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# SOFTWARE SUPPORT DEVELOPMENT FOR NUMERICAL SOLUTION OF ANSYS CFX

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**Abstract:** The paper deals with possibilities to apply a new developed software support for simulation programme ANSYS CFX. A direct export of heat-transfer coefficients into variables used under edge conditions as well as of physical properties of gas mixtures into material properties during simulation solution of technical tasks means a significant saving of time. The paper summarizes in detail description of the software for calculation of heat-transfer coefficient during free convection (HTC-FC) and of material properties of gas mixture (MPGM) that enable to export calculated data directly into the text files which can be imported then into the programme ANSYS CFX.

**Key words:** Software, Numerical Methods, Multidimensional Regression, Ansys CFX, Heat-Transfer Coefficient

## 1. INTRODUCTION

The design of the energy equipments is closely connected with the use of numerical methods based on the finite volume method (FVM). These methods pull down the barriers of classic solutions of problems through an analytical way and speed up the whole calculation (Badida et al, 2008; Trebuňa et al., 2013). The simulation is based on creation of mostly 3D geometry that is then discretized through mesh creation with a final number of elements (Michalec et al, 2010; Kapjor et al., 2010, Kizek et al., 1999). By setting conditions of uniqueness into the simulation tool as well as by applying needed models and differential equations, a numerical calculation is carried out after which it is possible to evaluate sought parameters (Oravec et al, 2010; Durdán et al, 2009, Vranay and Vranayová, 1999). Setting physical and boundary conditions is significantly time-consuming, especially, under dependent boundary conditions. Such a condition is the value of the heat-transfer coefficient (HTC) during simulations of transient phenomena of heating or cooling bodies. The heat-transfer coefficient is considerably dependent on the surface temperature of solved mesh boundary element during free convection, namely while considering radiation (Setoodeh et al, 2011; Mansoori et al., 2002 and Tauš and Kudelas, 2012).

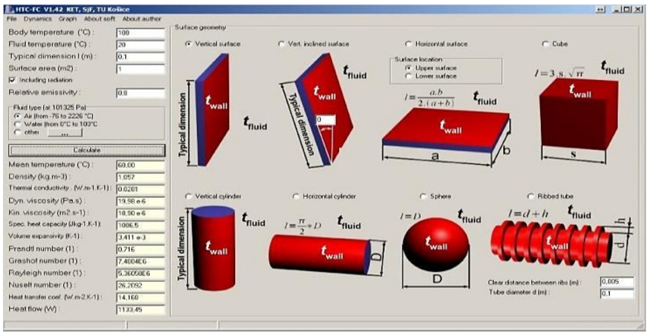
It is possible to use materials library data in the programme Ansys CFX during the simulation calculations in which a gas mixture is simulated. Setting individual parameters of the gas mixture sufficient for solution gives also the possibility to make up the mathematical dependence of the quantities on pressure and temperature of the solved element by means of the multidimensional regression.

The subject of this paper is the description of new created subroutines that facilitate the engineering work at numerical methods in ANSYS CFX.

## 2. HTC-FC SOFTWARE DEVELOPMENT

Calculations of the heat-transfer coefficient is a time-consuming matter not only with a view to the subtraction of physical properties of fluids, that are needed for setting criteria of similarity, but also with a view to the cyclic solution for more values of the surface temperatures. With regard to the requirement for speeding up the setting the boundary condition of the 3rd kind, an impulse arose for development of HTC-FC (heat-transfer coefficient – free convection) software that enables to calculate the heat-transfer coefficient for the surface temperature range of geometry specified by the user up to the scope of the criterions equation (Frestl and Masaryk, 2011; Kalaš et al., 2000).

Graphical window is divided for selection of basic geometry types from vertical areas up to the ribbed tubes where a typical dimension l (Fig. 1) is represented at each type. After starting calculation, the programme will read body temperature, fluid temperature, typical dimensions and surface emissivity while considering radiation. In the case of the requirement for storing data into a file, it is possible to set the surface temperature range of the wall as well as the temperature step, by which the calculation will be executed, in the tool bar. An inherent part of the programme is the material selection. Today, it is possible to select air, water or to set the physical properties of any fluid. All material properties are dependent on the temperature. In order to guarantee a right calculation, the programme will check not only the ranges of permissible temperatures, but also the range of individual criterion equations or similarity criteria.



Body temperature (°C) : 100
Fluid temperature (°C) : 20
Typical dimension l (m) : 0,1
Surface area (m2) : 1
☑ Including radiation
Relative emissivity : 0,8

Fluid type (at 101325 Pa)
● Air (from -76 to 2226 °C)
○ Water (from 0°C to 100°C
○ other

Mean temperature (°C) : 60,00
Density (kg.m-3) : 1,057
Thermal conductivity . (W.m-1.K-1) : 0,0281
Dyn. viscosity (Pa.s) : 19,98 e-6
Kin. viscosity (m2.s-1) : 18,90 e-6
Spec. heat capacity (Jkg-1.K-1) : 1006,5
Volume expansivity (K-1) : 3,411 e-3
Prandtl number (1) : 0,716
Grashof number (1) : 7,4004E6
Rayleigh number (1) : 5,36058E6
Nuselt number (1) : 26,2092
Heat transfer coef. (W.m-2.K-1) : 14,168
Heat flow (W) : 1133,45

● Vertical surface
○ Vert. inclined surface
○ Horizontal surface
○ Cube
Surface location
● Upper surface
○ Lower surface
○ Vertical cylinder
○ Horizontal cylinder
○ Sphere
○ Ribbed tube
Clear distance between ribs (m) : 0,005
Tube diameter d (m) : 0,1

**Fig. 1.** View of graphical window of the HTC-FC programme

The main advantage of using HTC-FC software is the speeding up the setting the boundary condition of the 3rd kind into the simulation programme ANSYS CFX, as the programme enables to export files with the extension “ccl”. They are the text files containing settings in CFX. After selection of the export into the “ccl” file, the programme will ask for the name of the boundary condition by which a duplicate setting will be avoided in case of more boundary conditions in one simulation.

The number of exported values of HTC is dependent on set temperature range and step in the tool bar. Only the total heat-transfer coefficient (Fig. 2 Total HTC - $\alpha_c$) will be recorded in the file for simulation programme. If the user decides to add radiation into the calculation, it will be reflected in the total HTC as the sum of HTC of free convection and of equivalent HTC from the radiative thermal flux (Pyszko et al., 2010):

$$\alpha_c = \alpha(Pr,Gr) + \varepsilon\cdot\sigma\cdot\left(T_s^2+T_t^2\right)\cdot\left(T_s+T_t\right) \qquad (\mathrm{W\cdot m^{-2}\cdot K^{-1}}) \qquad (1)$$

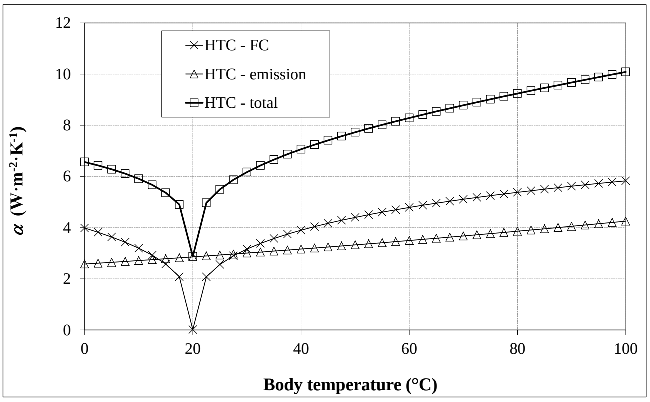


**Fig. 2.** Course of the heat-transfer coefficient in dependence on the body temperature

Fig. 2 shows the course of the heat-transfer coefficients during free convection calculated by means of the HTC-FC programme for vertical plate with typical dimension 1 m, fluid temperature 20 °C and emissivity 0.5. The fluid used was air.

## 2.1. HTC - FC software usage

The possibilities of the software usage will be demonstrated by means of cooling a horizontal steel bar of 50 mm in diameter. A CFX domain for ambient air was created during the first simulation and the entire computation of convective heat demand was directly simulated for free convection along with air movement. Radiation was computed using the “Discrete Transfer" model. A domain was created only for the steel bar during the second simulation, whereas the third type boundary condition was applied to the outer cylindrical surface area. The HTC value, computed by the HTC - FC software, and the ambient temperature are known for this condition. The numerical computation without using the fluid domain, and hence without having to solve the Navier-Stokes differential equations, is much faster.

For the horizontal cylinder shown in Fig. 3, dependence of HTC upon the surface temperature of the cylinder (Fig. 4) was generated. The initial temperature of the cylinder was 300 °C and the cooling computation lasted for an hour. The ambient air temperature was set at 25 °C and the radiation ambient was of the same value. The mean air temperature was used for computation of physical quantities of air.

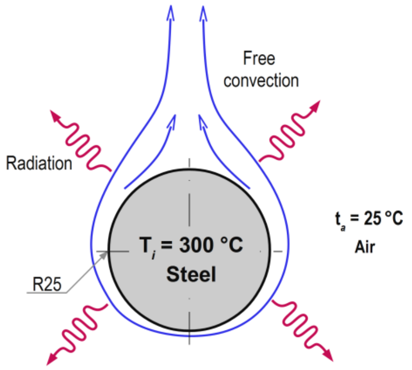


**Fig. 3.** Description of cooling of a horizontal cylinder

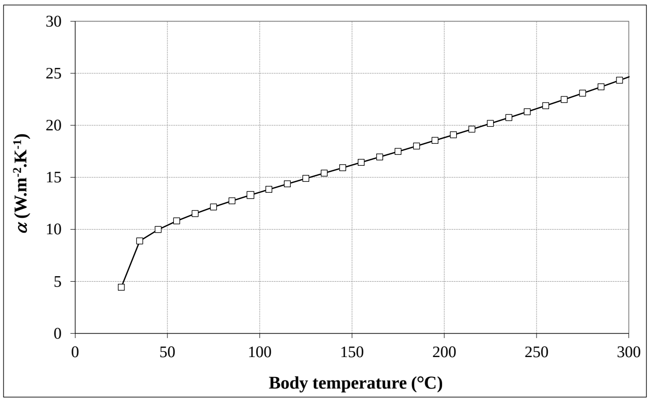


**Fig. 4.** Dependence of HTC - horizontal cylinder upon temperature

The surface emissivity was assumed to be 0.7 and the constant value was considered in the whole temperature range. The thermal field of the steel bar along with ambient air after 600 seconds from the beginning of the initial time is plotted in Fig. 5. Air heating results in free convection, which cools the cylinder along with radiation.

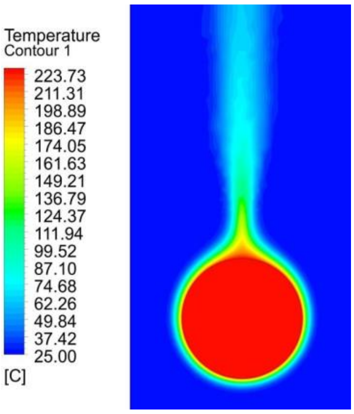


**Fig. 5.** The thermal field of air and the bar after 600 s for solution of air flow and radiation

The thermal field after 600 s without solution of the ambient air flow, only by applying the third type boundary condition, is shown in Fig. 6 to compare temperatures. In addition to free convection, HTC also includes radiation HTC equivalent. Given the low value of the Biot number in the range from 0.002 to 0.011 the temperature difference is minimal between the core of the rod and its surface.

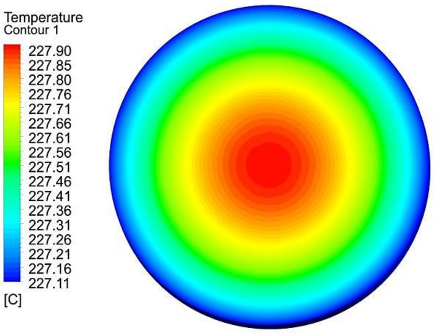


**Fig. 6.** The thermal field of the bar after 600 s without solution of the air flow and by applying the HTC

The deviation of the average temperature of the horizontal bar after 600 s from the beginning using the different approaches is only 0.06 °C. The comparison of temperature change during the entire solution time and the percentage deviation are shown in Fig. 7. The diagram shows that the time-consuming computation of the cooling fluid flow can be replaced by using HTC in those cases. The computation without considering the air flow was approximately twenty-six times faster in this case while the same iterative accuracy was maintained.

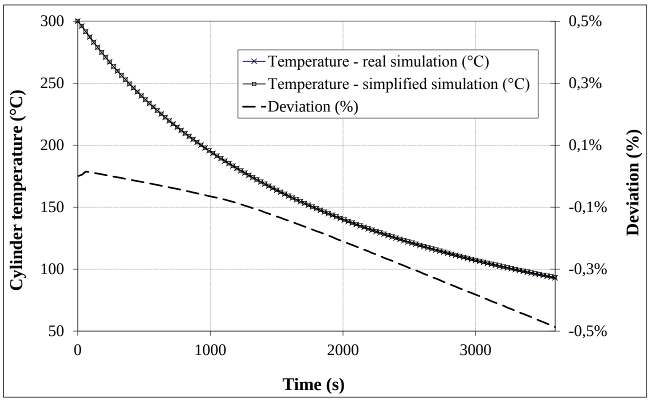
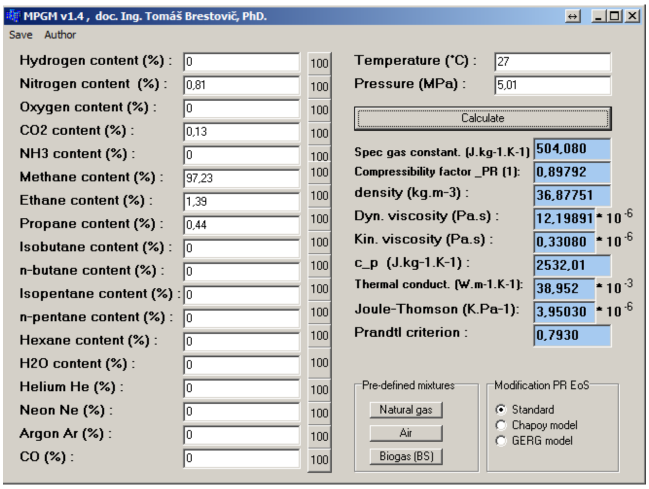


**Fig. 7.** The course of temperatures and their mutual deviation at simulations

Adequacy of using the simpler approach is strongly dependent upon the type of the solved issue. For complex geometrical shapes, the simulation of fluid flow is more advantageous and accurate due to the effect of mutual radiation of surfaces and the complex fluid flow.

## 3. MPGM (MATERIAL PROPERTIES OF GAS MIXTURES) SOFTWARE DEVELOPMENT

In ANSYS CFX, it is possible to create the gas mixtures, e. g. by import of clean gases of which the state quantities are calculated by means of Peng-Robinson equatation of state (PR EoS) with consecutive defining their mutual relation. The aim to facilitate setting and defining of gas mixture with its material properties resulted in development of MPGM software (Material Properties of Gas Mixtures,(Tkáč and Hvizdoš, 2008) that has 18 preset gases for any mixture production (Fig. 8).



MPGM v1.4 , doc. Ing. Tomáš Brestovič, PhD.

Hydrogen content (%) : 0
Nitrogen content (%) : 0,81
Oxygen content (%) : 0
CO2 content (%) : 0,13
NH3 content (%) : 0
Methane content (%) : 97,23
Ethane content (%) : 1,39
Propane content (%) : 0,44
Isobutane content (%) : 0
n-butane content (%) : 0
Isopentane content (%) : 0
n-pentane content (%) : 0
Hexane content (%) : 0
H2O content (%) : 0
Helium He (%) : 0
Neon Ne (%) : 0
Argon Ar (%) : 0
CO (%) : 0

Temperature (°C) : 27
Pressure (MPa) : 5,01

Spec gas constant. (J.kg-1.K-1) 504,080
Compressibility factor _PR (1): 0,89792
density (kg.m-3) : 36,87751
Dyn. viscosity (Pa.s) : 12,19891 * 10 -6
Kin. viscosity (Pa.s) : 0,33080 * 10 -6
c_p (J.kg-1.K-1) : 2532,01
Thermal conduct. (W.m-1.K-1): 38,952 * 10 -3
Joule-Thomson (K.Pa-1): 3,95030 * 10 -6
Prandtl criterion : 0,7930

Modification PR EoS
● Standard
○ Chapoy model
○ GERG model

**Fig. 8.** Graphical window of the MPGM programme

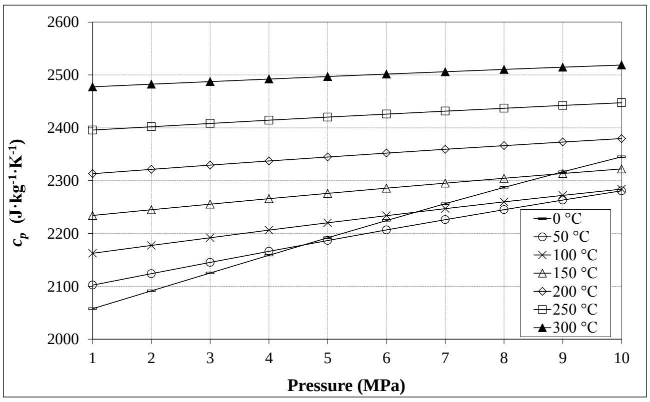


**Fig. 9.** Course of specific heat $c_p$ = f(p,T) for gas mixture 30 % $H_2$, 30 % $N_2$, 40 % $CH_4$

The programme calculates the compressibility factor according to PR EoS (from which the density is calculated), the specific heat (Fig. 9), transport properties as well as Joule-Thomson coefficient and Prandtl criterion for any gas mixture. These parameters can be used in practice for any of the processes using a mixture of gases at higher pressures, such as the cooling natural gas in compressor station. When the dependencies of physical quantities are exported to HTC- FC program, it can be calculated HTC on the internal heat exchange surfaces of coolers and thus cooling performance can be quantified.

### 3.1. Peng - Robinson equation of state

The Peng-Robinson equation of state (PR EOS) is a three-parameter modification of the Redlich-Kwong equation of state. The third parameter, which led to the more accurate results, is the acentric factor ω. The constant a was converted into a temperature-dependent one at the same time (Svoboda et al, 2007). The basic form of the equation of state is as follows:

$$p = \frac{R \cdot T}{V - b} - \frac{a}{V \cdot (V + b) + b \cdot (V - b)} \quad \text{(Pa)} \qquad (2)$$

To compute the compressibility factor, the equation can be derived as follows:

$$z^3 - (1-B)\cdot z^2 + \left(A - 3\cdot B^2 - 2\cdot B\right)\cdot z - \left(A\cdot B - B^2 - B^3\right) = 0 \tag{3}$$

Where the constants A and B are expressed as follows:

$$A = \frac{p\cdot a(T)}{R^2\cdot T^2} \tag{4}$$

$$B = \frac{b\cdot p}{R\cdot T} \tag{5}$$

The computation of the equation (2) is carried out using the Newton-Raphson method. The parameter *a*(*T*) is dependent on the reduced temperature, which represents the ratio of the thermodynamic temperature and the critical temperature of the *i*th component of a gas.

$$a(T) = 0.45724\cdot\frac{R^2\cdot T_k^2}{p_k}\cdot\left[1+\kappa\cdot\left(1-\sqrt{\frac{T}{T_k}}\right)\right]^2 \quad (\mathrm{J^2\cdot mol^{-2}\cdot Pa^{-1}}) \tag{6}$$

$$b = 0.0778\cdot\frac{R\cdot T_k}{p_k} \quad (\mathrm{J^2\cdot mol^{-2}\cdot Pa^{-1}}) \tag{7}$$

$$\kappa = 0.37464 + 1.54226\cdot\omega - 0.26992\cdot\omega^2 \tag{8}$$

Where $\omega$ is the acentric factor (1), whose value for the particular components of a mixture of gases is given by references (Svoboda et al, 2007). In respect of compution of the compressibility factor for a mixture of gases, it is necessary to use the mixing rule to calculate the constants *a*(*T*) and *b*. The rule is in the form as follows:

$$a_{zp}(T) = \sum_i\sum_j x_i\cdot x_j\cdot\sqrt{a_i\cdot a_j}\cdot\left(1-K_{ij}\right) \tag{9}$$

$$b_{zp} = \sum_i b_i\cdot x_i \tag{10}$$

For the larger number of gas components, it is more appropriate to use computer software for this type of computation. It is also due to the need for implementation of the binary interaction coefficients $K_{ij}$, which are given in (Knapp, H. et al., 1982).

### 3.2. Dynamic viscosity of pure gases at high pressures

Dynamic viscosity is considered to be constant up to the pressure below 1 MPa. Above the pressure, the viscosity increases with the pressure, whereas the most common method of its calculation is the Jossi-Stiel-Thodos method (Jossi, 1962). This indicates the dependence of the additional viscosity $(\eta-\eta_0)$ on the reduced density, which is defined by the ratio of the gas density at the determining conditions to the critical density (density at the critical pressure and critical temperature). The empirical relationship applies to the non-polar gases (CH4, CO2, N2, H2, etc.). It is valid in terms of the reduced densities $\rho_r \le 3$ and is in the form:

$$(\eta-\eta_0)\cdot\xi_\mathrm{d} = \left(0.506\cdot e^{1.584\cdot\rho_r} - 0.506\right)\cdot 10^{-6} \tag{11}$$

If the reduced density ranges $0.3 \le \rho_r \le 2$ , the following applies:

$$(\eta-\eta_0)\cdot\xi_\mathrm{d} = \left(1.0637\cdot e^{1.079\cdot\rho_r} - 1.15\right)\cdot 10^{-6} \tag{12}$$

The constant $\xi_d$ is a function of the critical temperature $T_\mathrm{k}$ (K), critical pressure $p_\mathrm{k}$ (MPa) and the molar mass *M* (kg·kmol$^{-1}$) and is in the form:

$$\xi_\mathrm{d} = \left(\frac{T_\mathrm{k}}{M^3\cdot p_\mathrm{k}^4}\right)^{\frac{1}{6}} \tag{13}$$

For polar gases (CO, HCl, $H_2O$), the empirical relationships obtained by experiments were classified according to the reduced density as follows:

$$\rho_\mathrm{r} \le 0.1 \qquad (\eta-\eta_0)\cdot\xi_\mathrm{d} = 0.7619\cdot 10^{-6}\cdot\rho_\mathrm{r}^{1.111} \tag{14}$$

$$0.1 \le \rho_\mathrm{r} \le 0.9 \qquad (\eta-\eta_0)\cdot\xi_\mathrm{d} = 2.793\cdot(9.045\cdot\rho_\mathrm{r} + 0.63)^{1.739}\cdot 10^{-8} \tag{15}$$

$$\begin{aligned} 0.9 \le \rho_\mathrm{r} \le 2.2 \qquad & \log\{-\log[(\eta-\eta_0)\cdot\xi_\mathrm{d}] - 2.3372\} = \\ & = 0.6439 - 0.1005\cdot\rho_r \end{aligned} \tag{16}$$

#### 3.2.1. Dynamic viscosity of a mixture of gases

The Dean and Stiel method, which is designed for hydrogen-free and helium-free non-polar gases, can be used for the calculation of the viscosity of a mixture of gases:

$$(\eta-\eta_0)\cdot\xi_\mathrm{dh} = 0.496\cdot\left(e^{1.439\cdot\rho'_\mathrm{r}} - e^{-1.111\cdot\rho_\mathrm{r}'^{1.858}}\right) \tag{17}$$

The constant $\xi_{dh}$ is calculated similarly to the consideration $\xi_d$ of the mean molar mass of a mixture of gases:

$$\xi_\mathrm{dh} = \left[\frac{T_\mathrm{k}}{\left(\sum x_i\cdot M_i\right)^3\cdot p_\mathrm{k}^4}\right]^{\frac{1}{6}} \tag{18}$$

The reduced density of a mixture of gases is calculated based on the average specific critical volume of particular components by means of a weighted mole fraction:

$$\rho'_\mathrm{r} = \rho\cdot\sum_i\left(x_i\cdot v_{\mathrm{k}i}\right) \tag{19}$$

### 3.3. Thermal conductivity of gases at high pressures

Thermal conductivity has the same properties as viscosity at low pressures. Its value is virtually unchanged with the changing pressure up to the pressure of 100 kPa. Thermal conductivity increases with the increasing pressure at a higher pressure (Heinrich, 1982).

Stiel and Thodos developed equations for different ranges of the reduced density based on the dimensional analysis:

$$\rho_\mathrm{r} \le 0.5 \qquad (\lambda-\lambda_0)\cdot\vartheta_d\cdot z_k^5 = 2.697\cdot 10^{-4}\cdot\left(e^{-0.535\cdot\rho_r} - 1\right) \tag{20}$$

$$0.5 < \rho_\mathrm{r} \le 2 \qquad (\lambda-\lambda_0)\cdot\vartheta_d\cdot z_k^5 = 2.523\cdot 10^{-4}\cdot\left(e^{0.67\cdot\rho_r} - 1.069\right) \tag{21}$$

$$2 < \rho_\mathrm{r} \le 2.8 \qquad (\lambda-\lambda_0)\cdot\vartheta_d\cdot z_k^5 = 0.5733\cdot 10^{-4}\cdot\left(e^{1.555\cdot\rho_r} - 2.016\right) \tag{22}$$

The relative error of these equations ranges from 10 to 20 %.

The dependence according to (Ullmann, 2005, Purcz, 2006) is an equation commonly used for calculation of the thermal conductivity of mixtures of gases of low density. It is in the form:

$$\lambda_{GM} = \sum_i \frac{\lambda_i}{1 + \sum_{j \neq i} 1.065 \cdot \Phi_{ij} \cdot \frac{x_j}{x_i}} \qquad (\mathrm{W \cdot m^{-1} \cdot K^{-1}}) \qquad (23)$$

The constant $\Phi_{ij}$ is defined by the formula:

$$\Phi_{ij} = \frac{\left[1 + \left(\frac{\eta_{0,i}}{\eta_{0,j}}\right)^{\frac{1}{2}} \cdot \left(\frac{M_j}{M_i}\right)^{\frac{1}{4}}\right]^2}{\sqrt{8} \cdot \left[1 + \frac{Mi}{Mj}\right]^{\frac{1}{2}}} \qquad (24)$$

## 3.4. Computation of the heat capacity and implementation of the multi-dimensional regression

The calculation of thermal capacity at higher pressures is based on the differential equation (Heinrich, 1980, Rajzinger, 2012, Purcz, 2001):

$$\left(\frac{\partial c_p}{\partial p}\right)_T = -T \cdot \left(\frac{\partial^2 v}{\partial T^2}\right)_p \qquad (\mathrm{m^3 \cdot kg^{-1} \cdot K^{-1}}) \qquad (25)$$

By equation integration, we receive a relation by which it is possible, at known courses of state quantities, to calculate the thermal capacity at high pressures in the form:

$$c_{p_2} = c_{p_1} - \int_{p_1}^{p_2} T \cdot \left(\frac{\partial^2 v}{\partial T^2}\right)_p \mathrm{d}p \qquad (\mathrm{J \cdot kg^{-1} \cdot K^{-1}}) \qquad (26)$$

With regard to the complexity of calculation of the compressibility factor needed for the calculation of specific volume and its second-order derivative according to the temperature at a constant pressure, it is favourable to use the numerical solution by means of Taylor expansion:

$$c_{p2} = c_{p1} - \frac{p_2 - p_1}{n} \cdot \sum_{j=1}^{n} T \cdot \left[\frac{v_{i-1} - 2 \cdot v_i + v_{i+1}}{(\Delta T)^2}\right]_{p_1 + j \cdot \frac{p_2 - p_1}{n}} \qquad (\mathrm{J \cdot kg^{-1} \cdot K^{-1}}) \qquad (27)$$

It is not possible to add an expression according to the relation (27) to the CFX simulation, as it requires to define only a simple function $c_p$ = f($p$,$T$). In case of creating dependence of the thermal capacity on pressure and temperature, it is necessary to analyse calculated values by multidimensional regression in the programme MPGM. For approximation of a physical quantity depending on pressure and temperature, a linear model was selected with a form of an approximated function:

$$c_p = a_1 + a_2 \cdot p + a_3 \cdot T + a_4 \cdot p \cdot T + a_5 \cdot p^2 + a_6 \cdot T^2 \qquad (\mathrm{J \cdot kg^{-1} \cdot K^{-1}}) \qquad (28)$$

After generating the table with calculated values of a physical quantity, the programme will calculate coefficients $a_1$ to $a_6$ on the basis of the method of least squares. By using this method, it is necessary to reach a minimum sum of squares of deviations between the real values and an approximated function given by the relation:

$$s = \sum (a_1 + a_2 \cdot p + a_3 \cdot T + a_4 \cdot p \cdot T + a_5 \cdot p^2 + a_6 \cdot T^2 - c_p)^2 \qquad (\mathrm{J^2 \cdot kg^{-2} \cdot K^{-2}}) \qquad (29)$$

In order to meet the condition of the least deviation $s$, it is necessary to differentiate the function according to all sought coefficients:

$$\frac{\partial s}{\partial a_\mathrm{i}} = 0 \qquad (30)$$

For example, it is possible to write for the coefficient $a_4$ on the basis of the relation (30):

$$\frac{\partial s}{\partial a_4} = 2 \cdot \sum (a_1 + a_2 \cdot p + a_3 \cdot T + a_4 \cdot p \cdot T + a_5 \cdot p^2 + a_6 \cdot T^2 - c_p) \cdot p \cdot T = 0 \qquad (31)$$

By differentiation and modification according to all coefficients $a_1$ to $a_6$, it is possible to create the system of linear equations written in the matrix form as follows:

$$\begin{vmatrix} n & \sum p & \sum T & \sum p \cdot T & \sum p^2 & \sum T^2 \\ \sum p & \sum p^2 & \sum p \cdot T & \sum p^2 \cdot T & \sum p^3 & \sum p \cdot T^2 \\ \sum T & \sum p \cdot T & \sum T^2 & \sum p \cdot T^2 & \sum p^2 \cdot T & \sum T^3 \\ \sum p \cdot T & \sum p^2 \cdot T & \sum p \cdot T^2 & \sum p^2 \cdot T^2 & \sum p^3 \cdot T & \sum p \cdot T^3 \\ \sum p^2 & \sum p^3 & \sum p^2 \cdot T & \sum p^3 \cdot T & \sum p^4 & \sum p^2 \cdot T^2 \\ \sum T^2 & \sum p \cdot T^2 & \sum T^3 & \sum p \cdot T^3 & \sum p^2 \cdot T^2 & \sum T^4 \end{vmatrix} \cdot \begin{vmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{vmatrix} = \begin{vmatrix} \sum c_p \\ \sum p \cdot c_p \\ \sum T \cdot c_p \\ \sum p \cdot T \cdot c_p \\ \sum p^2 \cdot c_p \\ \sum T^2 \cdot c_p \end{vmatrix} \qquad (32)$$

The MPGM software uses also a programme unit for matrix adjustment by means of Gauss method of elimination during calculation. Fig. 9 shows the thermal capacity for a particular gas mixture composition (30 % $H_2$, 30 % $N_2$, 40 % $CH_4$). The function (for range 0 to 300 °C and 1 to 10 MPa) was created by regression analysis in the form:

$$c_p = 2399 + 6.131 \cdot 10^{-7} \cdot p - 1.78 \cdot T + 2.2196 \cdot 10^{-8} \cdot p \cdot T + 5.919 \cdot 10^{-14} \cdot p^2 + 3.212 \cdot 10^{-3} \cdot T^2 \qquad (\mathrm{J \cdot kg^{-1} \cdot K^{-1}}) \quad (33)$$

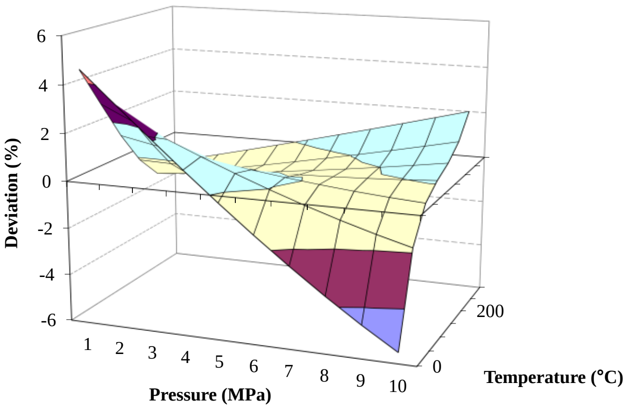


**Fig. 10.** Deviation between real and calculated value of the thermal capacity from regression analysis for the pressure range 1 to 10 MPa and the temperature range 0 to 300 °C

An average percentage deviation of calculated value cp according to (27) and (33) is on the level of 1 %. The least deviation is 5.2 %, and when the range of temperatures and pressures is decreasing at approximation, the accuracy is increasing.

If it is necessary to obtain mathematical dependence of thermal capacity for the pressure range from 1 to 3 MPa and for the temperature range from 0 to 60 °C, the deviation between real values and values from the regression analysis is only up to 0.5 % (Fig. 11). The least deviations at mean values are reached from the temperature and pressure range at used form of the regression function according to (28). Table 1 shows the regression coefficients a1 to a6 of other physical quantities for model gas composition (30 % H2, 30 % N2, 40 % CH4) and the range 0 to 300 °C and 1 to 10 MPa.

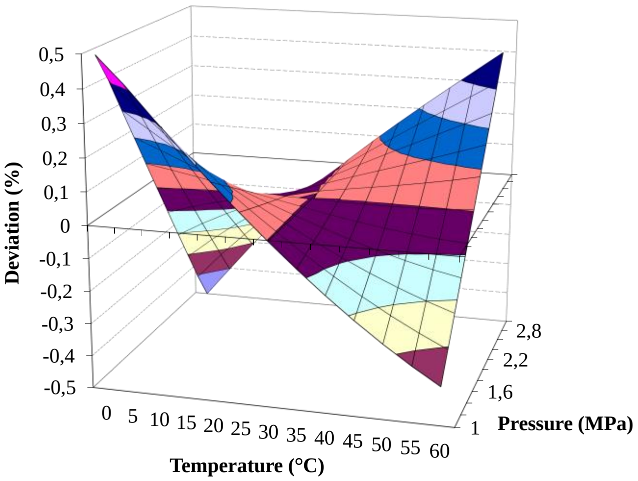


**Fig. 11.** Deviation between real and calculated value of the thermal capacity from regression analysis for the pressure range 1 to 3 MPa and the temperature range 0 to 60 °C

**Tab. 1.** Regression coefficients for selected physical quantities solved by the MPGM software

| Physical quantity | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ | $a_6$ |
|---|---|---|---|---|---|---|
| Dynamic viscosity ($kg \cdot m^{-1} \cdot s^{-1}$) | 4,554 | $5{,}401 \cdot 10^{-9}$ | $3{,}5025 \cdot 10^{-2}$ | $2{,}309 \cdot 10^{-10}$ | $4{,}257 \cdot 10^{-16}$ | $-8{,}7318 \cdot 10^{-6}$ |
| Compressibility factor (-) | 0,79994 | $-1{,}0102 \cdot 10^{-10}$ | $8{,}1263 \cdot 10^{-4}$ | $2{,}5849 \cdot 10^{-12}$ | $-1{,}1717 \cdot 10^{-17}$ | $-7{,}9707 \cdot 10^{-7}$ |
| Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$) | $17{,}99 \cdot 10^{-3}$ | $1{,}5527 \cdot 10^{-11}$ | $1{,}1709 \cdot 10^{-4}$ | $9{,}8254 \cdot 10^{-13}$ | $1{,}388 \cdot 10^{-18}$ | $6{,}9015 \cdot 10^{-8}$ |
| Thermal capacity ($J \cdot kg^{-1} \cdot K^{-1}$) | 2399 | $6{,}131 \cdot 10^{-7}$ | -1,78 | $2{,}2196 \cdot 10^{-8}$ | $5{,}919 \cdot 10^{-14}$ | $3{,}212 \cdot 10^{-3}$ |

It is possible to use such obtained courses of physical quantities for any gas mixture as input defining of material in the HTC-FC software. Export of equations directly into the file *.ccl* that is an input file of the ANSYS CFX programme enables the import of material properties of gas mixture. With regard to the fact that the simulation tool does not have to calculate material properties of each solved element for a long time, but it uses the approximation equations, the time needed for simulation gets short.

## 4. CONCLUSION

The introduction of numerical calculations into engineering method of solving various tasks becomes a necessary part of complex demands of the praxis. It is often necessary to realize solution in a relatively short time. I such a case, the designer engineer will welcome a supporting software that enables to facilitate and, especially, to speed up the whole process of solution of research as well as commercial tasks.

A full application of mentioned software requires its comprehensive treatment and tests at various types of set physical parameters. In case of the MPGM software, it is necessary to search approximation functions that describe physical properties of the gas mixtures better and more accurate and, therefore, minimize the deviations from real values.

**Notations:** $a_{1,2,..}$ – regression coefficients; $c_p$ – specific thermal capacity, $J \cdot kg^{-1} \cdot K^{-1}$; $c_{p1}$ – specific thermal capacity at $p_1$, $J \cdot kg^{-1} \cdot K^{-1}$; $c_{p2}$ – specific thermal capacity at $p_2$, $J \cdot kg^{-1} \cdot K^{-1}$; $n$ – number of integral divisions, 1; $p$ – pressure, Pa; $p_1$ – initial pressure, Pa; $p_2$ – final pressure, Pa; $R$ – universal gas constant, $J \cdot mol^{-1} \cdot K^{-1}$; $T$ – gas temperature, K; $T_s$ – surface temperature, K; $T_t$ – fluid temperature, K; $V$ – molar volume, $m^3 \cdot mol^{-1}$; $z$ – compressibility factor, 1; $v$ – specific volume, $m^3 \cdot kg^{-1}$; $\alpha$ – free convection HTC, $W \cdot m^{-2} \cdot K^{-1}$; $\alpha_c$ – total HTC, $W \cdot m^{-2} \cdot K^{-1}$; $\varepsilon$ – surface emissivity, 1; $\sigma$ – Stefan-Boltzmann constant, $W \cdot m^{-2} \cdot K^{-4}$; $\omega$ – acentric factor.

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