frac{dh}{dT}(\frac{\partial T}{\partial t}+u_x\frac{\partial T}{\partial x}+u_r\frac{\partial T}{\partial r})=\frac{\partial}{\partial x}(\lambda\frac{\partial T}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\lambda r\frac{\partial T}{\partial r})+\kappa[(\frac{\partial U}{\partial x})^2+(\frac{\partial U}{\partial r})^2]+Q-ST \quad (4.1.4\text{-}3)$$

where the derivative of enthalpy with respect temperature is approximated by different formulas, see Lewis (1996)

Phase changes=2
$$\frac{dh}{dT}=\sqrt{\frac{(\frac{\partial h}{\partial x})^2+(\frac{\partial h}{\partial r})^2}{(\frac{\partial T}{\partial x})^2+(\frac{\partial T}{\partial r})^2}} \quad (4.1.4\text{-}4)$$

Phase changes=3
$$\frac{dh}{dT}=\sqrt{\left(\frac{\frac{\partial h}{\partial x}}{\frac{\partial T}{\partial x}}\right)^2+\left(\frac{\frac{\partial h}{\partial r}}{\frac{\partial T}{\partial r}}\right)^2} \quad (4.1.4\text{-}5)$$

Phase changes=4 $$\frac{dh}{dT}=\frac{1}{2}\left|\frac{\frac{\partial h}{\partial x}}{\frac{\partial T}{\partial x}}+\frac{\frac{\partial h}{\partial r}}{\frac{\partial T}{\partial r}}\right| \qquad (4.1.4\text{-}6)$$

Phase changes=5 $$\frac{dh}{dT}=\frac{\frac{\partial h}{\partial x}\frac{\partial T}{\partial x}+\frac{\partial h}{\partial r}\frac{\partial T}{\partial r}}{(\frac{\partial T}{\partial x})^2+(\frac{\partial T}{\partial r})^2} \qquad (4.1.4\text{-}7)$$

Spatial derivatives of enthalpy h in Eqs.(4-7) are approximated by nodal enthalpy h_j calculated only temporarily from actual nodal temperatures T_j

$$\frac{\partial h}{\partial x}=\frac{\partial N_j}{\partial x}h_j, \qquad \text{where } h_j=c_pT_j \text{ for } T_j<T_M \text{ else } h_j=h_M+c_p(T_j-T_M) \qquad (4.1.4\text{-}8)$$

From now on the numerical solution is the same as in the previous chapter, it is nodal temperatures at a new time level are calculated from the old temperatures solving the system of equations

$$(M_{ij}+\theta\Delta tA_{ij})T_j=[M_{ij}-(1-\theta)\Delta tA_{ij}]T_j^0+\Delta tb_i \ , \qquad (4.1.4\text{-}9)$$

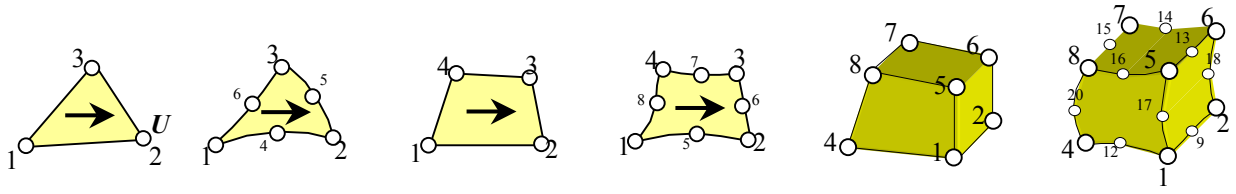
where

$$M_{ij}=\iint\rho\frac{dh}{dT}rN_iN_jd\Omega \qquad (4.1.4\text{-}10)$$

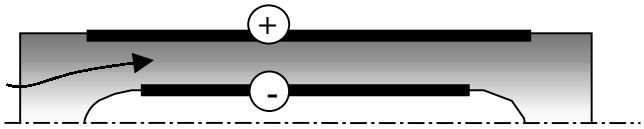
$$A_{ij}=\iint_\Omega r\{W_i[\rho\frac{dh}{dT}(u_x\frac{\partial N_j}{\partial x}+u_r\frac{\partial N_j}{\partial r})+SN_j]+\lambda(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r})]drdx+\int_\Gamma rkN_iN_jd\Gamma \qquad (4.1.4\text{-}11)$$

$$b_i=\iint_\Omega rW_i\{\kappa[(\frac{\partial U}{\partial x})^2+(\frac{\partial U}{\partial r})^2]+Q\}drdx+\int_\Gamma rkT_eN_id\Gamma \ . \qquad (4.1.4\text{-}12)$$

4.1.5. Electric potential distribution



Electric potential distribution is not a transport problem; however its solution is a necessary prerequisite for solution of heat transport equations (direct ohmic heating).



The distribution is described by the Laplace equation, expressed e.g. for the cylindrical coordinate system as

$$0 = \frac{\partial}{\partial x}(\kappa \frac{\partial U}{\partial x}) + \frac{1}{r}\frac{\partial}{\partial r}(\kappa r \frac{\partial U}{\partial r}) \qquad (4.1.5\text{-}1)$$

where U is electric potential and κ [S/m] is specific electrical conductivity of material. Fixed voltage U can be prescribed on a part of boundary as a strong boundary condition, electric insulation is a natural boundary condition (zero normal gradient), and the imperfect insulation characterised by electric conductivity of an equivalent resistive layer k_e [S/m^2] can be prescribed as a boundary condition of the third kind

$$\kappa \frac{\partial U}{\partial n} = k_e (U_e - U) \qquad (4.1.5\text{-}2)$$

where U_e is voltage (el. potential) outside the calculated region.

Galerkin method can be applied to the equation (1) with boundary conditions (2) using identical base and weighting functions $N_i(x,y)$, giving

$$A_{ij} U_j = b_i \qquad (4.1.5\text{-}3)$$

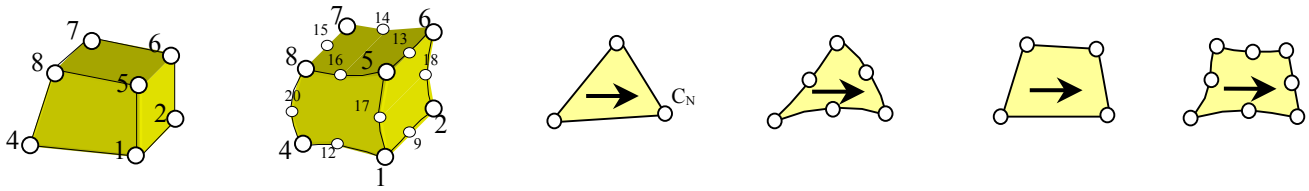
$$A_{ij} = \iint_\Omega r \left[\kappa \left(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r} \right) \right] d\Omega + \int_\Gamma r k_e N_i N_j d\Gamma \qquad (4.1.5\text{-}4)$$

$$b_i = \int_\Gamma r k_e U_e N_i d\Gamma \quad . \qquad (4.1.5\text{-}5)$$

Formulation and solution of the problem in Cartesian coordinate system is the same, only the multiplication by radius r is omitted in integrals (4-5).

This procedure is implemented for elements T3, T6, Q4, Q8, B8, B20 and variable number of integration points (Gauss integration) can be selected.

4.1.6. Mass transport with chemical reaction



The mass transport of up to three different components denoted by N (as Native proteins), D (denaturated, unfolded proteins) and A (as agglomerates) can be solved using concentrations c_N, c_D, c_A of the three mentioned components (kg/m^3). It is possible to define any production and sink terms in transport equations, corresponding for example to an arbitrary chemical reactions or injections of tracer in a stimulus response experiments. However it is not necessary to interpret the concentrations c_N, c_D, c_A as the concentrations of chemical species in a mixture, but for example as structural parameters (for modelling of thixotropic liquids), concentration of bubbles or discrete particles in multiphase flows. In these cases the source and sink terms describe mechanisms of structure decay or restoration.

The mass balance of the component N can be described by the transport equation written e.g. for cylindrical coordinate system

$$\frac{\partial c_N}{\partial t} + u_x \frac{\partial c_N}{\partial x} + u_r \frac{\partial c_N}{\partial r} = \frac{\partial}{\partial x}(D_N \frac{\partial c_N}{\partial x}) + \frac{1}{r}\frac{\partial}{\partial r}(D_N r \frac{\partial c_N}{\partial r}) + Q_N - S_N c_N, \qquad S_N = S_{Nu} + A_N \qquad (4.1.6\text{-}1)$$

together with the boundary condition of the third kind

$$D_N \frac{\partial c_N}{\partial n} = k_N (c_e - c_N) \qquad (4.1.6\text{-}2)$$

and it is obvious that these equations are exactly the same as the transport equations and boundary conditions for heat transfer (mass transfer coefficient k_N is interactively defined as a function). Also the solution method is the same, and equations (1) for c_N, c_D, c_A are solved in this order (Femina calculates in each time step first electric potential U, then the flow field, temperature field and even then c_N followed by c_D and finally c_A).

A slight difference is in definition of production and sink terms: Production term Q_N [kg of A produced in m^3 per second] is defined by user, while the sink S_N is the sum of the user defined function and the rate coefficient A_N corresponding to the chemical reaction of the first order

$$\frac{dc_N}{dt} = -A_N(T) c_N \qquad . \qquad (4.1.6\text{-}3)$$

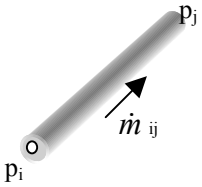
While the sink S_{Nu} must be defined as a function with index referred in EGROUP, the rate coefficient A_N is a material parameter and its corresponding material function represents the Arrhenius term

$$A_N = A_{N0} \exp(-\frac{E}{RT}). \qquad (4.1.6\text{-}4)$$

4.1.7. Pipeline networks – pressure distribution

Let us assume that the flow of an incompressible liquid in a pipe segment is fully developed and isothermal. Then the axial pressure profile is linear and only 2-node elements (elements PIPE2D or PIPE3D) having pressure as a nodal parameter are sufficient.

Element PIPE



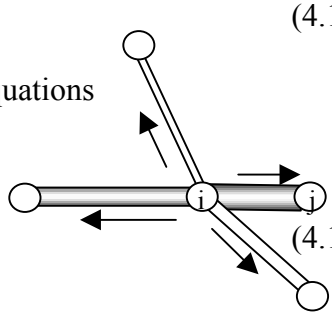
The most important characteristics of the pipe element is relationship between the mass flowrate and the pressure drop which can be expressed in the following way assuming no gravity effects

$$m_{ij} = \varphi_{ij}(|\, p_i - p_j \,|) \cdot (p_i - p_j) \tag{4.1.7-1}$$

Mass balancing[3] in nodal points will be used instead of the weighted residual method: Sum of oriented mass flowrates $\dot{m}$ in a node without a source (a pump), or a sink (leakage), is to be zero

$$\sum_j \varphi_{ij}(|p_i - p_j|).(p_i - p_j) = 0 \tag{4.1.7-2}$$

The whole network is therefore described by the following system of equations



$$\begin{bmatrix} \sum_{i=2,3,\ldots} \varphi_{1i} & -\varphi_{12} & \ldots \\ -\varphi_{21} & \sum_{i=1,3,\ldots} \varphi_{2i} & \ldots \\ \ldots & & \end{bmatrix} \cdot \begin{bmatrix} p_1 \\ p_2 \\ \ldots \end{bmatrix} = \begin{bmatrix} \dot{m}_1 \\ \dot{m}_2 \\ \ldots \end{bmatrix} \tag{4.1.7-3}$$

where the right hand side terms $\dot{m}_1, \dot{m}_2, \ldots$ are non zero only in nodes where a source pumping liquid into the network exists, or in discharge points. This global matrix of flow coefficients is assembled from the local element matrices

$$\left[K_{ij}\right] = \begin{bmatrix} \varphi_{ij} & -\varphi_{ij} \\ -\varphi_{ij} & \varphi_{ij} \end{bmatrix} \tag{4.1.7-4}$$

where flow coefficients φ depend upon the viscous properties of fluid, flow regime, channel geometry (diameter of pipe d and length L_{ij}) and local losses:

$$\varphi_{ij} = \frac{\pi \rho d^4}{128 \mu L_{ij}}, \qquad \text{holds for laminar flow of Newtonian liquid Re<2300} \tag{4.1.7-5}$$

and

$$\varphi_{ij} = \left(\frac{0.558}{L_{ij}}\right)^{4/7} \frac{\rho \pi\, d^{19/7}}{(\rho|\Delta p|)^{3/7}\, \mu^{1/7}}, \qquad \text{holds for } 2300<Re<10^5 \text{ (Blasius).} \tag{4.1.7-6}$$

[3] Mass balancing is quite general, however if density of liquid is constant, the same approach can be applied for volumetric flowrates and this method has been used in versions FEMINA 3.4 and older.

The flow coefficients are constant and the whole problem is linear only in the case of Newtonian liquids and laminar flows. If it is not the case, iterations are necessary and coefficients φ_{ij} must be repeatedly evaluated from Eq. (6) for pressures from the previous iteration. Decision whether the flow regime is laminar or turbulent is based upon the value of Re calculated from the hypothesis of laminar flow

$$\mathrm{Re} = \frac{d^3 \mid \Delta p \mid}{32 \mu^2 L_{ij}} \ . \tag{4.1.7-7}$$

Starting from the version FEMINA 3.3 the element PIPE2D has been improved so that the wall roughness k as well as the local resistance ζ (e.g. Borda's losses) is respected in the turbulent regime. The Blasius correlation (6) is used only as an initial estimate, followed by iterations based upon the Churchill's correlation for pressure drop

$$\Delta p = \frac{1}{2} \rho u^2 (\lambda \frac{L}{d} + \zeta) \tag{4.1.7-7}$$

where λ is the friction factor (Churchill 1977),

$$\lambda = 8[(\frac{8}{\mathrm{Re}})^{12} + \frac{1}{(a+b)^{3/2}}]^{1/12} \tag{4.1.7-8}$$

$$a = [2.457 \ln \frac{1}{(\frac{7}{\mathrm{Re}})^{0.9} + 0.27 \frac{k}{d}}]^{16} \qquad b = (\frac{37530}{\mathrm{Re}})^{16} \ . \tag{4.1.7-9}$$

Parameter ζ in (7) is the coefficient of local losses specified as an element parameter RCONST – in this way it is possible to account for additional pressure losses in sudden contraction or expansion of pipe, influence of elbows or T-pipes.

Using Eq.(7) the flow coefficient can be expressed in terms of pressure drop as

$$\varphi_{ij}(\Delta p, \lambda, \zeta) = \pi d^2 \sqrt{\frac{\rho}{8 \lambda \Delta p (\frac{L}{d} + \zeta)}} \ . \tag{4.1.7-10}$$

Non-Newtonian liquids

Viscosity of liquid need not be a constant, but can be defined as a function of temperature, pressure or shear stress as a table (CURDEF) or as a function (FUNDEF). Non-Newtonian liquids are characterised by dependency of apparent viscosity upon the shear rate or upon the shear stress (TAU). If such a form of dependency (e.g. FUNDEF 1,tau**a) is specified[4], the calculation of flow coefficients must be quite different. Radial velocity profile is no longer a parabolic but a more complicated function, and only the radial profile of shear stress remains linear even for an arbitrary non-Newtonian liquid (for an arbitrary rheological model with the exception of viscoelastic liquids). Knowing the shear stress at the wall (τ_w) it is therefore possible to integrate the mass flowrate according to the Rabinowitsch Mooney Weissenberg equation

[4] FEMINA identifies the nonnewtonian liquid automatically, therefore it need not be specified explicitly by a switch. However, it is possible to enforce the RMW integration even in the case, when viscosity function is independent of stress, i.e. if it is only Newtonian but temperature sensitive liquid. This is accomplished by selection the index of viscosity funkcion higher than 10.

$$\dot{m}_{ij} = \frac{8\rho\pi L_{ij}^3}{\Delta p_{ij}^3}\int_0^{\tau_w}\tau^2\dot{\gamma}d\tau = \frac{8\rho\pi L_{ij}^3}{\Delta p_{ij}^3}\int_0^{\tau_w}\frac{\tau^3}{\mu}d\tau \qquad (4.1.7\text{-}10)$$

for a specified function $\mu(\tau)$ - apparent viscosity as a function of shear stress. This integration must be carried out numerically in each element and in each iteration, because the upper bound of integral, the wall shear stress τ_w, is changing with the iterated value of pressure drop:

$$\tau_w = \frac{d\Delta p_{ij}}{4L_{ij}}. \qquad (4.1.7\text{-}11)$$

Let us show how the constitutive equations for the most frequently used models are formulated: Power law liquid (two parameters, *K*-coefficient of consistency, *n*-power law index)

$$\tau = K\dot{\gamma}^n \qquad \mu(\tau) = \frac{K^{1/n}}{\max(10^{-10},\tau)^{(1-n)/n}} \qquad (4.1.7\text{-}12)$$

Bingham liquid (two parameters, yield stress τ_0, plastic viscosity μ_p)

$$\tau = \tau_0 + \mu_p\dot{\gamma} \qquad \mu(\tau) = \frac{\mu_p\tau}{\max(10^{-10},\tau-\tau_0)} \qquad (4.1.7\text{-}13)$$

Herschel Bulkley liquid (three parameters *K*- consistency, *n*-power law index, yield stress τ_0)

$$\tau = \tau_0 + K\dot{\gamma}^n \qquad \mu(\tau) = \frac{K^{1/n}\tau}{\max(10^{-10},\tau-\tau_0)^{1/n}}. \qquad (4.1.7\text{-}14)$$

Note: The reason why the function *max* has been used is to avoid overflow if the shear stress is zero (at axis) or less than the yield stress (within the piston flow region) – in these cases apparent viscosity should be infinity.

Thixotropic liquids

A specific form on non-Newtonian liquids are liquids exhibiting thixotropic behaviour, which means that the consistency of liquid depends not only upon the actual deformation (or upon an actual wall shear stress) but upon the whole history of deformation. This is typical for example for paints which increase consistency after application when stay at rest, or for food products like a yoghurt or mayonnaise which gradually decrease consistency when mixed and regenerate their structure at rest. Thixotropic liquids are usually modelled by previously mentioned power law or Bingham like models when model parameters, e.g. coefficient of consistency or the yield stress are functions of the so called structural parameter $\lambda_s \in(0,1)$ which is a transported property of liquid decreasing towards zero in regions with high rates of deformation (or with high level of stresses) and returning back to the state of fully regenerated liquid ($\lambda_s \to 1$) at rest or at very slow flow regions. Rather general thixotropic model EHZS (extended Houska, Zitny, Sestak) originated from the model of Cheng (see Šesták 1990) can be expressed as

$$\frac{\partial\lambda_s}{\partial t} + \vec{u}\cdot\nabla\lambda_s = \nabla\cdot D\nabla\lambda_s + a(1-\lambda_s) - b\lambda_s\dot{\gamma}^m \qquad (4.1.7\text{-}15)$$

where the first term on the right hand side represents dispersion of structural parameter (in the same way as for example dispersion of a component in a mixture), the second term describes regeneration of structure and the last term the structure decay due to actual rate of deformation. There is no thixotropic model implemented in FEMINA explicitly, however it is possible to make use the FEMINA's capability to solve concentration changes and for example the concentration c_N can be interpreted as the structural parameter λ_s. Parameters of rheological model, for example consistency coefficient, can be therefore expressed as interactively defined functions of structural parameter c_N.

Example: How to implement Cheng's model of thixotropy using interactively defined functions.

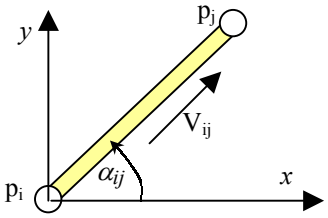
```
FUNDEF 1,A+B*TAU**P              FUNDEF 2,A
FUNDEF 3,(C*CN/max(1e-10,TAU)**(1-Q))**(1/Q)
```

The function 1 and 2 define source and sink of Cheng model (15) where the wall shear stress TAU is used instead of shear rate (these functions must be specified as parameters in EGROUP as sources and sink). Parameters of Cheng's model are user variables A (restoration coefficient), B (decay coefficient) and P (exponent). The function 3 defines the power law model of viscosity (variable Q is a power law index) with the consistency coefficient proportional to the structural parameter CN, see Eq.(12). This function 3 has to be specified as a viscosity function in MPROP and because it depends on the shear stress TAU the Rabinowitsch method will be automatically applied for solution of flow.

Hydrostatic pressure (buoyancy)

Gravity changes the distribution of pressures and flowrates. These effects must be considered if we want to study buoyancy and natural circulation loops formed in a non-isothermal field of liquid as soon as its density depends upon temperature (and it always depends). Straightforward approach follows from the following force balance, which is a slight modification of the straight pipe characteristics Eq.(1)

$$m_{ij} = \varphi_{ij}[p_i - p_j + \rho L_{ij}(g_y \sin\alpha_{ij} + g_x \cos\alpha_{ij})] \qquad (4.1.7\text{-}16)$$



or more generally for a pipe in the *x,y,z* space

$$m_{ij} = \varphi_{ij}[p_i - p_j + \rho(g_x h_x + g_y h_y + g_z h_z)] \qquad (4.1.7\text{-}17)$$

where h_x, h_y, h_z are projections of L_{ij} onto coordinate axes *x,y,z*.

The mass flowrate balance at a general node *i* can be expressed using (16) as

$$\sum_j \dot{m}_{ij} = \sum_j \varphi_{ij}(p_i - p_j) + \sum_j \rho L_{ij}\varphi_{ij}(g_y \sin\alpha_{ij} + g_x \cos\alpha_{ij}) = 0\,. \qquad (4.1.7\text{-}18)$$

The global system of equations for nodal pressures

$$\begin{bmatrix} \sum_{i=2,3,\ldots}\varphi_{1i} & -\varphi_{12} & \ldots \\ -\varphi_{21} & \sum_{i=1,3,\ldots}\varphi_{2i} & \ldots \\ \ldots & & \end{bmatrix} \cdot \begin{bmatrix} p_1 \\ p_2 \\ \ldots \end{bmatrix} = \begin{bmatrix} \dot{m}_1 - \sum_{i=2,3,\ldots}\rho L_{1i}\varphi_{1i}(g_y \sin\alpha_{1i} + g_x \cos\alpha_{1i}) \\ \dot{m}_2 - \sum_{i=1,3,\ldots}\rho L_{2i}\varphi_{2i}(g_y \sin\alpha_{2i} + g_x \cos\alpha_{2i}) \\ \ldots \end{bmatrix} \qquad (4.1.7\text{-}19)$$

can be obtained by assembly of local element matrices (considering element with nodes i and j)

$$\begin{bmatrix} \varphi_{ij} & -\varphi_{ij} \\ -\varphi_{ij} & \varphi_{ij} \end{bmatrix} \cdot \begin{bmatrix} p_i \\ p_j \end{bmatrix} = \begin{bmatrix} -\rho L_{ij}\varphi_{ij}(g_y \sin\alpha_{ij} + g_x \cos\alpha_{ij}) \\ \rho L_{ij}\varphi_{ij}(g_y \sin\alpha_{ij} + g_x \cos\alpha_{ij}) \end{bmatrix} + \begin{bmatrix} \dot{m}_{ij} \\ -\dot{m}_{ij} \end{bmatrix} \qquad (4.1.7\text{-}20)$$

Note 1: Assembly of the last vector on the right hand side over all elements gives vector of residual flowrates $\dot{m}_i$ which are zero at all inner nodes of network. Therefore this vector is omitted when

contributions of individual elements are calculated (modelling of wall permeability is an exception, see later). It should be stressed that at any end point of network one and only one boundary condition must be prescribed: either pressure as a strong boundary condition, or flowrate which is in fact residual of the mass flowrates in the respective point.

Note 2: When calculating coefficients φ_{ij} it is necessary to take into account that these coefficients correspond only to friction or kinetic energy losses (and thus the hydrostatic pressure must be subtracted from the pressure difference p_i-p_j , which is used as an argument of the function φ_{ij}).

Buoyancy can be modelled by prescribing temperature dependent density $\rho(T)$ in previous equations, either as an expression (FUNDEF) or a table (CURDEF) with index of function specified in MPROP. However, there is another option, Boussinesq approximation, operating with a constant density but with the material parameter β, thermal expansion coefficient, prescribed as a material parameter. In this case (which is better for example when considering round-off errors during assembly) the Eq.(16) is replaced by equation

$$\dot{m}_{ij} = \varphi_{ij}[p_i - p_j + \rho_0 \beta (T - T_0)(g_x h_x + g_y h_y + g_z h_z)] \qquad (4.1.7\text{-}21)$$

where ρ_0 is a *constant* density corresponding to a constant reference temperature T_0. Use the command OPTION or the drop-down menu Solution - OPTION for selection of the Boussinesq method.

Permeability of wall

There exist applications, especially at biological systems, where a pipe cannot be considered as perfectly tight and some leakage of liquid through the pipe wall is possible. Assuming that the leakage is proportional to the difference between the pressure inside a pipe and the external pressure, the mass flowrate [kg/s] assigned to the node *i* of the element with nodes *i,j* can be expressed as

$$\Delta\dot{m}_i = (p_i - p_e)\frac{\rho L_{ij} O \mu_p}{2 h_w \mu} \qquad (4.1.7\text{-}22)$$

where L_{ij} is length of element, O-perimeter of pipe, h_w wall thickness, μ viscosity of permeating liquid and μ_p permeability of wall material (unit of permeability is m^2). Parameters O, h_w, μ_p are specified in RCONST, while viscosity μ is an MPROP parameter. The leakage flowrate (22) is applied in the right hand side vector in Eq.(20) describing mass flowrate contributions of element i-j to the balance at nodes i and j.

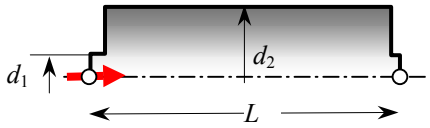
Local resistances

Pipeline network consists usually of other components like valves, pumps, heat exchangers and even mixed vessels. All the elements could be also described by two node elements (two pressures as nodal parameters and flowrate as a single element parameter), however with a different hydraulic characteristic. Some of these elements can be described in FEMINA as the element PIPE2D with a user defined hydraulic characteristic $\varphi_{ij}(\Delta p, Re, D_e, H)$ specified as a parameter of EGROUP (zero index of this function means standard empty pipe). This function can be defined in a standard way as an expression or as a table with arguments DP (pressure difference with subtracted hydrostatic head), RE (Reynolds number), DE (characteristic diameter), and HE (element length), TEMP (mean temperature of element). This function, if specified, multiplies hydraulic characteristic calculated by previously described methods for straight empty pipe.

Note: Some permanent characteristics, e.g. of elbows and t-pipes can be included into coefficient of local losses ζ which is much simple (but cannot by a function because ζ is a RCONST parameter).

Vessels (element CSTR)

Pressure drop through a vessel is calculated in the same way as the pressure drop in a circular pipe. The only difference is in the coefficient of local loss ζ which represents full loss of kinetic energy, corresponding mean velocity at inlet



$$\Delta p = \frac{1}{2}\rho(u_1^2 + \lambda_2 \frac{L}{d_2} u_2^2) \qquad (4.1.7\text{-}23)$$

Pumps

The element PUMP is designed in a specific way. The flow coefficient φ is set to zero (there is no contribution to the matrix of the algebraic equations system) and the right hand side vector is defined as the mass flowrate, calculated according to the characteristic of pump

$$\dot{m} = \rho(A + B\Delta p + C\Delta p^2) \qquad (4.1.7\text{-}24)$$

if the pressure height Δp is within the specified range for a given pump, or

$$\dot{m} = \rho(E + F\Delta p) \qquad (4.1.7\text{-}25)$$

if the pressure height calculated from the previous iteration exceeds capability of centrifugal pump. This approach is used for calculation of centrifugal pumps selected from a database (each pump is characterised by the coefficients A,B,C,E,F).

In the case that a wrong pump is selected and the pump is not able to deliver sufficient displacement head, an emergency modification of hydraulic characteristic is used (with an empirical parameter D)

$$\dot{m} = \frac{\rho D}{\Delta p} \qquad (4.1.7\text{-}26)$$

Positive displacement pumps or pumps with non-standard characteristics are calculated according to the prescribed function $\dot{V}(t, \Delta p)$.

Parallel pipes

The element PIPE2D can be extended for modelling of flow in N identical parallel pipes – this case is identified by parameter in EGROUP. Algorithm is almost the same and follows from the following equation

$$\dot{m}_{ij} = N\varphi_{ij}[p_i - p_j + \rho(g_x h_x + g_y h_y + g_z h_z)]. \qquad (4.1.7\text{-}27)$$

What can be misleading: Flowrates, calculated during postprocessing and presented as an element parameter (Q) are related only to single pipe in a bundle!

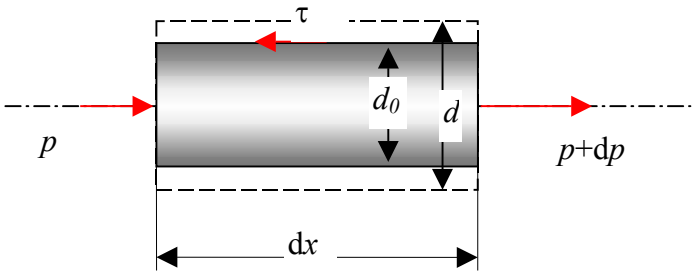
Elastic wall of pipe

Flow in an elastic pipe is especially important for modelling flows in arteries and veins. The simplest case assumes flexible walls of circular pipe, with elongation of diameter directly proportional to the internal pressure

$$p = e(d - d_0) \tag{4.1.7-28}$$

where the coefficient e [Pa/m] depends on modulus of elasticity of wall, its thickness and diameter.

An equation relating flowrate, pressure and diameter of elastic pipe can be derived from continuity equation (assuming incompressible liquid) and balance of forces, acting upon a short element of a circular pipe with inner diameter d



giving

$$\dot{m} = -\varphi_L \frac{\partial p}{\partial x} + \rho \varphi_L g_x - \rho \varphi_L \frac{\partial u}{\partial t} \quad , \tag{4.1.7-29}$$

with the coefficient of fluidicity φ_L ([m^{2}s], this coefficient represents effects of viscous friction). Fluidicity can be derived in the same way as in Eqs.(5-6), giving $\varphi_L = \varphi_{ij} L_{ij}$ and therefore

$$\varphi_L = \frac{\pi \rho d^4}{128 \mu} \qquad \text{holds for laminar flow of Newtonian liquid Re<2300} \tag{4.1.7-30}$$

and

$$\varphi_L = 0.558^{4/7} \frac{\rho \pi d^{19/7}}{(\rho \left|\frac{\partial p}{\partial x}\right|)^{3/7} \mu^{1/7}} \qquad \text{holds for } 2300<Re<10^5 \text{ (Blasius).} \tag{4.1.7-31}$$

Parameters in Eq.(29) have the following meaning: $\dot{m} = \rho u A$ is mass flowrate (kg/s in a given place x and time t), g_x is the x-component of gravity (acceleration m/s^2), and the last inertial term represents acceleration of liquid (u is mean velocity [m/s]).

Continuity equation must include also the time variable volume of element of a circular pipe

$$\frac{\partial \dot{m}}{\partial x} = -\frac{\rho \pi d}{2e} \frac{\partial p}{\partial t} \tag{4.1.7-32}$$

Combining the continuity equation (32) with the momentum balance (29) we can eliminate the mass flowrate and arrive to the differential equation for distribution of pressure

$$-\frac{\rho\pi d}{2e}\frac{\partial p}{\partial t}=\frac{\partial}{\partial x}(\varphi_L\frac{\partial p}{\partial x})+\frac{\partial}{\partial x}(\rho\varphi_L g_x)-\frac{\partial}{\partial x}(\rho\varphi_L\frac{\partial u}{\partial t}) \quad . \tag{4.1.7-33}$$

Few comments: The second term corresponds to the buoyancy – in the case that both density, gravity and flow resistance are constant, the term vanishes. Last term is caused by inertial forces and it will be neglected in the following analysis.

Let us consider dimensionless form of pressure equation without the buoyancy term. Introducing dimensionless pressure, normalised by the pressure drop corresponding to a steady viscous flow in a pipe with characteristic length L and

$$p^*=\frac{p}{\Delta p}=\frac{pd^2}{32L\mu u_0} \qquad x^*=\frac{x}{L}, \qquad t^*=\frac{tu_0}{L}, \qquad u^*=\frac{u}{u_0}. \tag{4.1.7-34}$$

we arrive to simplyfied form of (33)

$$-\frac{\partial p^*}{\partial t^*}=A\frac{\partial^2 p^*}{\partial x^{*2}}-B\frac{\partial^2 u^*}{\partial t^*\partial x^*} \tag{4.1.7-35}$$

with dimensionless numbers

$$A=\frac{d^3 e}{64L\mu u_0}, \qquad B=\frac{\rho d^5 e}{2048\mu^2 L^2}. \tag{4.1.7-36}$$

The last inertial term will be negligible if B/A << 1

$$\frac{B}{A}=\frac{\rho d^2 u_0}{32L\mu}=0.0315\,\mathrm{Re}\frac{d}{L} \tag{4.1.7-37}$$

therefore if Reynolds number and d/L simplex are sufficiently small.

Let us suppose that this assumption is satisfied. Then we can derive an integral form of Eq.(33), by using weighted residual method with arbitrary weight functions *W*(x)

$$\int_\Omega W[\frac{\rho\pi d}{2e}\frac{\partial p}{\partial t}-\frac{\partial}{\partial x}(\varphi_L\frac{\partial p}{\partial x})-\frac{\partial}{\partial x}(\rho\varphi_L g_x)]dx=0. \tag{4.1.7-38}$$

The unpleasant second derivative is eliminated by per partes integration

$$\int_\Omega (W\frac{\rho\pi d}{2e}\frac{\partial p}{\partial t}+\varphi_L\frac{\partial W}{\partial x}\frac{\partial p}{\partial x}+\frac{\partial W}{\partial x}\rho\varphi_L g_x)dx=0 \tag{4.1.7-39}$$

Further on we apply Galerkin method $W_i(x)=N_i(x)$, $p(t,x)=p_jN_j(x)$ and thus we obtain the following system of ordinary differential equations describing a time evolution of pressure

$$M_{ij}\frac{dp_j}{dt}+K_{ij}p_j=b_i \tag{4.1.7-40}$$

where

$$M_{ij} = \int_{\Omega} N_i N_j \frac{\rho \pi d}{2e} dx \tag{4.1.7-41}$$

$$K_{ij} = \int_{\Omega} \varphi_L \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} dx \tag{4.1.7-42}$$

and

$$b_i = -\int_{\Omega} \frac{\partial N_i}{\partial x} \rho \varphi_L g_x dx \,. \tag{4.1.7-43}$$

4.1.8. Pipeline networks – heat transfer fundamentals

Let us consider the network of pipes where pressures and flowrates are known. Knowing thermal characteristics of liquid, external temperature and having information on thermal resistances at wall (for example thickness of thermal boundary layer) it is possible to calculate axial temperature profiles in pipes using three different methods: method of weighted residuals, method of enthalpy balances and method of characteristics which will be described separately for the simplest element PIPE2D. All the three methods are based upon the Fourier Kirchhoff equation written in the following form

$$A\rho c_p(\frac{\partial T}{\partial t}+\bar{u}\frac{\partial T}{\partial x})=\frac{\partial}{\partial x}(A\rho c_p a_e\frac{\partial T}{\partial x})+kO(T_e-T)+A(Q-ST)$$

$$Q=\kappa[(\frac{\Delta U}{h})^2+E_y^2]+Q_u \qquad (4.1.8\text{-}1)$$

with boundary condition

$$\rho c_p a_e\frac{\partial T}{\partial n}=\alpha(T_e-T)|_\Gamma, \qquad (4.1.8\text{-}2)$$

where $T(t,x)$ is a mean calorimetric temperature in a cross section of pipe, a_e is axial dispersion, k is heat transfer coefficient to surrounding, O is perimeter, A cross section, and T_e is ambient temperature. The term Q represents a volumetric heat source [W/m^3] consisting of predefined contribution of electric field (κ is specific electrical conductivity [S/m], ΔU is voltage difference along the channel axis, while E_y is transversal component of electric field intensity) and a user defined source Q_e describing for example reaction heat. Sink term (ST) proportional to temperature is also defined by user as a function $S(T,t,c_N,\ldots)$. Unit of all terms in Eq.(1) is W/m i.e. power related to the unit length of pipe.

Note: Boundary condition (2) of the third kind is not typical for pipelines where convective heat transfer dominates. However, the Eq.(1) can be applied also for description of one dimensional temperature profile in a slab (in a layer or in a truss) where heat is transferred by conduction and the boundary condition (2) at surface is frequently applied.

Special attention should be paid to the coefficient of axial dispersion a_e which is not identical with the thermal diffusivity a. If the flow is laminar, if the tube is thermally insulated and if the thermal diffusivity a is sufficiently high

$$a>0.08\frac{\dot{V}}{L} \qquad (4.1.8\text{-}3)$$

the analogy with diffusion of a tracer holds and the Taylor Aris theory can be applied (see Thyn 2000) for theoretical prediction of dispersion coefficient as a function of tube diameter d, thermal diffusivity and mean velocity as

$$a_e=a+\frac{\bar{u}^2d^2}{192a}\qquad[\frac{m^2}{s}], \qquad (4.1.8\text{-}4)$$

while at turbulent regime the dispersion coefficients can be expressed as o function of Re

$$a_e=\bar{u}d(\frac{3\cdot10^7}{\mathrm{Re}^{2.1}}+\frac{1.35}{\mathrm{Re}^{0.125}}). \qquad (4.1.8\text{-}5)$$

Problem exists when the thermal diffusion is rather small and the flow is laminar. In this case neither Eq.(4) nor the formula (5) can be used and only as an emergency solution the expression

$$a_e = a + \frac{\bar{u}^2 \tau}{\pi} \tag{4.1.8-6}$$

could be tried, where characteristic time τ is a more or less empirical parameter.

Note: The formula (6) stems from requirement that the rate of dispersion of a narrow pulse is the same as the mean velocity $\bar{u}\,\tau = \sqrt{\pi a_e \tau}$.

Thermal resistances

Heat transfer coefficient *k* in Eq.(1) represents overall heat transfer from the liquid inside a pipe (characterized by the bulk temperature *T* - nodal parameter) to the surrounding (outer temperature T_e is specified as a RCONST parameter). The heat transfer through the pipe surface (or only through the part of the pipe surface, see parameter PERIMeter in RCONST) must overcome outer thermal resistance and thermal resistance of wall (given by ALPHA parameter in RCONST), then thermal resistance of deposited fouling layer (calculated according to selected model of fouling) and finally internal thermal resistance in liquid, characterised by heat transfer coefficient α which is related to the thermal boundary layer thickness δ as

$$\alpha = \frac{\lambda}{\delta}. \tag{4.1.8-7}$$

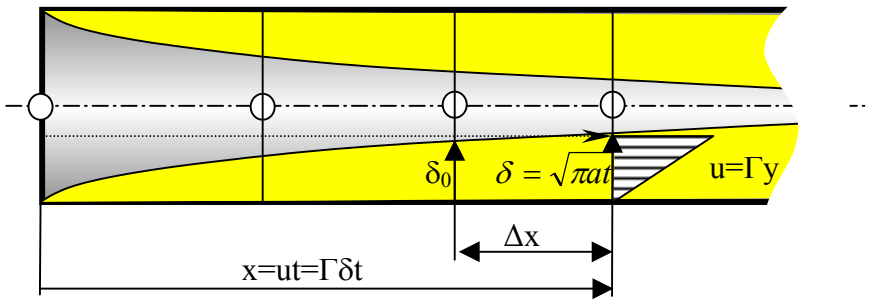
The thickness δ can be calculated from correlation for Nusselt number in turbulent regime

$$Nu = 0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.4}, \tag{4.1.8-8}$$

because arguments (Re and Pr) are independent of axial distance, and therefore δ can be calculated only from dimensions and flowrate in a given element. This is not so simple in laminar regime, because in this case thermal boundary layer is not disturbed by turbulent vortices and is only slowly developing along the pipe. The following figure shows, how the thickness δ can be estimated based upon assumption of linear velocity profile near the wall ($u=\Gamma y$, where Γ is velocity gradient and *y* is the distance from wall) and thermal penetration depth theory, giving

$$\delta = \sqrt[3]{\varphi \frac{\pi a x}{\Gamma}} \tag{4.1.8-9}$$

where the coefficient φ represents correction which is to be evaluated from experiments.



The assumptions used in derivation of Eq.(9) are consistent with the Leveque's solution for circular tube and thermally developing region (for a short pipes)

$$Nu_{\ln} = 1.618\sqrt[3]{Gz} = 1.618\sqrt[3]{\frac{\bar{u}d^2}{ax}} \qquad (4.1.8\text{-}10)$$

According to Eq.(9) we can express the thickness δ in terms of thickness δ_0 in the preceding element (preceding in the sense of flow direction):

$$\delta^3 = \delta_0^3 + \varphi\frac{\pi a \Delta x}{\Gamma} \qquad (4.1.8\text{-}11)$$

which is implemented in FEMINA in the form

DELTA=AMIN1((D/3.66)**3, DELTA0**3+1.845*PI*A*H/GAMMA)**0.3333333. (4.1.8-12)

The first term represent a limit – maximum thickness of thermal boundary layer, corresponding to limiting Nusselt number for circular tube and the case with constant wall temperature (Nu_∞=3.66).

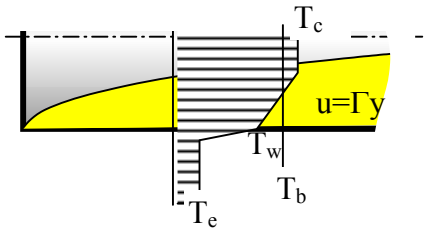
The symbol Γ is usually used for the so called consistency variable which is identical with the velocity gradient at wall for parabolic velocity profile, Γ=8u/d, but in FEMINA the Γ is evaluated as the actual gradient even for a general radial velocity profile, corresponding to variable apparent viscosity

$$\Gamma = \frac{\tau_w}{\mu_w(\tau_w, T_w)} \qquad (4.1.8\text{-}13)$$

where τ_w is wall shear stress calculated from axial pressure gradient

$$\tau_w = \frac{d}{4}\frac{dp}{dx}. \qquad (4.1.8\text{-}14)$$

It should be noted that the Eq.(14) holds for circular tube and narrow planar slit exactly (no matter what is the form of radial velocity profile) as soon as the parameter *d* is calculated as the equivalent hydraulic diameter. Apparent viscosity at wall generally depends upon unknown wall temperature T_w, and this temperature cannot be calculated exactly. Wall temperature estimate is based upon rather crude assumption of radial temperature profile in a circular tube, characterised by known temperatures T_e (ambient), T_b (mean calorimetric temperature – this is calculated nodal temperature) and unknown temperature T_w and T_c (temperature in core, outside the thermal boundary layer). Starting from the definition of mean calorimetric temperature and substituting boundary condition for temperature in the form



$$Bi(T_w - T_e) = \frac{T_c - T_w}{\delta^*},\ Bi = \frac{k_e R}{\lambda},\ \delta^* = \frac{\delta}{R} \qquad (4.1.8\text{-}15)$$

where k_e is 'outer' heat transfer coefficient (specified in RCONST) and R is radius of tube, the final equation for wall temperature can be derived

$$T_w = \frac{\frac{1}{4}T_b + (\delta^* A + C - B)BiT_e}{(1 + Bi\delta^*)A + (1 + Bi)C - BiB}. \qquad (4.1.8\text{-}16)$$

The coefficients A,B,C depend upon relative thickness of boundary layer

$$A = \frac{(1-\delta^*)^2}{2} - \frac{(1-\delta^*)^4}{4} \tag{4.1.8-17}$$

$$B = \frac{1-(1-\delta^*)^3}{3} - \frac{1-(1-\delta^*)^5}{5} \tag{4.1.8-18}$$

$$C = \frac{1-(1-\delta^*)^2}{2} - \frac{1-(1-\delta^*)^4}{4}. \tag{4.1.8-19}$$

Remark: Previous equations have been derived only for circular tube assuming parabolic velocity profile, therefore the calculated T_w is only an approximation.

Fouling in PIPE2D elements

Fouling is a nonstationary phenomenon because thickness of deposits on the tube wall is a function of time even for constant flowrate and inlet temperatures. Models have form of ordinary differential equations describing rate of fouling - time change of thermal resistance.

A very simple model suitable for oils and oil products has been suggested by Ebert and Panchal (1995) as an ordinary differential equation for thermal resistance r [m^2.K/W], or thickness of layer h

$$\frac{dr}{dt} = \frac{\alpha}{\mathrm{Re}^{0.88}} \exp(-\frac{E}{RT}) - \gamma\tau\,, \qquad h = \lambda_f r\,, \tag{4.1.8-20}$$

where α=8.39 [m^2K/J], E=68 [kJ/mol], $\gamma=4.03\cdot10^{-11}$ [Pa.m^2.K/J] are constants (determined experimentally for oils) and τ is wall shear stress.

Milk fouling has been studied by many authors, the key contributions are the work of Fryer at all and Lalande at all in France, who investigated the effect of β-lactoglobulin denaturation. De Jong et al (1992) applied the reaction kinetics of β-lactoglobulin in plate heat exchangers. Paterson and Fryer (1988) proved, that the fouling of milk cannot be considered as a surface reaction and that it is necessary to model the chemical reaction and mass transfer in the bulk region too. The native protein, denaturated protein and aggregated protein kinetics can be simplified in 1D form

$$\frac{\partial c_N}{\partial t} + u\frac{\partial c_N}{\partial x} = \frac{\partial}{\partial x}(D_{eN}\frac{\partial c_N}{\partial x}) - k_N \exp(-\frac{E_N}{RT})c_N \tag{4.1.8-21}$$

$$\frac{\partial c_D}{\partial t} + u\frac{\partial c_D}{\partial x} = \frac{\partial}{\partial x}(D_{eD}\frac{\partial c_D}{\partial x}) + k_N \exp(-\frac{E_N}{RT})c_N - k_D \exp(-\frac{E_D}{RT})c_D^2 \tag{4.1.8-22}$$

$$\frac{\partial c_A}{\partial t} + u\frac{\partial c_A}{\partial x} = \frac{\partial}{\partial x}(D_{eA}\frac{\partial c_A}{\partial x}) + k_D \exp(-\frac{E_D}{RT})c_D^2 \tag{4.1.8-23}$$

The rate of deposition is related to the concentration of aggregated proteins and can be expressed again as a differential equation for the thermal resistance r or equivalent thickness h of fouling layers

$$\frac{dr}{dt} = \beta c_A\,, \qquad \frac{dh}{dt} = \lambda_f \beta c_A\,. \tag{4.1.8-24}$$

Crystallisation fouling analysed by Brahmin et al, can be described by a similar model as Ebert Panchal

$$\frac{dr}{dt} = k_N (c_N - c_{Nsat})^2 - a c_N u^2 \tag{4.1.8-25}$$

where the first term describes deposit and the second term removal of layer formed from salt having concentration c_N in the main stream flowing with the mean velocity u.

4.1.9. Pipeline networks – heat transfer in pipes, CSTR and heat exchangers

In this chapter three fundamental finite methods for solution of previously formulated problem (heat transfer in pipe) will be presented.

Weighted residual method for element PIPE2D

This is a standard procedure: The Fourier Kirchhoff Eq.(1) in previous chapter is multiplied by a weighting function $W(x)$ and integrated over the whole region (interval a,b), giving weak formulation

$$\int_a^b [W\rho c_p A(\frac{\partial T}{\partial t} + \bar{u}\frac{\partial T}{\partial x}) + \rho c_p A a_e \frac{\partial W}{\partial x}\frac{\partial T}{\partial x} - WkO(T_e - T) - WA(Q - ST)]dx = [WA\alpha(T_e - T)]_{x=a,b} \tag{4.1.9-1}$$

Temperature is approximated by linear base functions $N_j(x)$ and asymmetric weighting functions $W_i(x)$ are derived according to Zienkiewicz as

$$T = N_j T_j \qquad W_i = N_i + \frac{\alpha h \bar{u}}{2|\bar{u}|}\frac{dN_i}{dx} \tag{4.1.9-2}$$

with the optimal value of coefficient of asymmetry α

$$\alpha_{opt} = \coth Pe - \frac{1}{Pe}, \qquad Pe = \frac{|u|h\rho}{2a_e}. \tag{4.1.9-3}$$

Substituting approximation (2) into Eq.(1) we arrive to the system of ordinary differential equations

$$M_{ij}\frac{dT_j}{dt} + A_{ij}T_j = b_i \tag{4.1.9-4}$$

where the matrix of heat capacities M, matrix of heat transfer A and the vector of heat sources are

$$M_{ij} = \int_a^b A\rho c_p W_i N_j dx \tag{4.1.9-5}$$

$$A_{ij} = \int_a^b [\rho c_p A(W_i\bar{u}\frac{\partial N_j}{\partial x} + a_e\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}) + W_i N_j(kO + AS)]dx + [A\alpha W_i N_j]_{i=j=a,b} \tag{4.1.9-6}$$

$$b_i = \int_a^b W_i(kOT_e + AQ)dx + [A\alpha T_e W_i]_{i=a,b} \tag{4.1.9-7}$$

The system of ordinary differential equations (4) is solved by Euler's method (θ=0 explicit, θ=1 implicit)

$$M_{ij}\frac{T_j - T_j^0}{\Delta t} + A_{ij}[\theta T_j + (1-\theta)T_j^0] = b_i, \tag{4.1.9-8}$$

it means that in each time step new temperatures are solution of the following system of linear algebraic equations

$$(M_{ij} + \Delta t\theta A_{ij})T_j = [M_{ij} - \Delta t(1-\theta)A_{ij}]T_j^0 + \Delta t b_i. \tag{4.1.9-9}$$

Method of characteristics for PIPE2D

With the aim to reduce numerical diffusion error the method of characteristics, decomposing a time step to a convective and a diffusive phase, has been developed. The convective phase solves the hyperbolic differential equation (integration along characteristics)

$$\frac{\partial T_c^*}{\partial t} + \bar{u}\frac{\partial T_c^*}{\partial x} = 0 \qquad (4.1.9\text{-}10)$$

(any function $T(x\text{-}ut)$ is solution), while the parabolic differential equation, without convective terms

$$A\rho c_p \frac{\partial T_d^*}{\partial t} = \frac{\partial}{\partial x}(A\rho c_p a_e \frac{\partial T_d^*}{\partial x}) + kO(T_e - T_d^*) + A(Q - ST_d^*) \qquad (4.1.9\text{-}11)$$

is solved in the second phase, by the previously described Galerkin method, it means, that temperatures are calculated according to Eq.(9) where

$$M_{ij} = \int_a^b A\rho c_p N_i N_j dx \qquad (4.1.9\text{-}12)$$

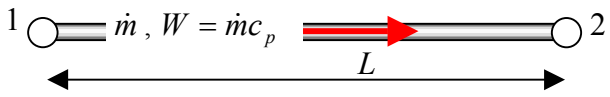
$$A_{ij} = \int_a^b [\rho c_p A a_e \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + N_i N_j (kO + AS)]dx + [A\alpha N_i N_j]_{i=j=a,b} \qquad (4.1.9\text{-}13)$$

$$b_i = \int_a^b N_i (kOT_e + AQ)dx + [A\alpha T_e N_i]_{i=a,b} \qquad (4.1.9\text{-}14)$$

Remark:
This decomposition is not quite accurate, which can be demonstrated on a simplified problem $\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = a\frac{\partial^2 T}{\partial x^2}$ with the initial condition T^0. The solution is searched in the form $T=T_c+\Delta T_d$ where the convective part satisfies initial condition T^0 and hyperbolic equation $\frac{\partial T_c}{\partial t} + u\frac{\partial T_c}{\partial x} = 0$, while the diffusive part should be solution of $\frac{\partial \Delta T_d}{\partial t} + u\frac{\partial \Delta T_d}{\partial x} = a\frac{\partial^2 T}{\partial x^2}$, however the convective term $u\frac{\partial \Delta T_d}{\partial x}$ is neglected.

Method of enthalpy balances for PIPE2D

This is in fact control volume method, however even if balances are formulated at an element level, equations are written for nodes, stating that the sum of oriented enthalpy flows must be zero at any nodal point (if it is not a point source or a sink of heat of course). Let us assume an element PIPE, with mass flowrate oriented from node 1 to node 2.



We shall suppose that the mass flowrate and also the specific heat capacity is constant and that the temperature profile is linear. Then the enthalpy flow to the node 1 is negative

$$\dot{H}_1 = -WT_1 - A\lambda_e \frac{T_1 - T_2}{L}. \qquad (4.1.9\text{-}15)$$

The enthalpy flow *into* the node 2 can be expressed as the sum of enthalpy flow from the node 1 plus the internal heat source plus the heat transferred from surrounding, minus heat sink and accumulation

$$\dot{H}_2 = WT_1 + A\lambda_e \frac{T_1 - T_2}{L} + ALQ + kLO(T_e - \frac{T_1 + T_2}{2}) - ALS\frac{T_1 + T_2}{2} - \frac{AL\rho c_p}{2}\frac{d(T_1 + T_2)}{dt} \quad (4.1.9\text{-}16)$$

where W is heat capacity of stream, A is cross section and L length of pipe, O is perimeter (therefore LO is heat transfer surface), Q is volumetric heat source, and S is volumetric sink term.

These two contributions of element to enthalpy flows can be expressed in matrix form

$$\begin{pmatrix} 0 & 0 \\ -\frac{AL\rho c_p}{2} & -\frac{AL\rho c_p}{2} \end{pmatrix}\begin{pmatrix} \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{pmatrix} + \begin{pmatrix} -W - \frac{A\lambda_e}{L} & \frac{A\lambda_e}{L} \\ W + \frac{A\lambda_e}{L} - \frac{kLO + ALS}{2} & -\frac{A\lambda_e}{L} - \frac{kLO + ALS}{2} \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \end{pmatrix} = \begin{pmatrix} \dot{H}_1 \\ \dot{H}_2 - ALQ - kLOT_e \end{pmatrix} \quad (4.1.9\text{-}17)$$

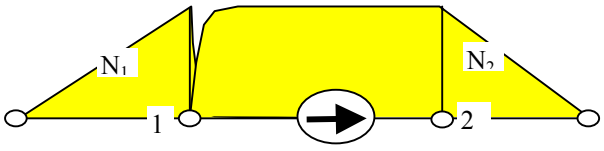
and similar expression holds for the opposite flow direction (W<0),

$$\begin{pmatrix} -\frac{AL\rho c_p}{2} & -\frac{AL\rho c_p}{2} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{pmatrix} + \begin{pmatrix} -\frac{A\lambda_e}{L} - \frac{kLO + ALS}{2} & \frac{A\lambda_e}{L} - \frac{kLO + ALS}{2} - W \\ \frac{A\lambda_e}{L} & W - \frac{A\lambda_e}{L} \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \end{pmatrix} = \begin{pmatrix} \dot{H}_1 - ALQ - kLOT_e \\ \dot{H}_2 \end{pmatrix} \quad (4.1.9\text{-}18)$$

Assembly of these contributions gives again the system of ordinary differential equations (4).

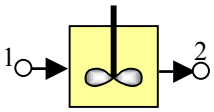
Pipelines with CSTR and PUMP

Elements CSTR and PUMP are calculated in a similar way as PIPE2D – they are also elements with two nodes and the three previously described methods are implemented with minor differences. When using weighted residual method, the element PUMP and CSTR had been initially implemented as a pipe, the only differences were in the definition of heat transfer surface. However, this is not a realistic description of mixed tanks and thus beginning from the version FEMINA 3.4 the base functions has been modified so that the weighted residual method would be compatible with the enthalpy balancing approach.



The enthalpy balancing assumes, that temperature inside an element is uniform and equal to the outlet temperature, which corresponds to the assumption that liquid inside a vessel or inside a pump is well mixed. The equations of enthalpy balances are therefore simplified:

$$\dot{H}_1 = -WT_1, \qquad \dot{H}_2 = WT_1 + VQ + kLO(T_e - T_2) - VST_2 - V\rho c_p \frac{dT_2}{dt}$$



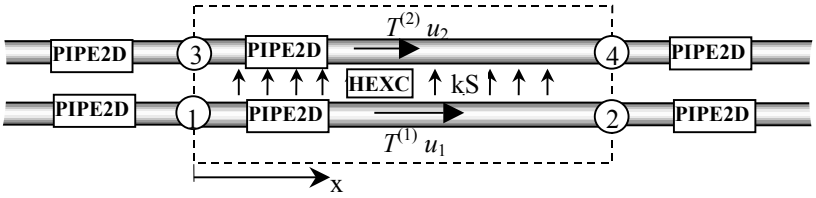
$$\begin{pmatrix} 0 & 0 \\ 0 & -V\rho c_p \end{pmatrix}\begin{pmatrix} \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{pmatrix} + \begin{pmatrix} -W & 0 \\ W & -kOL - VS \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \end{pmatrix} = \begin{pmatrix} \dot{H}_1 \\ \dot{H}_2 - VQ - kLOT_e \end{pmatrix} \quad \text{for W>0} \quad (4.1.9\text{-}19)$$

and $$\begin{pmatrix} -V\rho c_p & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{dT_1}{dt} \\ \frac{dT_2}{dt} \end{pmatrix}+\begin{pmatrix} -kOL-VS & -W \\ 0 & W \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \end{pmatrix}=\begin{pmatrix} \dot{H}_1 - VQ - kLOT_e \\ \dot{H}_2 \end{pmatrix} \quad \text{for W<0} \qquad (4.1.9\text{-}20)$$

Heat exchangers HEXC

Heat exchangers are modelled by HEXC elements of different kinds, determined by the EGROUP parameter TYPE.

The simplest Heat Exchanger (TYPE=0) is formed from two elements PIPE2D which must be defined separately and represent heat exchangers with parallel flows, in cocurrent and countercurrent flow orientation, e.g. a simple one pass double pipe or one pass plate heat exchanger. This approach has the advantage, that the element HEXC need not calculate the flow (pressure drop) and thermal resistances (fouling, heat transfer coefficients) in both streams, because this is accomplished by two elements PIPE2D



Equations describing temperature profiles along the heat exchanger in both streams are described by nearly the same equations as for temperature in pipe, the only difference is in the source/sink terms, describing heat exchange between the streams:

$$A_1\rho_1 c_{p1}\left(\frac{\partial T^{(1)}}{\partial t}+\bar{u}_1\frac{\partial T^{(1)}}{\partial x}\right)=A_1\rho_1 c_{p1}a_{e1}\frac{\partial^2 T^{(1)}}{\partial x^2}+k_1O_1(T_e-T^{(1)})+Q^{(1)}+kS(T^{(2)}-T^{(1)}) \qquad (4.1.9\text{-}21)$$

$$A_2\rho_2 c_{p2}\left(\frac{\partial T^{(2)}}{\partial t}+\bar{u}_2\frac{\partial T^{(2)}}{\partial x}\right)=A_2\rho_2 c_{p2}a_{e2}\frac{\partial^2 T^{(2)}}{\partial x^2}+k_2O_2(T_e-T^{(2)})+Q^{(2)}+kS(T^{(1)}-T^{(2)}) \qquad (4.1.9\text{-}22)$$

Weighted residual method for HEXC (TYPE=0)

is applied in the same way as for single pipe

$$M_{ij}^{(1)}\frac{dT_j^{(1)}}{dt}+A_{ij}^{(1)}T_j^{(1)}+B_{ij}^{(1)}(T_j^{(1)}-T_j^{(2)})=b_i^{(1)} \qquad (4.1.9\text{-}23)$$

$$M_{ij}^{(2)}\frac{dT_j^{(2)}}{dt}+A_{ij}^{(2)}T_j^{(2)}+B_{ij}^{(2)}(T_j^{(2)}-T_j^{(1)})=b_i^{(2)} \qquad (4.1.9\text{-}24)$$

where

$$B_{ij}^{(k)}=\int_\Omega (N_i+Z^{(k)}\frac{dN_i}{dx})N_j kS dx \quad , \quad Z^{(k)}=\frac{\alpha h\bar{u}_k}{2\,|\,\bar{u}_k\,|} \; . \qquad (4.1.9\text{-}25)$$

It should be noted, that matrices ***M, A*** and ***b*** are the same as integrals derived for single pipe, where the heat transfer coefficient k_k concerns only the heat transfer between pipe and surrounding (for a well insulated heat exchanger this coefficient is zero). Essential for the heat exchanger are only coefficients

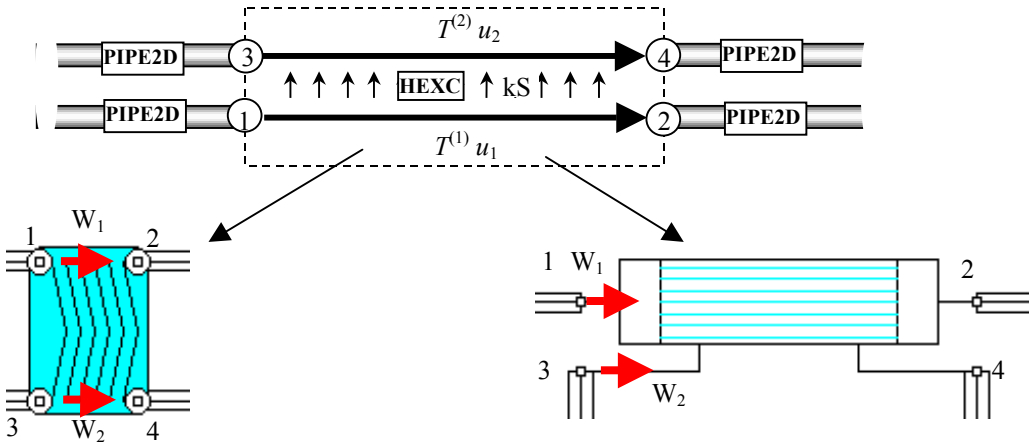
B, where *k* is heat transfer coefficient summarising thermal resistance of wall, thermal resistances of fouling and thermal boundary layers in channels 1 and 2. *S* in Eq. (25) is heat transfer area related to the unit length of heat exchanger (therefore the unit of S is meter). Not considering the asymmetric part of weighting function $Z^{(k)}$, the coefficients ***B*** would be independent of characteristics of individual pipes (e.g. independent on size, flowrates and so on).

Thus the element HEXC calculates only the following contribution to the matrix of the system of algebraic equation

$$\Delta t \begin{pmatrix} B_{11}^{(1)} & B_{12}^{(1)} & -B_{11}^{(1)} & -B_{12}^{(1)} \\ B_{21}^{(1)} & B_{22}^{(1)} & -B_{21}^{(1)} & -B_{22}^{(1)} \\ -B_{11}^{(2)} & -B_{12}^{(2)} & B_{11}^{(2)} & B_{12}^{(2)} \\ -B_{21}^{(2)} & -B_{22}^{(2)} & B_{21}^{(2)} & B_{22}^{(2)} \end{pmatrix} . \qquad (4.1.9\text{-}26)$$

Enthalpy balance method for HEXC (TYPE=0,1,2,…)

Heat exchangers HEXC TYPE=0 (formed by two elements PIP2D) can be calculated by the enthalpy balance method in the same way as by using weighted residuals, i.e. calculating only the contribution of heating power transferred between the both stream. However, the enthalpy balance method is applied also for more complex heat exchangers if TYPE>0. In this case the HEXC is a stand alone element and calculates both hydraulic and thermal characteristics of multipass plate and shell&tube heat exchangers. Nodes of these 4-nodes elements should be numbered as shown in the following figure (1,2 denote first stream, i.g. in a shell, while nodes 3,4 second stream, e.g. tube bundle, pair 1,3 are nodes at one end of heat exchanger, e.g. front head, while 2,4 are nodes at the opposite end, e.g. rear head):



W_1, W_2 are thermal capacities of streams ($W_1=\rho_1 c_{p1} A_1 u_1$) and positive values correspond to the orientation of flow in the previous figure. A general heat exchanger is characterised by the element matrix A (4 x 4), which enables to calculate a contribution of the element to the nodal enthalpy flows (positive value denotes heat flow towards a node)

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{pmatrix} \cdot \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \end{pmatrix} = \begin{pmatrix} \dot{H}_1 \\ \dot{H}_2 \\ \dot{H}_3 \\ \dot{H}_4 \end{pmatrix} \qquad (4.1.9\text{-}27)$$

Matrix of enthalpy flows A depends upon orientation of flow in both streams and there are four possible arrangements (entries of the matrix A are thermal capacities W_1, W_2 and heat exchanger duty $W=Q/\Delta T$ calculated according to Eq. (32)):

ΔT - difference of inlet temperatures

$W_1>0, W_2>0$ $\quad A=\begin{pmatrix} -W_1 & 0 & 0 & 0 \\ W_1-W & 0 & W & 0 \\ 0 & 0 & -W_2 & 0 \\ W & 0 & W_2-W & 0 \end{pmatrix}$ $\quad \Delta T = T_1 - T_3$ (4.1.9-28)

$W_1>0, W_2<0$ $\quad A=\begin{pmatrix} -W_1 & 0 & 0 & 0 \\ W_1-W & 0 & W & 0 \\ W & 0 & 0 & -W_2-W \\ 0 & 0 & 0 & W_2 \end{pmatrix}$ $\quad \Delta T = T_1 - T_4$ (4.1.9-29)

$W_1<0, W_2>0$ $\quad A=\begin{pmatrix} 0 & -W_1-W & W & 0 \\ 0 & W_1 & 0 & 0 \\ 0 & 0 & -W_2 & 0 \\ 0 & W & W_2-W & 0 \end{pmatrix}$ $\quad \Delta T = T_2 - T_3$ (4.1.9-30)

$W_1<0, W_2<0$ $\quad A=\begin{pmatrix} 0 & -W_1-W & 0 & W \\ 0 & W_1 & 0 & 0 \\ 0 & W & 0 & -W_2-W \\ 0 & 0 & 0 & W_2 \end{pmatrix}$ $\quad \Delta T = T_2 - T_4$ (4.1.9-31)

Heating power transferred between streams Q (heat exchanger duty) is calculated from the temperature difference of incoming streams ΔT and from the effectiveness of the heat exchanger ε_1 related to the first stream (tube side stream in case of shell&tube heat exchangers)

$$\varepsilon_1 = \frac{|T_1^{(1)} - T_2^{(1)}|}{\Delta T} = \frac{|W_1(T_1^{(1)} - T_2^{(1)})|}{|W_1|\Delta T} = \frac{Q}{|W_1|\Delta T}$$

$Q = |W_1|\varepsilon_1 \Delta T = W\Delta T$, where $W = |W_1|\varepsilon_1$. (4.1.9-32)

Note: For basic heat exchangers TYPE=0 the contributions corresponding to the terms W_1 and W_2 have been described in elements PIPE2D, therefore the HEXC elements needs to define only the entries W in the preceding matrices A.

Effectiveness ε_1 of heat exchanger depends upon heat transfer area, overall heat transfer coefficient and upon a specific flow arrangement (e.g. crossflow), and can be calculated from correlation as a function of NTU (Number of Transfer Units) and relative heat capacities of streams R.

Co-current flow arrangement

$$\varepsilon_1 = \frac{1-\exp[-NTU_1(1+R_1)]}{1+R_1} \quad (4.1.9\text{-}33)$$

counter-current

$$\varepsilon_1 = \frac{1-\exp[-NTU_1(1-R_1)]}{1-R_1\exp[-NTU_1(1-R_1)]}. \quad (4.1.9\text{-}34)$$

Number of transfer units is related to the heat capacity of stream 1 (therefore we do not distinguish weak and strong streams)

$$NTU_1 = \frac{kS}{|W_1|} \tag{4.1.9-35}$$

and R_1 is absolute value of ratio of heat capacities

$$R_1 = \left|\frac{W_1}{W_2}\right| . \tag{4.1.9-36}$$

A disadvantage of enthalpy balances method in comparison with weighted residuals is the fact, that there are no natural boundary conditions and therefore ending nodes must be treated differently (it does not hold that sum of enthalpy flows is zero in these nodes). Therefore the outlet nodes where the temperature cannot be described as a strong boundary condition must be labelled (in Femina status of temperature must be set to a value greater than 20 in these nodes) and matrix of enthalpy flows must be modified (this modification consists in adding heat capacity to the diagonal entry of $\boldsymbol{A}$)

$W_1>0, W_2>0$

$$A = \begin{pmatrix} -W_1 & 0 & 0 & 0 \\ W_1 - W & -\mathbf{W_1} & W & 0 \\ 0 & 0 & -W_2 & 0 \\ W & 0 & W_2 - W & -\mathbf{W_2} \end{pmatrix} \tag{4.1.9-37}$$

$W_1>0, W_2<0$

$$A = \begin{pmatrix} -W_1 & 0 & 0 & 0 \\ W_1 - W & -\mathbf{W_1} & W & 0 \\ W & 0 & \mathbf{W_2} & -W_2 - W \\ 0 & 0 & 0 & W_2 \end{pmatrix} \tag{4.1.9-38}$$

$W_1<0, W_2>0$

$$A = \begin{pmatrix} \mathbf{W_1} & -W_1 - W & W & 0 \\ 0 & W_1 & 0 & 0 \\ 0 & 0 & -W_2 & 0 \\ 0 & W & W_2 - W & -\mathbf{W_2} \end{pmatrix} \tag{4.1.9-39}$$

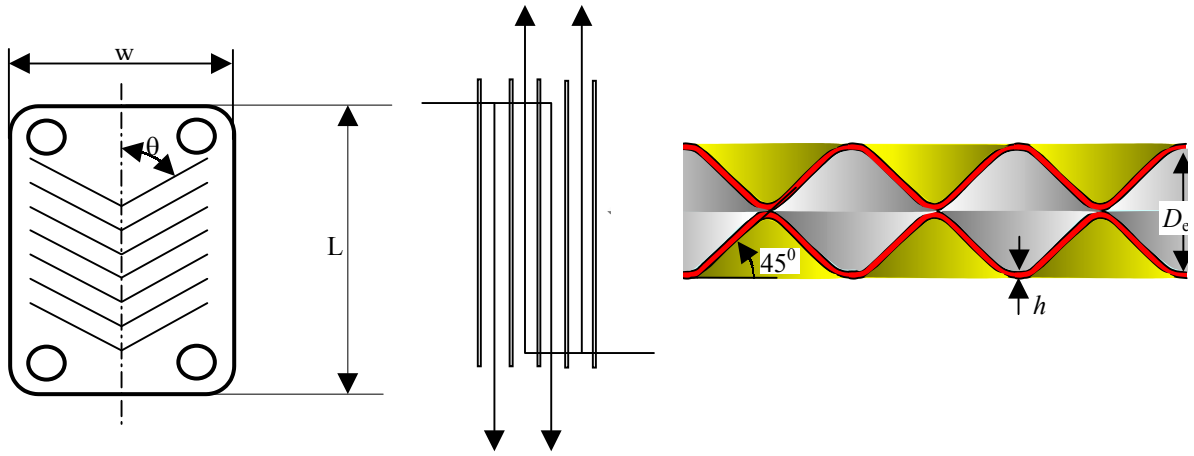
$W_1<0, W_2<0$

$$A = \begin{pmatrix} \mathbf{W_1} & -W_1 - W & 0 & W \\ 0 & W_1 & 0 & 0 \\ 0 & W & \mathbf{W_2} & -W_2 - W \\ 0 & 0 & 0 & W_2 \end{pmatrix} \tag{4.1.9-40}$$

Programming of a specific heat exchanger reduces to the calculation of pressure losses, i.e. calculation of flow coefficients $\varphi_{ij}(\Delta p)$ in both streams and to calculation of effectiveness ε_1, which represents calculation of overall heat transfer coefficient (including eventually fouling at both sides of heat transfer surface).

Chevron plate heat exchanger

In view of the fact that in FEMINA it is easy to combine heat exchangers in series or in parallel it seems sufficient to analyse only a heat exchanger with one pass and m parallel channels in one stream. These m-channels are formed by $2m+1$ plates having width w and height L. Distance of plates is $D_e/2$, where D_e is a hydraulic diameter of channel. We shall consider chevron type plates schematically shown in the following figure:



It follows from the preceding figure that the overall heat transfer area between stream 1 and 2 is

$$S=S_{plate}\,(2m-1) \qquad (4.1.9\text{-}41)$$

and that the heat transfer area of one plate is approximately

$$S_{plate}=\sqrt{2}wL \quad . \qquad (4.1.9\text{-}42)$$

Cross section of a channel is $A_{kanal}=\frac{D_e w}{2}$ and corresponding mean velocity u and Re number

$$u=\frac{2\dot{V}}{mD_e w},\qquad \mathrm{Re}=\frac{uD_e\rho}{\mu} \quad . \qquad (4.1.9\text{-}43)$$

Pressure drop along the plate of the length L can be expressed as a function of Fanning's friction factor

$$\Delta p=2f\frac{L}{D_e}\rho u^2=\frac{8fL\rho}{D_e^3 m^2 w^2}\dot{V}^2 \qquad (4.1.9\text{-}44)$$

therefore

$$\dot{V}_{ij}=\varphi_{ij}\Delta p_{ij},\qquad \varphi_{ij}=\frac{mwD_e^{3/2}}{\sqrt{8fL_{ij}\rho\Delta p_{ij}}} \quad . \qquad (4.1.9\text{-}45)$$

The Fanning's factor f has been derived by Martin (1996) as a function of chevron angle θ

$$\frac{1}{\sqrt{f}}=\frac{\cos\theta}{\sqrt{0.045\tan\theta+0.09\sin\theta+\frac{f_0}{\cos\theta}}}+\frac{1-\cos\theta}{\sqrt{3.8f_1}} \qquad (4.1.9\text{-}46)$$

Functions f_0 and f_1 depend upon flow regime, i.e. upon Reynolds number

Re<2000

$$f_0=\frac{16}{\mathrm{Re}}\quad ,\qquad f_1=\frac{149}{\mathrm{Re}}+0.9625$$

Re>2000

$$f_0=\frac{1}{1.56\ln\mathrm{Re}-3}\qquad f_1=\frac{9.75}{\mathrm{Re}^{0.289}} \quad . \qquad (4.1.9\text{-}47)$$

Heat transfer coefficient can be expressed using this Fanning factor as suggested by Martin (1996)

$$Nu = \frac{\alpha D_e}{\lambda} = 0.205\,\mathrm{Pr}^{1/3}\left(\frac{\mu}{\mu_w}\right)^{1/6}\left(f\,\mathrm{Re}^2\sin 2\theta\right)^{0.374} \quad . \qquad (4.1.9\text{-}48)$$

4.1.10. Pipeline networks – mass transport

Mass transfer in pipes is described by a similar transport equation as for heat transfer

$$A(\frac{\partial c_N}{\partial t}+\bar{u}\frac{\partial c_N}{\partial x})=\frac{\partial}{\partial x}(AD_{Ne}\frac{\partial c_N}{\partial x})+k_N O(c_{Ne}-c_N)+A(Q_N-S_N c_N) \tag{4.1.10-1}$$

where $S_N = A_N(T)+S_{Nu}$,

and these equations hold for three concentrations c_N, c_D, c_A , only coefficients differ. D_{Ne} is dispersion coefficient, calculated from the diffusion coefficient D_N in exactly the same way as the thermal dispersion a_e was calculated from the thermal diffusivity a. The coefficient k_N is mass transfer coefficient (m/s) corresponding to permeation of the component c_N through the tube wall into surrounding, with concentration c_{Ne} given as a RCONST parameter. Q_N is a production term defined by user (default zero), while S_N describes sink of component N, and consist of predefined chemical reaction of the first order with the frequency factor A_N defined as material parameter (possibly including the Arrhenius term) and of user defined part S_{Nu}, characterising for example other reactions).

Problem formulation is completed by the boundary condition

$$D_{Ne}\frac{\partial c_N}{\partial n}=\alpha_N(c_{Ne}-c_N)\,|_\Gamma \tag{4.1.10-2}$$

at endpoints of pipes.

Due to similarity of differential equations also the solution methods are the same. Weighted residual methods leads to the system of equations for element PIPE2D (and also PUMP,CSTR)

$$(M_{ij}+\Delta t\theta A_{ij})c_{Nj}=[M_{ij}-\Delta t(1-\theta)A_{ij}]c_{Nj}^0+\Delta t b_i \tag{4.1.10-3}$$

where

$$M_{ij}=\int_a^b AW_iN_j dx \tag{4.1.10-4}$$

$$A_{ij}=\int_a^b[A(W_i\bar{u}\frac{\partial N_j}{\partial x}+D_{Ne}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x})+W_iN_j(k_NO+AS_N)]dx+[A\alpha_N W_iN_j]_{i=j=a,b} \tag{4.1.10-5}$$

$$b_i=\int_a^b W_i(k_NOc_{Ne}+AQ_N)dx+[A\alpha_N c_{Ne}W_i]_{i=a,b} \quad . \tag{4.1.10-6}$$

Component balance leads to the equations written in matrix form for element 1-2. For positive velocity

$$\begin{pmatrix}0 & 0\\ -\frac{AL}{2} & -\frac{AL}{2}\end{pmatrix}\begin{pmatrix}\frac{dc_{N1}}{dt}\\ \frac{dc_{N2}}{dt}\end{pmatrix}+\begin{pmatrix}-A\bar{u}-\frac{AD_{Ne}}{L} & \frac{AD_{Ne}}{L}\\ A\bar{u}+\frac{AD_{Ne}}{L}-\frac{k_NLO+ALS_N}{2} & -\frac{AD_{Ne}}{L}-\frac{k_NLO+ALS_N}{2}\end{pmatrix}\begin{pmatrix}c_{N1}\\ c_{N2}\end{pmatrix}=\begin{pmatrix}\dot{m}_{N1}\\ \dot{m}_{N2}-ALQ_N-k_NLOc_{Ne}\end{pmatrix} \tag{7}$$

and similar expression holds for negative velocity (u<0),

$$\begin{pmatrix}-\frac{AL}{2} & -\frac{AL}{2}\\ 0 & 0\end{pmatrix}\begin{pmatrix}\frac{dc_{N1}}{dt}\\ \frac{dc_{N2}}{dt}\end{pmatrix}+\begin{pmatrix}-\frac{AD_{Ne}}{L}-\frac{k_NLO+ALS_N}{2} & \frac{AD_{Ne}}{L}-\frac{k_NLO+ALS_N}{2}-A\bar{u}\\ \frac{AD_{Ne}}{L} & A\bar{u}-\frac{AD_{Ne}}{L}\end{pmatrix}\begin{pmatrix}c_{N1}\\ c_{N2}\end{pmatrix}=\begin{pmatrix}\dot{m}_{N1}-ALQ_N-k_NLOc_{Ne}\\ \dot{m}_{N2}\end{pmatrix} \tag{8}$$

Component balance of elements PUMP and CSTR follows the same assumptions as the enthalpy balance, i.e. uniformity of concentration inside the apparatus

$$\begin{pmatrix} 0 & 0 \\ 0 & -V \end{pmatrix} \begin{pmatrix} \frac{dc_{N1}}{dt} \\ \frac{dc_{N2}}{dt} \end{pmatrix} + \begin{pmatrix} -A\bar{u} & 0 \\ A\bar{u} & -k_N OL - VS_N \end{pmatrix} \begin{pmatrix} c_{N1} \\ c_{N2} \end{pmatrix} = \begin{pmatrix} \dot{m}_{N1} \\ \dot{m}_{N2} - VQ_N - k_N LOc_{Ne} \end{pmatrix} \quad \text{for u>0} \qquad (4.1.10\text{-}9)$$

and

$$\begin{pmatrix} -V & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{dc_{N1}}{dt} \\ \frac{dc_{N2}}{dt} \end{pmatrix} + \begin{pmatrix} -k_N OL - VS_N & -A\bar{u} \\ 0 & A\bar{u} \end{pmatrix} \begin{pmatrix} c_{N1} \\ c_{N2} \end{pmatrix} = \begin{pmatrix} \dot{m}_{N1} - VQ_N - k_N LOc_{Ne} \\ \dot{m}_{N2} \end{pmatrix} \quad \text{for u<0 .} \qquad (4.1.10\text{-}10)$$

4.2. RTD processing and finite difference equation models

Matrix of observation point is used for comparison of transient FEM solution with experimental data, further on for lumped parameter models based upon assembly of ideally mixed tanks and plug flow units and finally for regression analysis of calculated or measured data. The first column of matrix of observation point is time, corresponding to data in the following columns (2,3,…,10). Therefore the matrix of observation points describes up to 9 functions of time represented by table of values with a common time base (there are 1024 rows – observation points by default).

There is a pair of parameters TYPE and INDEX associated to each column, these parameters are used for identification of columns

- TYPE=0 Empty (undefined) column)
- TYPE=1 Time (the first column by default)
- TYPE=2 Time course of nodal parameters (INDEX is the index of node)
- TYPE=3 Experimental data (usually imported by ROM command)
- TYPE=4 Stimulus function (INDEX identifies stimulus in the case of multiple inputs)
- TYPE=5 Response calculated by RTD model (INDEX identifies output of system with multiple outlets)
- TYPE=6 Regression model prediction
- TYPE=7 Standard deviation σ
- TYPE=8 Impulse response E(t)
- TYPE=9 Correlation function $R_{xy}(t)$

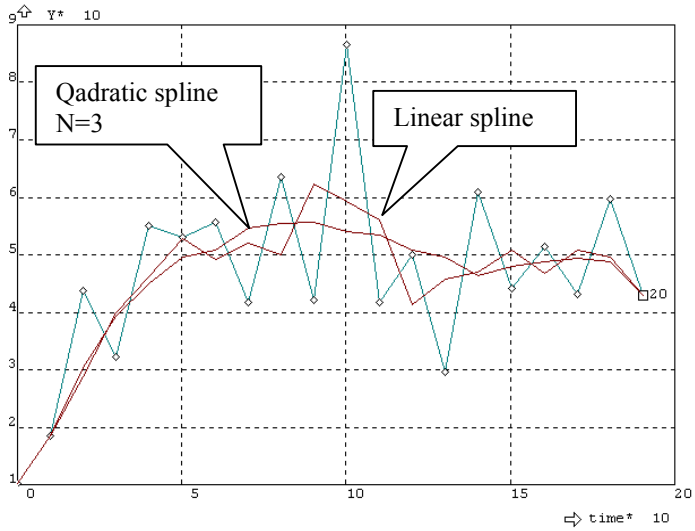
The following paragraphs are focused upon description of methods used for processing of time courses (evaluation, corrections and generation response).

	1	2	3	4	5	6	7	8	9	10
	TIME	EMPTY	EXPERI	EXPERI	EMPTY	EMPTY	EMPTY	EMPTY	EMPTY	EMPTY
1	.00E+00	.20E+00	.10E+00	.10E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
2	.10E+00	.29E+00	.19E+00	.19E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
3	.20E+00	.36E+00	.44E+00	.31E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
4	.30E+00	.42E+00	.32E+00	.39E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
5	.40E+00	.47E+00	.55E+00	.45E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
6	.50E+00	.50E+00	.53E+00	.50E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
7	.60E+00	.53E+00	.56E+00	.51E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
8	.70E+00	.55E+00	.42E+00	.55E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
9	.80E+00	.56E+00	.64E+00	.55E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
10	.90E+00	.57E+00	.42E+00	.56E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
11	.10E+01	.57E+00	.87E+00	.54E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
12	.11E+01	.57E+00	.42E+00	.53E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
13	.12E+01	.56E+00	.50E+00	.51E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
14	.13E+01	.55E+00	.30E+00	.50E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
15	.14E+01	.55E+00	.61E+00	.47E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
16	.15E+01	.53E+00	.44E+00	.48E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
17	.16E+01	.52E+00	.52E+00	.49E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
18	.17E+01	.51E+00	.43E+00	.49E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
19	.18E+01	.50E+00	.60E+00	.49E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0
20	.19E+01	.48E+00	.43E+00	.43E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+0

observation matrix 20-rows

4.2.1. Local smoothing

The operation SMOOTH comprises simple Method for local smoothing: median filtration and linear or quadratic regression splines. The coefficients of splines are not evaluated by a solution of system of equations, but recursively starting from the first data point. The idea of smoothing is simple: i+1 point is a value of linear or quadratic polynomial passing through the preceding point i and having the least sum of squares of deviations from N-preceding points and N-points behind the point i+1 (smoothing is suppressed for N=0).



In the following the symbol c is used for smoothed and y for original (noised) values:
Linear spline

$$c = y_i + a_i(t - t_i), \tag{4.2.1-1}$$

has coefficients a_i following from the requirement of minimum sum of squares

$$s_i^2 = \sum_{j=i-1}^{i+2}[y_j - y_i - a_i(t_j - t_i)]^2 \tag{4.2.1-2}$$

$$a_i = \frac{\sum_{j=i-1}^{i+2}(y_j - c_i\frac{t_{i+1} - t_j}{t_{i+1} - t_i})(t_j - t_i)}{\sum_{j=i-1}^{i+2}(t_j - t_i)^2} \tag{4.2.1-3}$$

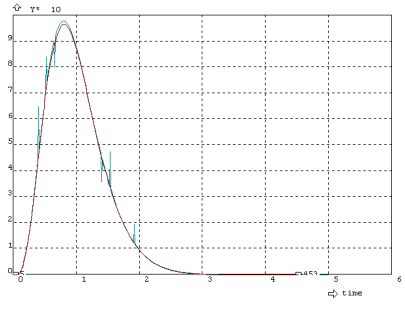
Quadratic spline

$$c = y_i + a_i(t - t_i) + b_i(t - t_i)^2 \tag{4.2.1-4}$$

has the coefficients a_i b_i which are derived in a similar way like the coefficients of linear splines

$$s_i^2 = \sum_{j=i-N+1}^{i+N}[y_j - y_i - a_i(t_j - t_i) - b_i(t_j - t_i)^2]^2 \tag{4.2.1-5}$$

$$\begin{pmatrix} \sum_{j=i-N+1}^{i+N}(t_j - t_i)^2 & \sum_{j=i-N+1}^{i+N}(t_j - t_i)^3 \\ \sum_{j=i-N+1}^{i+N}(t_j - t_i)^3 & \sum_{j=i-N+1}^{i+N}(t_j - t_i)^4 \end{pmatrix} \cdot \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} \sum_{j=i-N+1}^{i+N}(t_j - t_i)(y_j - c_i) \\ \sum_{j=i-N+1}^{i+N}(t_j - t_i)^2(y_j - c_i) \end{pmatrix} \tag{4.2.1-6}$$



The median filtration replaces y_i by median of values
$y_{i-N}, y_{i-N+1}, \ldots, y_{i-1}, y_i, y_{i+1}, \ldots, y_{i+N}$.

4.2.2. Data import with quadratic interpolation

Let us assume that the data, prepared in a file in form of pairs ($t_i\ y_i$), do not match the time base in MOP (sampled times do not conform with the first column, time, in the matrix of observation points). Standard approach based upon linear interpolation is substituted in FEMINA by quadratic local regression approximation. Quadratic polynomial passes through the pair of points enclosing the interpolated value of time t, and has the least sum of squares of deviations in two neighbouring points (left and right). The quadratic polynomials are therefore defined by tetrad of points labelled $t_0,\ldots,t_3$

$$c = y_1 + a(t - t_1) + b(t - t_1)^2 \tag{4.2.2-1}$$

where coefficients a,b follows from interpolating restriction

$$y_2 = y_1 + a(t_2 - t_1) + b(t_2 - t_1)^2 \tag{4.2.2-2}$$

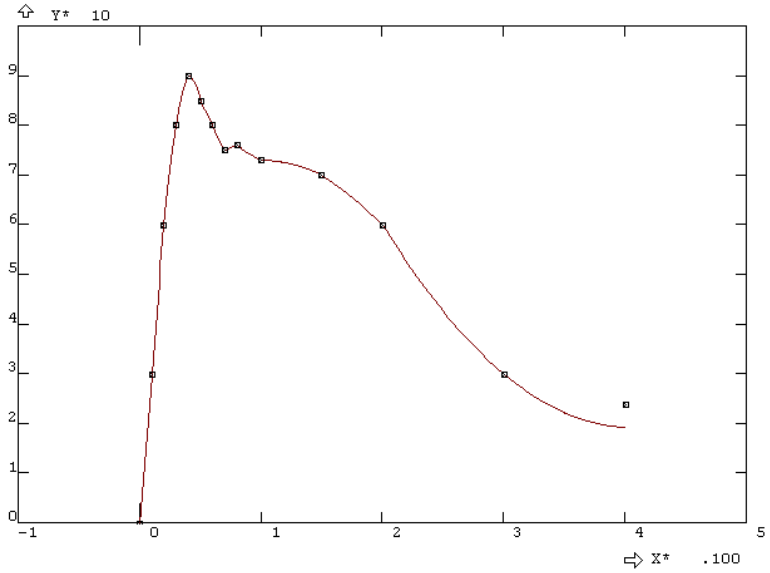
and from requirement of least squares

$$s^2 = \sum_{j=0,3}[y_j - y_1 - a(t_j - t_1) - b(t_j - t_1)^2]^2\ . \tag{4.2.2-3}$$

Solution of these equations gives

$$b = -\frac{\sum_{j=0,3}[y_j - y_1 - (y_2 - y_1)\frac{t_j - t_1}{t_2 - t_1}][(t_2 - t_1)(t_j - t_1) - (t_j - t_1)^2]}{\sum_{j=0,3}[(t_2 - t_1)(t_j - t_1) - (t_j - t_1)^2]^2} \tag{4.2.2-4}$$

$$a = \frac{y_2 - y_1}{t_2 - t_1} - b(t_2 - t_1) \tag{4.2.2-5}$$



4.2.3. Tail approximation

There are three options, three different functions, which can be used for tail approximation identified by non-linear regression analysis

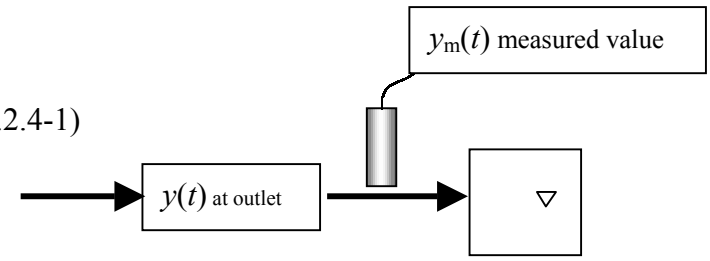
Mixed vessel	$c(t) = y_\infty + a\exp(-bt)$	(4.2.3-1)
Two mixed vessels	$c(t) = y_\infty + t\exp(a - bt)$	(4.2.3-2)
Convective model	$c(t) = y_\infty + a/t^3$	(4.2.3-3)

Parameter identification proceeds as follows: First the background level y_∞ is estimated according to minimum of processed response, the regression model is linearised and parameters *a,b* are evaluated by linear regression. This procedure is repeated several times for improved value of background y_∞ (bisection method).

4.2.4. Background raise correction

The case when the limiting value of measured response y_m for infinitely long time is greater than the initial value at time zero can be explained by the fact that the detector signal registers not only the radiation from the outlet stream but also the activity of tracer accumulated in a storage tank behind the apparatus outlet:

$$y_m(t) = y(t) + k\int_0^t y(u)du \qquad (4.2.4\text{-}1)$$



The constant *k* is fraction of radiation of the tracer in the storage tank recorded by detector and depends upon shielding of the detector. This constant is determined by the amount of tracer in infinite time, when all tracer is transported to the tank.

$$k = \frac{y_m(\infty) - y_m(0)}{\int_0^\infty y(u)du}. \qquad (4.2.4\text{-}2)$$

The integral equation (1) can be solved by the Laplace transform

$$y(t) = y_m(t) - k\int_0^t y_m(u)e^{-k(t-u)}du \qquad . \qquad (4.2.4\text{-}3)$$

In view of the fact that the constant *k* depends upon the unknown signal *y*(*t*) iterative solution is necessary, i.e. new approximation of *y*(*t*) is calculated from Eq. (3) using the value *k* from previous iteration and its value is updated according to Eq. (2). These relationships assume that the initial value (and also a final) value of signal *y*(*t*) is zero (zero concentration of tracer at inlet), however due to presence of a natural background radiation the value $y_m(0)$ is greater than zero and this value is to be subtracted from the measure signal (this operation is performed automatically).

4.2.5. Moment calculations

Moments of responses are calculated numerically, based upon linear interpolation of tabulated functions

$$M_0 = \int_0^\infty y(t)dt = \frac{1}{2}\sum_{i=1}^{N-1}(y_{i+1} + y_i)(t_{i+1} - t_i) \qquad (4.2.5\text{-}1)$$

$$M_1 = \int_0^\infty ty(t)dt = \frac{1}{6}\sum_{i=1}^{N-1}[y_i(t_{i+1}^2 + t_i t_{i+1} - 2t_i^2) - y_{i+1}(t_i^2 + t_i t_{i+1} - 2t_{i+1}^2)] \qquad (4.2.5\text{-}2)$$

$$M_2 = \int_0^\infty t^2 y(t)dt = \sum_{i=1}^{N-1}\{y_i\frac{t_{i+1}^3 - t_i^3}{3} - \frac{y_{i+1} - y_i}{t_{i+1} - t_i}[\frac{t_{i+1}^4 - t_i^4}{4} - \frac{t_i(t_{i+1}^3 - t_i^3)}{3}]\} \qquad (4.2.5\text{-}3)$$

4.2.6. Fast Fourier transform, convolution, deconvolution and correlations

Noise filtration, calculation of convolution, deconvolution and cross correlation of two functions are performed by using fast Fourier transform of N-sampled values (FFT),

$$\widetilde{E}(f) = \int_{-\infty}^{\infty} E(t) e^{2\pi i f t}\, dt, \qquad \widetilde{E}_n = \sum_{k=0}^{N-1} E_k e^{2\pi i k n/N}, \quad n = 0,1,...N-1. \tag{4.2.6-1,2}$$

Backward Fourier transform (inverse FFT) differs only by the sign in exponent

$$E(t) = \int_{-\infty}^{\infty} \widetilde{E}(f) e^{-2\pi i f t}\, df\,, \quad E_k = \frac{1}{N}\sum_{n=0}^{N-1} \widetilde{E}_n e^{-2\pi i k n/N}, \quad k = 0,1,...,N-1. \tag{4.2.6-3,4}$$

Convolution of functions x and y ($C_{xy}(t) = \int x(t-\tau) y(\tau) d\tau$) reduces to the product of Fourier images, it means to the product of Fourier coefficients

$$\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} x(t-\tau) y(\tau) d\tau\right) e^{2\pi i f t}\, dt = \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} x(t-\tau) e^{2\pi i f (t-\tau)} y(\tau) e^{2\pi i f \tau} d\tau\right) dt = \widetilde{x}(f)\widetilde{y}(f). \tag{4.2.6-5}$$

and correlation of the two functions x and y ($R_{xy}(t) = \int x(\tau) y(\tau + t) d\tau$) is product of complex conjugated x and y:

$$\widetilde{R}_{xy}(f) = \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} x(\tau) y(\tau + t) d\tau\right) e^{2\pi i f t}\, dt = \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} x(\tau) e^{-2\pi i f \tau} y(\tau + t) e^{2\pi i f (\tau + t)} d\tau\right) dt =$$

$$= \left(\int_{-\infty}^{\infty} x(\tau) e^{-2\pi i f \tau} d\tau\right)\left(\int_{-\infty}^{\infty} y(\tau) e^{2\pi i f \tau} d\tau\right) = \widetilde{x}(-f)\,\widetilde{y}(f) = \widetilde{x}^{*}(f)\,\widetilde{y}(f), \tag{4.2.6-6}$$

Note: Preceding relationships written for continuous FT hold also for discrete DFT.

Deconvolution, i.e. evaluation of impulse response $E(t)$ by the solution of Volterra integral equation of the first kind will be described in more details

$$y(t) = \int_{-\infty}^{\infty} E(t-\tau) x(\tau) d\tau\,. \tag{4.2.6-7}$$

The coefficients FFT of sought impulse response are calculated from the FFT coefficients of stimulus function $x(t)$ and response $y(t)$ by using regularisation procedure

$$\widetilde{E}_i = \frac{\widetilde{y}_i \widetilde{x}_i^{*} + W(i-1)^4 \widetilde{r}_i}{\widetilde{x}_i \widetilde{x}_i^{*} + W(i-1)^4}, \qquad W \approx w^2\left(\frac{2\pi}{N\Delta t}\right)^4 \tag{4.2.6-8}$$

where W is a weight of regularisation (user specified value of optimal regularisation w is independent of the period length NΔt and is typically of the order 10^{-3}). It is obvious that for W=0 it is a classical method of deconvolution, calculating FT of impulse response simply as a ratio of FT response y and stimulus function x. W>0 can be specified only if there are some reasons to believe that a specific analytical model should be a good representation of impulse response: $\widetilde{r}_i$ is Fourier coefficient of this analytical model. In the program FEMINA the impulse response of a serie of M-ideal mixers is used as a regularisation model

$$\widetilde{r}_i = \frac{1}{(1 - \frac{2\pi(i-1)\bar{t}}{MN\Delta t})^M}, \tag{4.2.6-9}$$

where $\bar{t}$ is the mean time of impulse response and NΔt is overall time – it is period of Fourier transform.

4.2.7. Solution of ordinary differential equations system

For the solution of ordinary differential equations of the first order (initial problem)

$$\begin{aligned}
&\frac{dc_1}{dt} = f_1(t, c_1, c_2, ..., c_M) \\
&\frac{dc_2}{dt} = f_2(t, c_1, c_2, ..., c_M) \qquad \frac{d\vec{c}}{dt} = \vec{f}(t, \vec{c}) \qquad (4.2.7\text{-}1) \\
&.... \\
&\frac{dc_M}{dt} = f_M(t, c_1, c_2, ..., c_M)
\end{aligned}$$

can be used either a classical Euler‘s method

$$\vec{c}(t + \Delta t) = \vec{c}(t) + \Delta t \vec{f}(t, \vec{c}(t)) \qquad (4.2.7\text{-}2)$$

or Runge Kutta method of the 4-th order

$$c(t + \Delta t) = c(t) + \frac{\vec{k}_1}{6} + \frac{\vec{k}_2}{3} + \frac{\vec{k}_3}{3} + \frac{\vec{k}_4}{6} \qquad (4.2.7\text{-}3)$$

where

$$\begin{aligned}
&\vec{k}_1 = \Delta t \vec{f}(t, \vec{c}(t)) \qquad (4.2.7\text{-}4,5,6,7) \\
&\vec{k}_2 = \Delta t \vec{f}(t + \frac{\Delta t}{2}, \vec{c}(t) + \frac{\vec{k}_1}{2}) \\
&\vec{k}_3 = \Delta t \vec{f}(t + \frac{\Delta t}{2}, \vec{c}(t) + \frac{\vec{k}_2}{2}) \\
&\vec{k}_4 = \Delta t \vec{f}(t + \Delta t, \vec{c}(t) + \vec{k}_3)
\end{aligned}$$

.

It is possible to select a constant time step Δt of integration when using Runge Kutta method (this integration time step should not be identified with the time step in the matrix of observation points because only each m-th integration step is stored in this matrix). However, it is also possible to use variable time step dynamically adjusting so that required accuracy ε will be achieved. The accuracy is estimated in the following way: each integration step is performed once with the full length Δt and than again with two smaller steps $\Delta t/2$ – its difference is a measure of approximation error and according to comparison with prescribed error the time step is either increased or decreased. Amount of necessary operations is little bit greater, nevertheless the fact that there exist two results obtained with different time steps can be exploited by Aitken extrapolation method for accuracy improvement.

The following relationships are used

Estimated relative error in one step is $$\varepsilon_{\max} = \max_j \frac{| y_{j,\Delta t/2} - y_{j,\Delta t} |}{| y_{j,\Delta t/2} |}, \; \varepsilon^* = \frac{\varepsilon_{\max}}{\varepsilon}. \qquad (4.2.7\text{-}8)$$

If $\varepsilon^*>1$, required accuracy has not been achieved and integration step is reduced according to the expression

$$\Delta t \leftarrow \frac{0.9\Delta t}{\sqrt[4]{\varepsilon^*}}. \qquad (4.2.7\text{-}9)$$

In the opposite case ($\varepsilon^*<1$) and if it has not been necessary to perform step reduction in the actual time step, the integration step is increased (maximum is 4 times)

$$\Delta t \leftarrow \frac{0.9\Delta t}{\sqrt[5]{\varepsilon^*}}. \qquad (4.2.7\text{-}10)$$

The extrapolation refining of results follows from the fact, the Runge Kutta method is of the 4th order which means, that it holds approximately

$$y_{\Delta t} = y + k\Delta t^4 \qquad (4.2.7\text{-}11)$$

$$y_{\Delta t/2} = y + k(\Delta t/2)^4 \quad .$$

Because the values $y_{\Delta t}$ and $y_{\Delta t/2}$ are known, it is possible to calculate the unknown coefficient k and therefore also the „true“ value y

$$y_j = y_{j,\Delta t/2} + \frac{1}{15}(y_{j,\Delta t/2} - y_{j,\Delta t}). \qquad (4.2.7\text{-}12)$$

4.3. Linear and nonlinear regression analysis

Linear polynomial regression is based upon procedures described in Press (1986)

$y = a_1 + a_2 x + ... + a_{N+1} x^N$

Models for nonlinear analysis (the list in not complete, only 8 initially implemented models are presented) are solve by standard Marquardt Levenberg method, see Press (1986)

EXPONENTIAL

$y = a_1 + a_2 e^{-a_3 x}$

$\frac{\partial y}{\partial a_1} = 1$

$\frac{\partial y}{\partial a_2} = e^{-a_3 x}$

$\frac{\partial y}{\partial a_3} = -a_2 x e^{-a_3 x}$

1

DOUBLE EXPON.

$y = a_1 + a_2 e^{-a_4 x} + a_3 e^{-a_5 x}$

$\frac{\partial y}{\partial a_1} = 1$

$\frac{\partial y}{\partial a_2} = e^{-a_4 x}$

$\frac{\partial y}{\partial a_3} = e^{-a_5 x}$

$\frac{\partial y}{\partial a_4} = -a_2 x e^{-a_4 x}$

$\frac{\partial y}{\partial a_5} = -a_3 x e^{-a_5 x}$

2

GAUSS FUNCTION

$y = a_1 + a_2 e^{-(\frac{x-a_3}{a_4})^2}$

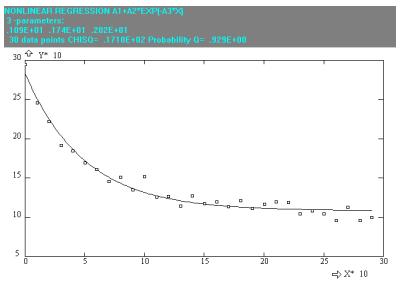
$\frac{\partial y}{\partial a_1} = 1$

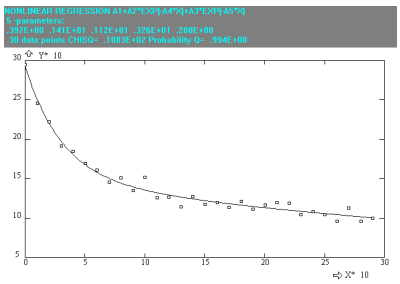
$\frac{\partial y}{\partial a_2} = e^{-(\frac{x-a_3}{a_4})^2}$

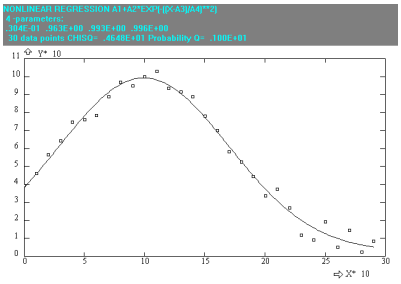
$\frac{\partial y}{\partial a_3} = 2a_2 \frac{x-a_3}{a_4^2} e^{-(\frac{x-a_3}{a_4})^2}$

$\frac{\partial y}{\partial a_4} = 2a_2 \frac{(x-a_3)^2}{a_4^3} e^{-(\frac{x-a_3}{a_4})^2}$

3







RATIONAL FUNCTION

$y = \frac{a_1 + a_2 x}{1 + a_3 x}$

$u_x = \frac{\partial \psi}{\partial y}$

$\frac{\partial y}{\partial a_2} = \frac{x}{1 + a_3 x}$

$\frac{\partial y}{\partial a_3} = -x \frac{a_1 + a_2 x}{1 + a_3 x}$

4

LOGISTICS

$y = \frac{a_1}{1 + a_2 e^{-a_3 x}}$

$\frac{\partial y}{\partial a_1} = \frac{1}{1 + a_2 e^{-a_3 x}}$

$\frac{\partial y}{\partial a_2} = -\frac{a_1 e^{-a_3 x}}{(1 + a_2 e^{-a_3 x})^2}$

$\frac{\partial y}{\partial a_3} = \frac{a_1 a_3 x e^{-a_3 x}}{(1 + a_2 e^{-a_3 x})^2}$

5

SERIE

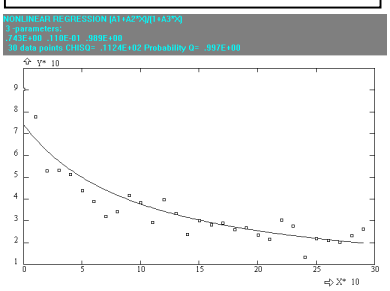
$y = a_1 x^{a_3 - 1} e^{-a_2 x}$

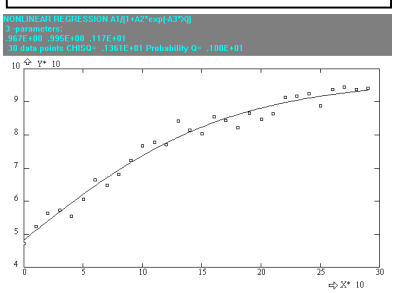
$\frac{\partial y}{\partial a_1} = x^{a_3 - 1} e^{-a_2 x}$

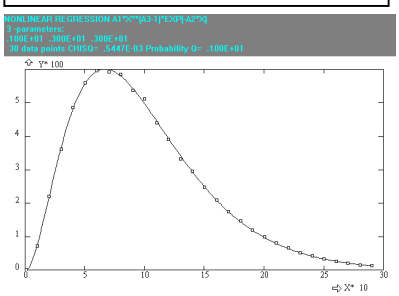
$\frac{\partial y}{\partial a_2} = -a_1 x^{a_3} e^{-a_2 x}$

$\frac{\partial y}{\partial a_3} = a_1 x^{a_3 - 1} e^{-a_2 x} \ln x$

6







AXIAL DISPERSION I.

$$y = \frac{a_1}{\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

7

$$\frac{\partial y}{\partial a_1} = \frac{1}{\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

$$\frac{\partial y}{\partial a_2} = -\frac{a_1 (x-a_3)^2}{x\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

$$\frac{\partial y}{\partial a_3} = \frac{2a_1 a_2 (x-a_3)}{x\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

AXIAL DISPERSION II.

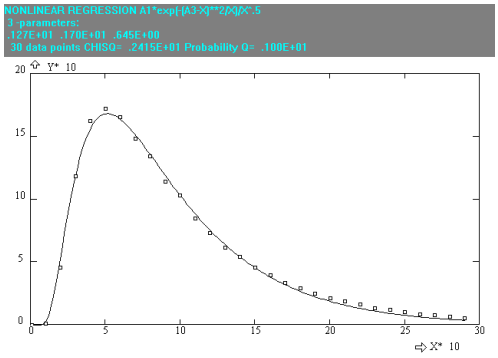
$$y = \frac{a_1}{x\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

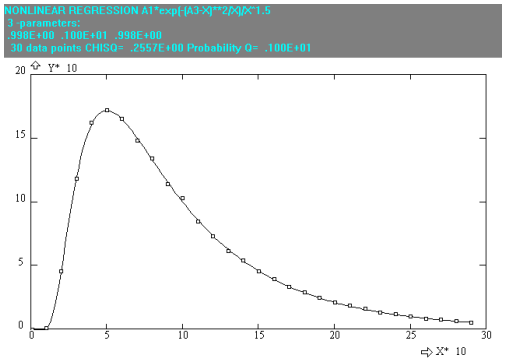
8

$$\frac{\partial y}{\partial a_1} = \frac{1}{x\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

$$\frac{\partial y}{\partial a_2} = -\frac{a_1 (x-a_3)^2}{x^2\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$

$$\frac{\partial y}{\partial a_3} = \frac{2a_1 a_2 (x-a_3)}{x^2\sqrt{x}} e^{-a_2 \frac{(x-a_3)^2}{x}}$$





The following models with two independent variables are available

Linear polynomial	$y = a_1 + a_2 x_1 + a_3 x_2$
Bilinear polynomial	$y = a_1 + a_2 x_1 + a_3 x_2 + a_4 x_1 x_2$
Quadratic polynomial	$y = a_1 + a_2 x_1 + a_3 x_2 + a_4 x_1 x_2 + a_5 x_1^2 + a_6 x_2^2$
Exponential model	$y = a_1 + (a_2 + a_3 x_1 + a_4 x_2)\exp(a_5 x_1 + a_6 x_2)$
Power law model	$y = a_1 x_1^{a_2} x_2^{a_3}$, $y = a_1 + a_2 x_1^{a_3} x_2^{a_4}$
Rational power law	$y = a_1 + a_2 \frac{x_1^{a_3} x_2^{a-4}}{1 + a_5 x_1^{a_6} x_2^{a_7}}$

4.4. Optimisation (operation OPTIMA and SOMA)

The basic method used for optimisation of a general mathematical model OPTIMA is in principle the same as the method used for nonlinear regression – Marquardt Levenberg. The method is based upon linearisation of optimised model $f(x_i,p_1,\ldots,p_M)=f_i$, where x_i are independent variables of the i-th observation point and $p_1,\ldots,p_M$ are optimised parameters of model. The least squares criterion is used for optimisation

$$s^2 = \sum_i (y_i - f_i)^2 w_i \tag{4.4-1}$$

$$\frac{\partial s^2}{\partial p_j} = 2\sum_i (y_i - f_i)\frac{\partial f_i}{\partial p_j} w_i \equiv 0 \tag{4.4-2}$$

$$\sum_i (y_i - f_{i0} - \sum_k \frac{\partial f_i}{\partial p_k}\Delta p_k)\frac{\partial f_i}{\partial p_j} w_i \equiv 0\,, \tag{4.4-3}$$

where $\Delta p_k = p_k - p_{k0}$ is the sought increment of k-th parameter in current iteration step. Therefore we arrive to the system of linear algebraic equations for the vector of increments

$$\sum_k C_{jk}\Delta p_k = B_j \tag{4.4-4}$$

where

$$C_{jk} = \sum_i \frac{\partial f_i}{\partial p_j}\frac{\partial f_i}{\partial p_k} w_i\,, \qquad B_j = \sum_i \frac{\partial f_i}{\partial p_j}(y_i - f_{i0}) w_i\,. \tag{4.4-5}$$

In the case, that the model is linear with respect to calculated parameters, the system of equations (4) is linear and only one iteration is sufficient. However, even if some parameters are non-linear iterations are necessary: first the values of linear parameters are calculated from reduced system (4) for fixed values of nonlinear parameters. Event than the full system of equations for linear and nonlinear parameters is solved, with modified matrix of the system (4), where a positive value λ is added to all diagonal entries of the matrix. Before adding the parameter λ the whole system of equations is scaled, which represents matrix transformation giving equivalent system of equations with matrix having ones on diagonal (this scaling is optional but recommended):

$$\sum_k C^*_{jk}\Delta p^*_k = B^*_j \tag{4.4-6}$$

$$C^*_{jk} = \frac{C_{jk}}{\sqrt{C_{jj}C_{kk}}}, \qquad C^*_{jj} = 1+\lambda\,, \quad B^*_j = \frac{B_j}{\sqrt{C_{jj}}}, \quad \Delta p^*_k = \Delta p_k\sqrt{C_{kk}} \tag{4.4-7}$$

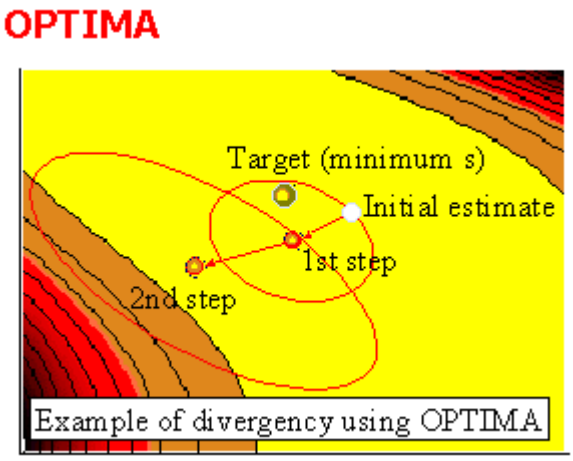
Gauss Jordan reduction is used for solution of (6) and calculated vector of increments is unscaled

$$\Delta p_k = \frac{\Delta p^*_k}{\sqrt{C_{kk}}} \tag{4.4-8}$$

and added to the vector of optimised parameters from the previous iteration.

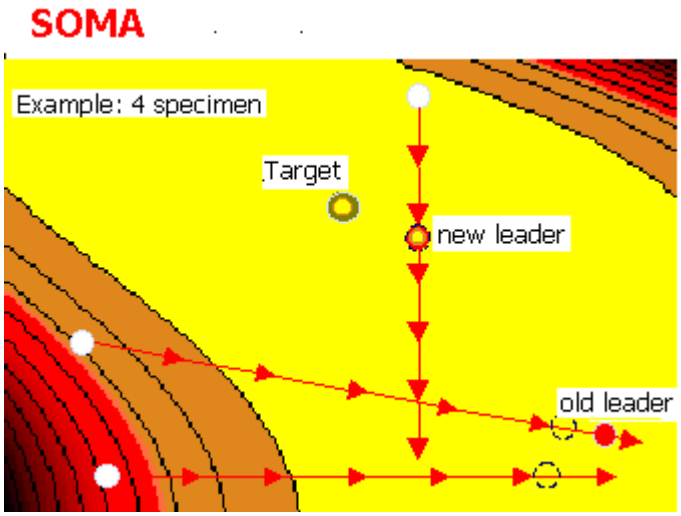
The value of parameter λ is dynamically adjusted in each iteration: if the result is improved, it means if the sum of weighted squares of differences decreased, the value λ is several times decreased (for zero λ, it is for system (4) without modification, the method reduces to the classical Gauss method), while in the opposite case the parameter λ is increased (thus the diagonal dominance of the matrix is increased, which means that the algorithm reduces to the gradient method if the scaling has been suppressed).

OPTIMA sometimes fails – it usually depends upon quality of the initial estimate, however even if it is close to the target convergency cannot be ensured, see the following figure



Beside this deterministic Marquardt Levenberg method also the stochastic method SOMA (Zelinka 2002) can be selected (usually for rough estimate of optimal parameters only). The method SOMA (Self Organising Migration Algorithm) need not calculate model derivatives, and therefore is much more simpler, robust but also significantly slower. This is so called memetic algorithm, modelling movement of several specimen in a hyperspace (under the term specimen we have in mind a solution of the optimised mathematical model). Principle is trivial:

- First several specimen NSPEC is generated by using pseudorandom number generator. All specimen must be within the specified range of model parameters.
- The best specimen, called LEADER, is selected.
- Iterations, in SOMA terminology called migration laps, begins. In each lap each of NSPEC specimen is moving towards LEADER in small steps of the length STEP (the parameter STEP is relative length of step with respect to the initial distance between specimen and leader), number of steps is MASS (MASS is specified control parameter, like STEP and NSPEC). In the space of parameter the trajectories of specimen are lines which aiming toward leader. Not exactly, the direction specimen-leader is perturbed intentionally by using random number generator. The measure of perturbation is specified by parameter PRT: if PRT=1 no disturbance is applied and the smaller (but still positive)is PRT, the greater is the deviation of direction toward the leader (this is realised in fact so that some randomly fixed parameters are fixed, and the smaller is PRT, the more parameters is fixed). Migration lap ends by transfer of all specimen to their best position and by election of new LEADER.



4.5. Structural analysis

4.5.1. Trusses (large deformation using Monte Carlo, command TRUSS)

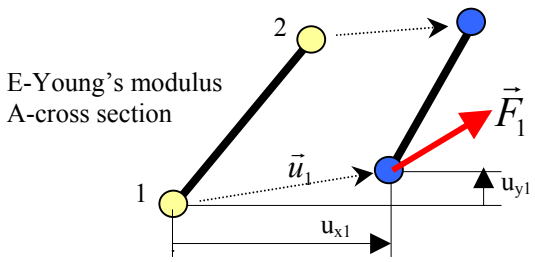
This example is more or less only a fun. System of trusses loaded by nodal forces is not solved by using equations describing nodal displacements, rather total energy is calculated for randomly selected configurations of nodal points displacements and the configuration exhibiting the least energy is selected (solution is not invoked by the command SOLVE, but using the command TRUSS). This approach is extremely slow, however it avoids complicated solution of nonlinear equations describing large displacements.

Total potential energy is the sum of internal energy of deformation (e) and potential energy of external forces (n).

$$W_{total} = \frac{1}{2}\sum_e \int_e E_e \varepsilon_e^2 dl - \sum_n (F_{xn}u_{xn} + F_{yn}u_{yn}) =$$

$$= \frac{1}{2}\sum_e E_e \frac{[\sqrt{(x_{e2}+u_{xe2}-x_{e1}-u_{xe1})^2+(y_{e2}+u_{ye2}-y_{e1}-u_{ye1})^2} - \sqrt{(x_{e2}-x_{e1})^2+(y_{e2}-y_{e1})^2}\,]^2}{\sqrt{(x_{e2}-x_{e1})^2+(y_{e2}-y_{e1})^2}} +$$

$$- \sum_n (F_{xn}u_{xn} + F_{yn}u_{yn}) \qquad (4.5\text{-}1)$$



4.5.2. Trusses (large deformation, incremental method, command SOLVE)

The same element TRUSS2D can be solved in a standard way (command SOLVE), it means as a solution of system of equations for nodal displacements. Element stiffness matrix is expressed in the following way, following from the previous equation (4.5-1) for total energy of a truss element

$$[K] = EA\begin{bmatrix} A_xE_x & A_yE_x & -A_xE_x & -A_yE_x \\ A_xE_y & A_yE_y & -A_xE_y & -A_yE_y \\ -A_xE_x & -A_yE_x & A_xE_x & A_yE_x \\ -A_xE_y & -A_yE_y & A_xE_y & A_yE_y \end{bmatrix} \qquad (4.5\text{-}2)$$

where $A_x, E_x, \ldots$ are not constants, but functions of nodal displacements from previous iteration:

$$A_x = \frac{1}{2L^2}(2\Delta x + \Delta u_x - \frac{\Delta x\Delta u_x + \Delta y\Delta u_y}{L^2}\Delta x)\,,\quad A_y = \frac{1}{2L^2}(2\Delta y + \Delta u_y - \frac{\Delta x\Delta u_x + \Delta y\Delta u_y}{L^2}\Delta y)$$

$$E_x = \frac{\Delta x + \Delta u_x}{\sqrt{(\Delta x + \Delta u_x)^2 + (\Delta y + \Delta u_y)^2}}\,,\quad E_y = \frac{\Delta y + \Delta u_y}{\sqrt{(\Delta x + \Delta u_x)^2 + (\Delta y + \Delta u_y)^2}} \qquad (4.5\text{-}3)$$

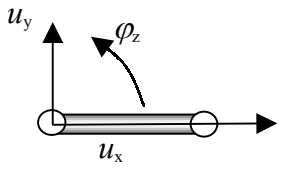
and

$$\Delta x = x_2 - x_1\,, \Delta y = y_2 - y_1 \qquad \Delta u_x = u_{x2} - u_{x1}\,,\ \Delta u_y = u_{y2} - u_{y1}\,.$$

4.5.3. Beams, pipelines (PIPE2D, BEAM2D)

Let us assume two dimensional beams, for example a pipeline. Stiffness matrix of beam having two nodes with nodal parameters u_x u_y φ_z can be expressed in the form

$$K_{\text{lokální}} = \begin{bmatrix} \frac{AE}{L} & 0 & 0 & -\frac{AE}{L} & 0 & 0 \\ 0 & \frac{12EJ}{L^3} & \frac{6EJ}{L^2} & 0 & -\frac{12EJ}{L^3} & \frac{6EJ}{L^2} \\ 0 & \frac{6EJ}{L^2} & \frac{4EJ}{L} & 0 & -\frac{6EJ}{L^2} & \frac{2EJ}{L} \\ -\frac{AE}{L} & 0 & 0 & \frac{AE}{L} & 0 & 0 \\ 0 & -\frac{12EJ}{L^3} & -\frac{6EJ}{L^2} & 0 & \frac{12EJ}{L^3} & -\frac{6EJ}{L^2} \\ 0 & \frac{6EJ}{L^2} & \frac{2EJ}{L} & 0 & -\frac{6EJ}{L^2} & \frac{4EJ}{L} \end{bmatrix} \qquad (4.5.3\text{-}1)$$



where A is cross section area of beam with length L and inertial moment J with respect to the axis z. For a tube with outer diameter D_2 , inner diameter D_1 (wall thickness $h=(D_2-D_1)/2$) the moment J can be expressed as

$$J = \frac{\pi}{64}(D_2^4 - D_1^4)\,, \qquad (4.5.3\text{-}2)$$

while for rectangular cross section b x h holds

$$J = \frac{bh^3}{12}. \qquad (4.5.3\text{-}3)$$

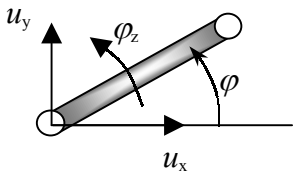
Right hand side vector represents loads (axial force F_a, transversal force F_t and bending moment M) – besides explicitly specified nodal forces, continuous loads corresponding to thermal dilatation and volumetric forces q [N/m], acting normal to the beam axis (for example dead weight, snow loading), and in the case that the element is a pipe (PIPE2D), also the axial force, caused by the contraction of pipe due to internal overpressure p:

$$F_{\text{lokální}} = \begin{bmatrix} \alpha(T_1 - T_e)AE - \mu\frac{p_1 DA}{2h} \\ -\frac{qL}{2} \\ 0 \\ -\alpha(T_2 - T_e)AE + \mu\frac{p_2 DA}{2h} \\ -\frac{qL}{2} \\ 0 \end{bmatrix} \qquad (4.5.3\text{-}4)$$

In Eq.(4) the α is a coefficient of thermal dilatation of wall material, T_e is a reference mounting temperature, and T_1, T_2 are nodal temperatures (we assume, that the wall temperature is the same as the temperature of fluid).

Stiffness matrix (1) corresponds to the beam, having axis aligned with the axis x of the global coordinate system ($K_{\text{lokální}}$ is stiffness matrix in a local coordinate system). For a beam inclined by the angle φ with respect to the axis x, it is necessary to transform the matrix $K_{lokální}$ by multiplying with the rotation matrix Q from left and right, and similar transformation (rotation) is to be applied also for the vector of loads F:

$$Q = \begin{bmatrix} C & S & 0 & 0 & 0 & 0 \\ -S & C & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & C & S & 0 \\ 0 & 0 & 0 & -S & C & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \qquad \mathrm{C} = \cos\varphi, \quad \mathrm{S} = \sin\varphi$$



(4.5.3-5)

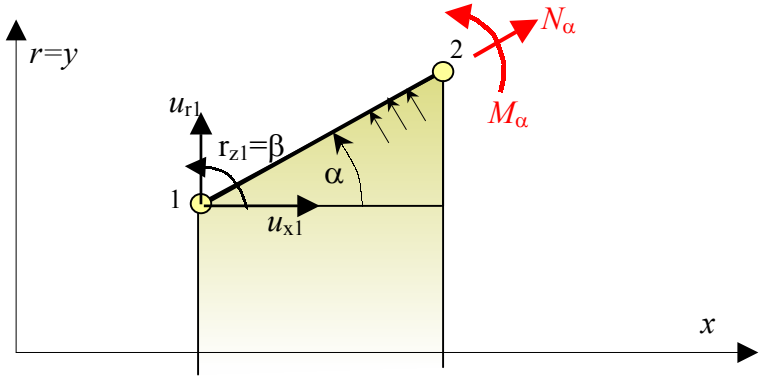
$$[F_{lokální}] = [Q][F_{globální}], \qquad [Q^T][K_{lokální}][Q] = [K_{globální}] \tag{4.5.3-6}$$

In view of the fact that the rotation matrix Q is orthogonal, $Q^{\mathrm{T}}Q=I$, it is possible to evaluate internal forces (axial force, transversal force and bending moment) from computed displacements in global coordinate system and from the stiffness matrix in the local coordinate system from the following expression

$$[F_{lokální}] = [K_{lokální}][Q][q_{globální}] \qquad . \tag{4.5.3-7}$$

4.5.4. Rotationally symmetric shells (SHELLAX)

Rotationally symmetric shell elements are very important for calculation of secondary stresses in vessels and pipes. Finite element representing a thin conical ring is based upon Vykutil's algorithm, see Schneider 1990. The element has 6 degrees of freedom (two displacements and rotation in a node)



Results of FE computations are displacements u_x, u_r and rotation of shell β in nodes. These values are used in postprocessing for calculation of internal forces, unit forces acting at the meridian direction N_α [N/m], unit forces in the circumferential direction N_β [N/m] (positive values correspond to tensile forces) and unit moments M_α [N] a M_β [N], whose positive values correspond to the *opening* of shell (tensile stresses at the inner surface of the shell, see figure). Further on the unit transversal force Q [N/m] and therefore the corresponding shear stresses is calculated.

$$N_\alpha = \frac{Eh}{1-\mu^2}(\varepsilon_\alpha + \mu\varepsilon_\beta) = \frac{Eh}{1-\mu^2}[\frac{u_{x2}-u_{x1}}{L}\cos\alpha + \frac{u_{r2}-u_{r1}}{L}\sin\alpha + \mu\frac{u_{r2}+u_{r1}}{2R}] \quad (4.5.4\text{-}1)$$

$$N_\alpha = \frac{Eh}{1-\mu^2}(\varepsilon_\beta + \mu\varepsilon_\alpha) = \frac{Eh}{1-\mu^2}[\mu(\frac{u_{x2}-u_{x1}}{L}\cos\alpha + \frac{u_{r2}-u_{r1}}{L}\sin\alpha) + \frac{u_{r2}+u_{r1}}{2R}] \quad (4.5.4\text{-}2)$$

$$M_\alpha = \frac{Eh^3}{12(1-\mu^2)}(\kappa_\alpha + \mu\kappa_\beta) = \frac{Eh^3}{12(1-\mu^2)}[\frac{\beta_2-\beta_1}{L} + \mu\sin\alpha\frac{\beta_2+\beta_1}{2R}] \quad (4.5.4\text{-}3)$$

$$M_\beta = \frac{Eh^3}{12(1-\mu^2)}(\kappa_\beta + \mu\kappa_\alpha) = \frac{Eh^3}{12(1-\mu^2)}[\mu\frac{\beta_2-\beta_1}{L} + \sin\alpha\frac{\beta_2+\beta_1}{2R}] \quad (4.5.4\text{-}4)$$

$$Q = \frac{5Eh}{12(1+\mu)}[\frac{u_{x2}-u_{x1}}{L}\sin\alpha + \frac{u_{r2}-u_{r1}}{L}\cos\alpha + \frac{\beta_2+\beta_1}{2}] \quad (4.5.4\text{-}5)$$

4.5.5. Plane stress/strain, rotationally symmetric bodies (elements PLANE2)

Plane stress

The only nonzero componets of stress are in the *x-y* plane, two normal and one shear stress.. Deformation in the normal direction to the plane *x-y* is allowed, however the corresponding normal stress s_{zz} is zero, and therefore is zero also the contribution of the transversal deformation to the deformation energy. Corresponding stiffness matrix of an element is expressed by integrals

$$[K]=\iint[B]^T.[D].[B]dS=\iint\begin{bmatrix}[B_1]^T\\ [B_2]^T\\ \dots\end{bmatrix}.[D].\begin{bmatrix}[B_1] & [B_2] & \dots\end{bmatrix}dS=\begin{bmatrix}[K_{11}] & [K_{12}] & \dots\\ [K_{21}] & [K_{22}] & \\ \dots & & \end{bmatrix} \qquad (4.5.5\text{-}1)$$

where D is the matrix of elastic constants and the submatrices K_{ij} with dimension 2 x 2 correspond to the combination of nodes *i* and *j*

$$[K_{ij}]=\iint[B_i]^T.[D].[B_j]dS=\frac{E}{1-\mu^2}\iint\begin{bmatrix}\frac{\partial N_i}{\partial x} & 0\\ 0 & \frac{\partial N_i}{\partial y}\\ \frac{\partial N_i}{\partial y} & \frac{\partial N_i}{\partial x}\end{bmatrix}.\begin{bmatrix}1 & \mu & 0\\ \mu & 1 & 0\\ 0 & 0 & \frac{1-\mu}{2}\end{bmatrix}.\begin{bmatrix}\frac{\partial N_j}{\partial x} & 0\\ 0 & \frac{\partial N_j}{\partial y}\\ \frac{\partial N_j}{\partial y} & \frac{\partial N_j}{\partial x}\end{bmatrix}dS= \qquad (4.5.5\text{-}2)$$

$$=\frac{E}{1-\mu^2}\iint\begin{bmatrix}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{1-\mu}{2}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} & \mu\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial y}+\frac{1-\mu}{2}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial x}\\ \mu\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial x}+\frac{1-\mu}{2}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial y} & \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}+\frac{1-\mu}{2}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}\end{bmatrix}dS$$

Plena strain

The case, when the component of deformation e_{zz} is zero differs only in a different matrix of elastic constants

$$[D]=\frac{E(1-\mu)}{(1+\mu)(1-2\mu)}\begin{bmatrix}1 & \frac{\mu}{1-\mu} & 0\\ \frac{\mu}{1-\mu} & 1 & 0\\ 0 & 0 & \frac{1-2\mu}{2(1-\mu)}\end{bmatrix}. \qquad (4.5.5\text{-}3)$$