# Natural gas properties and flow computation 

Ivan Marić and Ivan Ivek<br>Ruđer Bošković Institute<br>Croatia

## 1. Introduction

Precise measurement of fluid flow rate is essential in commercial and in process control applications. The flow rate can be measured using different principles and devices (Baker, 2000, Miller, 1996): Orifice, Turbine, Venturi, Nozzle, Target, V-cone, Pitot, Multiport averaging, Elbow, Wedge, Laminar flow, Gilfo, Positive displacement, Thermal mass, Ultrasonic-time of flight, Variable area, Vortex, Coriolis. The measurement accuracy varies from $\pm 5 \%$ of rate (Pitot) down to $\pm 0.2 \%$ of rate (Coriolis). The Coriolis mass flowmeters are generally used to measure the mass flow of liquids but have been also used for the measurement of flow of high density gases. The turbine meters are widely used for the measurement of the volumetric flow rate of clean gases ( $\pm 0.5 \%$ of rate) and liquids ( $\pm 1 \%$ of rate). The flow rate measurements based on orifice meters are less accurate ( $1-2 \%$ URV) but the orifice plates are the most widely used devices in natural gas flow rate measurements due to their simplicity and robustness. We will here illustrate the thermodynamic effects that may cause significant error in measurements of natural gas flow rate based on orifice meters. We will also demonstrate how they could be efficiently compensated.
In measurements based on orifice plates the temperature of the fluid measured upstream of the orifice plate is used for the calculation of the flow rate but the fluid temperature is preferably measured downstream of the orifice plate (ISO-5167-1, 2003). When a gas is forced to flow through an orifice its temperature is changed due to the Joule-Thomson (JT) effect. The effect can be generally neglected for low flow rates i.e. for low differential pressures measured across the orifice meter (ISO-5167-1, 2003). At higher differential pressures and at lower temperatures the flow rate error increases and generally needs to be compensated (Marić, 2007). The precise compensation of flow rate error implies double calculation of natural gas properties and the flow rate, which extends the calculation time significantly and may become impractical for implementation in low-computing-power embedded systems. To avoid the computational burden the original high complexity models of natural gas properties can be replaced by the corresponding low-complexity surrogate models (Marić \& Ivek, IEEE, Marić \& Ivek, 2010) with no significant deterioration of flow rate accuracy.
Comprehensive presentation of modern methods of estimating the physical properties of gases and liquids can be found in (Poling at al., 2000). Formulations explicit in the Helmholtz energy have been widely used to represent the properties of natural gas because of the ease of calculating all other thermodynamic properties by mathematical
differentiation (Lemmon \& Starling, 2003, Span \& Wagner, 1996, Span \& Wagner, 2003). The Helmholtz energy is a fundamental thermodynamic property from which all other thermodynamic properties can be calculated as derivatives with respect to molar density or temperature. The detailed procedure for the calculation of thermodynamic properties based on formulations explicit in Helmholtz energy (Lemmon \& Starling, 2003) and on AGA-8 detail characterization equation (Starling \& Savidge, 1992) is given in (ISO-207651-1, 2005). Here we will elaborate an alternative procedure for the calculation of properties of a natural gas that was originally published in the Journal Flow Measurement and Instrumentation (Marić, 2005 \& 2007). The procedure is derived using fundamental thermodynamic equations (Olander, 2007), DIPPR AIChE (DIPPR® Project 801, 2005) generic ideal heat capacity equations, and AGA-8 (Starling \& Savidge, 1992) extended virial-type equations of state. The procedure specifies the calculation of specific heat capacities at a constant pressure $c_{p}$ and at a constant volume $c_{v}$, the JT coefficient $\mu_{I T}$, and the isentropic exponent $\kappa$ of a natural gas. The effect of a JT expansion on the accuracy of natural gas flow rate measurements will be pointed out.
The possibilities of using the computational intelligence methods - Artificial Neural Networks - ANNs (Ferrari \& Stengel, 2005, Wilamowski et al., 2008) and machine learning tools - Group Method of Data Handling - GMDH (Ivakhnenko, 1971, Nikolaev \& Iba, 2003) for meta-modeling the effects of natural gas properties in flow rate measurements (Marić \& Ivek, 2010) will be illustrated. The practical examples of ANN and GMDH surrogate models for the compensation of natural gas flow rate measurement error caused by the thermodynamic effects, with the corresponding accuracies and execution times will be given. The models are particularly suitable for implementation in low computing power embedded systems.

## 2. A procedure for the calculation of thermodynamic properties of natural gas

This section summarizes the procedure (Maric, 2007) for the calculation of specific heat capacity at constant pressure $c_{\mathrm{p}}$ and at constant volume $c_{\mathrm{V}}$, JT coefficient $\mu_{\mathrm{JT}}$ and isentropic exponent $\kappa$ of a natural gas based on thermodynamic equations, AGA- 8 extended virial type characterization equation (Starling \& Savidge, 1992, ISO-12213-2, 2006) and DIPPR generic ideal heat capacity equations (DIPPR ${ }^{\circledR}$ Project 801, 2005). First, the relation of the molar heat capacity at constant volume to equation of state will be derived. Then the relation will be used to calculate a molar heat capacity at constant pressure, which will be then used for the calculation of the JT coefficient and the isentropic exponent. The total differential for entropy (Olander, 2007), related to temperature and molar volume, is:

$$
\begin{equation*}
d s=\left(\frac{\partial s}{\partial T}\right)_{v_{m}} d T+\left(\frac{\partial s}{\partial v_{m}}\right)_{T} d v_{m} \tag{1}
\end{equation*}
$$

where $s$ denotes entropy, $T$ denotes temperature and $v_{m}$ is a molar volume of a gas. By dividing the fundamental differential for internal energy $d u=T \cdot d s-p \cdot d v_{m}$ by $d T$ while holding $v_{m}$ constant the coefficient of $d T$ in Eq. (1) becomes $c_{m, v} / T$ since the molar heat at constant volume is defined by $c_{m, v}=(\partial u / \partial T)_{v_{m}}$. The Maxwell relation
$\left(\partial s / \partial v_{m}\right)_{T}=(\partial p / \partial T)_{v_{m}}$, is used to substitute the coefficient of $d v_{m}$. Finally, the Eq. (1) becomes:

$$
\begin{equation*}
d s=\frac{c_{m, v}}{T} d T+\left(\frac{\partial p}{\partial T}\right)_{v_{m}} d v_{m} \tag{2}
\end{equation*}
$$

Similarly, starting from a total differential for entropy related to temperature and pressure (Olander, 2007) $d s=(\partial S / \partial T)_{p} d T+(\partial S / \partial p)_{T} d p$ and by dividing the fundamental differential for enthalpy $d h=T \cdot d s+v_{m} \cdot d p$ by $d T$ while holding $p$ constant, the coefficient of $d T$ in total differential becomes $c_{m, p} / T$ since the molar heat capacity at constant pressure is defined by: $c_{m, p}=(\partial h / \partial T)_{p}$. The Maxwell relation $(\partial s / \partial p)_{T}=\left(\partial v_{m} / \partial T\right)_{p}$ is used to substitute the coefficient of $d p$ and the following relation is obtained:

$$
\begin{equation*}
d s=\frac{c_{m, p}}{T} d T+\left(\frac{\partial v_{m}}{\partial T}\right)_{p} d p \tag{3}
\end{equation*}
$$

Subtracting Eq. (2) from Eq. (3), then dividing the resulting equation by $d v_{m}$ while holding $p$ constant and finally inverting the partial derivative $\left(\partial T / \partial v_{m}\right)_{p}$ the following equation is obtained:

$$
\begin{equation*}
c_{m, p}-c_{m, v}=T\left(\frac{\partial v_{m}}{\partial T}\right)_{p}\left(\frac{\partial p}{\partial T}\right)_{v_{m}} \tag{4}
\end{equation*}
$$

A total differential of thermodynamic property, Eqs. (2) and (3), must be the exact differential i.e. the order of forming the mixed second derivative is irrelevant. The partial derivative of the first coefficient with respect to the second variable equals to the partial derivative of the second coefficient with respect to the first variable. By applying this property to Eq. (2) and by assuming $T$ to be the first variable with the corresponding coefficient $c_{m, v} / T$ and $v_{m}$ the second variable with the corresponding coefficient $(\partial p / \partial T)_{v_{m}}$ we obtain:

$$
\begin{equation*}
\left(\frac{\partial c_{m, v}}{\partial v_{m}}\right)_{T}=T\left(\frac{\partial^{2} p}{\partial T^{2}}\right)_{v_{m}} \tag{5}
\end{equation*}
$$

The Eq. (5) can be rewritten in the following integral form:

$$
\begin{equation*}
c_{m, v}=c_{m, v I}+T \int_{v_{m I} \rightarrow \infty(T=\text { const })}^{v_{m}}\left(\frac{\partial^{2} p}{\partial T^{2}}\right)_{v_{m}} d v_{m} \tag{6}
\end{equation*}
$$

where $c_{m, v I}, v_{m I}$ and $v_{m}$ denote the ideal molar heat capacity at constant volume and the corresponding molar volume of ideal and real gas at temperature $T$. Real gases behave more like ideal gases as pressure approaches zero or $v_{m I} \rightarrow \infty$. After substituting $v_{m}=1 / \rho_{m}$, $p=R T Z \rho_{m}$ and $c_{m, v I}=c_{m, p I}-R$ the Eq. (6) transforms to:

$$
\begin{equation*}
c_{m, v}=c_{m, p I}-R-R T \int_{\rho_{m I} \rightarrow 0(T=c o n s t)}^{\rho_{m}} \frac{1}{\rho_{m}}\left(2\left(\frac{\partial Z}{\partial T}\right)_{\rho_{m}}+T\left(\frac{\partial^{2} Z}{\partial T^{2}}\right)_{\rho_{m}}\right) d \rho_{m} \tag{7}
\end{equation*}
$$

where $c_{m, p I}$ denotes the temperature dependent molar heat capacity of ideal gas at constant pressure, $R$ is the universal gas constant, $Z$ is the compression factor and $\rho_{m I}$ and $\rho_{m}$ are the corresponding molar densities of ideal and real gas at temperature T. After substituting the first and the second derivative of the AGA-8 compressibility equation (Starling \& Savidge, 1992, ISO-12213-2, 2006)

$$
\begin{equation*}
Z=1+B \rho_{m}-\rho_{r} \sum_{n=13}^{18} C_{n}^{*}+\sum_{n=13}^{58} C_{n}^{*}\left(b_{n}-c_{n} k_{n} \rho_{r}^{k_{n}}\right) \rho_{r}^{b_{n}} e^{-c_{n} \rho_{r}^{k_{n}}} \tag{8}
\end{equation*}
$$

into the Eq. (7) and after integration we obtain

$$
\begin{equation*}
c_{m, v}=c_{m, p I}-R+R T \rho_{r}\left(2 C_{0}+T C_{1}-C_{2}\right) \tag{9}
\end{equation*}
$$

with

$$
\begin{gather*}
C_{0}=\sum_{n=13}^{18} C_{n}^{*^{\prime}}-\frac{B^{\prime}}{K^{3}},  \tag{10}\\
C_{1}=\sum_{n=13}^{18} C_{n}^{*^{\prime \prime}}-\frac{B^{\prime \prime}}{K^{3}},  \tag{11}\\
C_{2}=\sum_{n=13}^{58}\left(2 C_{n}^{*^{\prime}}+T C_{n}^{*^{\prime \prime}}\right) \rho_{r}^{b_{n}-1} e^{-c_{n} \rho_{r}^{k_{n}}}, \tag{12}
\end{gather*}
$$

where $\rho_{r}$ is the reduced density $\left(\rho_{r}=K^{3} \rho_{m}\right), B$ is the second virial coefficient, $\left\{C_{n}^{*}\right\}$ are the temperature dependent coefficients, $K$ is the mixture size parameter while $\left\{b_{n}\right\},\left\{c_{n}\right\}$ and $\left\{k_{n}\right\}$ are the equation of state parameters. The mixture size parameter $K$ is calculated using the following equation (ISO-12213-2, 2006):

$$
\begin{equation*}
K^{5}=\left(\sum_{i=1}^{N} y_{i} K_{i}^{5 / 2}\right)^{2}+2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} y_{i} y_{j}\left(K_{i j}^{5}-1\right)\left(K_{i} K_{j}\right)^{5 / 2} \tag{13}
\end{equation*}
$$

where $y_{i}$ denotes the molar fraction of the component $i$, while $\left\{K_{i}\right\}$ and $\left\{K_{i j}\right\}$ are the corresponding size parameters and the binary interaction parameters given in [ISO-12213-2, 2006]. According to (ISO-12213-2, 2006) the second virial coefficient is calculated using the following equation:

$$
\begin{equation*}
B=\sum_{n=1}^{18} a_{n} T^{-u_{n}} \sum_{i=1}^{N} \sum_{j=1}^{N} y_{i} y_{j} B_{n i j}^{*} E_{i j}^{u_{n}}\left(K_{i} K_{j}\right)^{3 / 2}, \tag{14}
\end{equation*}
$$

and the coefficients $\left\{B_{n i j}^{*}\right\},\left\{E_{i j}\right\}$ and $\left\{G_{i j}\right\}$ are defined by

$$
\begin{gather*}
B_{n i j}^{*}=\left(G_{i j}+1-g_{n}\right)^{g_{n}}\left(Q_{i} Q_{j}+1-q_{n}\right)^{q_{n}}\left(F_{i}^{1 / 2} F_{j}^{1 / 2}+1-f_{n}\right)^{f_{n}}, \\
\cdot\left(S_{i} S_{j}+1-s_{n}\right)^{s_{n}}\left(W_{i} W_{j}+1-w_{n}\right)^{w_{n}}  \tag{15}\\
E_{i j}=E_{i j}^{*}\left(E_{i} E_{j}\right)^{1 / 2}, \tag{16}
\end{gather*}
$$

and

$$
\begin{equation*}
G_{i j}=G_{i j}^{*}\left(G_{i}+G_{j}\right) / 2, \tag{17}
\end{equation*}
$$

where $T$ is temperature, $N$ is the total number of gas mixture components, $y_{i}$ is the molar fraction of the component $i,\left\{a_{n}\right\},\left\{f_{n}\right\},\left\{g_{n}\right\},\left\{q_{n}\right\},\left\{s_{n}\right\},\left\{u_{n}\right\}$, and $\left\{w_{n}\right\}$ are the equation of state parameters, $\left\{E_{i}\right\},\left\{F_{i}\right\},\left\{G_{i}\right\},\left\{K_{i}\right\},\left\{Q_{i}\right\},\left\{S_{i}\right\}$ and $\left\{W_{i}\right\}$ are the corresponding characterization parameters while $\left\{E_{i j}^{*}\right\}$ and $\left\{G_{i j}^{*}\right\}$ are the corresponding binary interaction parameters. The main symbols and units are given in Table 1.
The temperature dependent coefficients $\left\{C_{n}^{*} ; n=1, \ldots, 58\right\}$ and the mixture parameters $U, G$, $Q$ and $F$ are calculated using the equations (ISO-12213-2, 2006):

$$
\begin{equation*}
C_{n}^{*}=a_{n}\left(G+1-g_{n}\right)^{g_{n}}\left(Q^{2}+1-q_{n}\right)^{q_{n}}\left(F+1-f_{n}\right)^{f_{n}} U^{u_{n}} T^{-u_{n}} \tag{18}
\end{equation*}
$$

| Symbols and units |  |  |
| :---: | :---: | :---: |
| Symbol | Description | Unit |
| B | Second virial coefficient | $\mathrm{m}^{3 *} \mathrm{kmol}^{-1}$ |
| $B_{n i j}^{*}$ | Mixture interaction coefficient | - |
| C | Coefficient of discharge | - |
| $c_{m, p}$ | Molar heat capacity at constant pressure | $\mathrm{J} /(\mathrm{mol} \cdot \mathrm{K})$ |
| $c_{m, v}$ | Molar heat capacity at constant volume | $\mathrm{J} /(\mathrm{mol} \cdot \mathrm{K})$ |
| $\mathrm{C}_{n}^{*}$ | Temperature and composition dependent coefficients | - |
| $c_{n}$ | AGA-8 equation of state parameter | - |
| $c_{p}$ | Specific heat capacity at constant pressure | $\mathrm{J} /(\mathrm{kg} \cdot \mathrm{K})$ |
| $c_{m, p I}$ | Ideal molar heat capacity of the natural gas mixture | $\mathrm{J} /(\mathrm{mol} \cdot \mathrm{K})$ |
| $c_{m, p i}^{j}$ | Ideal molar heat capacity of the gas component $j$ | $\mathrm{J} /(\mathrm{mol} \mathrm{K})$ |
| D | Upstream internal pipe diameter | m |
| $d$ | Diameter of orifice | m |
| $h$ | Specific enthalpy | J/kg |
| K | Size parameter | - |
| M | Molar mass of the gas mixture | kg kmol ${ }^{-1}$ |
| $p$ | Absolute pressure | Pa |
| $q$ | Mass flow rate | kg/s |
| R | Molar gas constant 8314.51 | $\mathrm{J} /(\mathrm{kmol} \mathrm{K})$ |
| $s$ | Specific entropy | J/(kg K) |
| T | Absolute temperature | K |
| $v_{m}$ | Molar specific volume | $\mathrm{m}^{3} / \mathrm{kmol}$ |
| $v_{m I}$ | Molar specific volume of ideal gas | $\mathrm{m}^{3} / \mathrm{kmol}$ |
| $y_{i}$ | Molar fraction of $i$-th component in gas mixture | - |
| Z | Compression factor | - |
| $\beta$ | Diameter ratio d/D | - |
| $\Delta p$ | Differential pressure | Pa |
| $\Delta \omega$ | Pressure loss | Pa |
| $\kappa$ | Isentropic exponent | - |
| $\mu_{J T}$ | Joule-Thomson coefficient | K/Pa |
| $\rho_{m}$ | Molar density | $\mathrm{kmol} / \mathrm{m}^{3}$ |
| $\rho_{m I}$ | Molar density of ideal gas | $\mathrm{kmol} / \mathrm{m}^{3}$ |
| $\rho_{r}$ | Reduced density | - |

Table 1. Symbols and units (for additional symbols and units refer to (ISO-12213-2, 2006).

$$
\begin{gather*}
U^{5}=\left(\sum_{i=1}^{N} y_{i} E_{i}^{5 / 2}\right)^{2}+2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} y_{i} y_{j}\left(U_{i j}^{5}-1\right)\left(E_{i} E_{j}\right)^{5 / 2},  \tag{19}\\
G=\sum_{i=1}^{N} y_{i} G_{i}+2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} y_{i} y_{j}\left(G_{i j}^{*}-1\right)\left(G_{i}+G_{j}\right),  \tag{20}\\
Q=\sum_{i=1}^{N} y_{i} Q_{i}, \tag{21}
\end{gather*}
$$

and

$$
\begin{equation*}
F=\sum_{i=1}^{N} y_{i}^{2} F_{i} \tag{22}
\end{equation*}
$$

where, $U_{i j}$ is the binary interaction parameter for mixture energy. The first and the second derivatives of the coefficients $B$ and $C_{n}^{*}$, with respect to temperature are:

$$
\begin{gather*}
B^{\prime}=-\sum_{n=1}^{18} a_{n} u_{n} T^{-u_{n}-1} \sum_{i=1}^{N} \sum_{j=1}^{N} y_{i} y_{j} B_{n i j}^{*} E_{i j}^{u_{n}}\left(K_{i} K_{j}\right)^{3 / 2},  \tag{23}\\
B^{\prime \prime}=\sum_{n=1}^{18} a_{n} u_{n}\left(u_{n}+1\right) T^{-u_{n}-2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_{i} y_{j} B_{n i j}^{*} E_{i j}^{u_{n}}\left(K_{i} K_{j}\right)^{3 / 2},  \tag{24}\\
C_{n}^{*^{\prime}}=-\frac{u_{n}}{T} C_{n}^{*},  \tag{25}\\
C_{n}^{*^{\prime \prime}}=-\frac{u_{n}+1}{T} C_{n}^{*^{\prime}}, \tag{26}
\end{gather*}
$$

The ideal molar heat capacity $c_{p I}$ is calculated by

$$
\begin{equation*}
c_{m, p I}=\sum_{j=1}^{N} y_{j} c_{m, p i}^{j}, \tag{27}
\end{equation*}
$$

where $y_{j}$ is the molar fraction of component $j$ in the gas mixture and $c_{m, p i}^{j}$ is the molar heat capacity of the same component. The molar heat capacities of the ideal gas mixture components can be approximated by DIPPR/AIChE generic equations (DIPPR ${ }^{\circledR}$ Project 801, 2005), i.e.

$$
\begin{equation*}
c_{m, p i}^{j}=a_{j}+b_{j}\left(\frac{c_{j} / T}{\sinh \left(c_{j} / T\right)}\right)^{2}+d_{j}\left(\frac{e_{j} / T}{\cosh \left(e_{j} / T\right)}\right)^{2} \tag{28}
\end{equation*}
$$

where $c_{m, p i}^{j}$ is the molar heat capacity of the component $j$ of the ideal gas mixture, $a_{j}, b_{j}$, $c_{j}, d_{j}$ and $e_{j}$ are the corresponding constants, and $T$ is the temperature.

The partial derivative of pressure with respect to temperature at constant molar volume and the partial derivative of molar volume with respect to temperature at constant pressure are defined by the equations:

$$
\begin{equation*}
\left(\frac{\partial p}{\partial T}\right)_{v_{m}}=R \rho_{m}\left[Z+T\left(C_{3}-\rho_{r} C_{0}\right)\right] \tag{29}
\end{equation*}
$$

and

$$
\begin{equation*}
\left(\frac{\partial v_{m}}{\partial T}\right)_{p}=\frac{R}{p}\left[Z+\left(\frac{\partial Z}{\partial T}\right)_{p} T\right], \tag{30}
\end{equation*}
$$

where,

$$
\begin{gather*}
C_{3}=\sum_{n=13}^{58}\left(C_{n}^{*^{\prime}} D_{n}^{*}\right),  \tag{31}\\
D_{n}=\left(b_{n}-c_{n} k_{n} \rho_{r}^{k_{n}}\right) \rho_{r}^{b_{n}} e^{-c_{n} \rho_{r}^{k_{n}},}  \tag{32}\\
\left(\frac{\partial Z}{\partial T}\right)_{p}=\frac{R(T Z)^{2} C_{3}-p Z\left[T K^{3} C_{0}+C_{4}\right]}{R(T Z)^{2}+p T C_{4}},  \tag{33}\\
C_{4}=C_{5}+\sum_{n=13}^{58} C_{n}^{*} D_{1 n},  \tag{34}\\
C_{5}=B-K^{3} \sum_{n=13}^{18} C_{n}^{*} \tag{35}
\end{gather*}
$$

and

$$
\begin{equation*}
D_{1 n}=K^{3}\left[b_{n}^{2}-c_{n} k_{n}\left(2 b_{n}+k_{n}-c_{n} k_{n} \rho_{r}^{k_{n}}\right) \rho_{r}^{k_{n}} \rho_{r}^{b_{n}-1} e^{-c_{n} \rho_{r}^{k_{n}}}\right. \tag{36}
\end{equation*}
$$

The isentropic exponent is defined by the following relation

$$
\begin{equation*}
\kappa=-\frac{c_{m, p}}{c_{m, v}}\left(\frac{\partial p}{\partial v_{m}}\right)_{T}\left(\frac{v_{m}}{p}\right)=-\frac{c_{m, p}}{c_{m, v} \rho_{m} p}\left(\frac{\partial p}{\partial v_{m}}\right)_{T} \tag{37}
\end{equation*}
$$

where

$$
\begin{equation*}
\left(\frac{\partial p}{\partial v_{m}}\right)_{T}=\left(\frac{\partial p}{\partial \rho_{m}}\right)_{T}\left(\frac{\partial \rho_{m}}{\partial v_{m}}\right)_{T}=-R T \rho_{m}^{2}\left(Z+\rho_{m} C_{4}\right) \tag{38}
\end{equation*}
$$

The JT coefficient is defined by the following equation:

$$
\begin{equation*}
\mu_{J T}=\frac{R T^{2}}{p c_{m, p}}\left(\frac{\partial Z}{\partial T}\right)_{p} \tag{39}
\end{equation*}
$$

The derivation of the Eq. (39) is elaborated in (Olander, 2007 \& Maric, 2005).

## 3. Implementation in software

The procedure for the calculation of natural gas density, compression, molar heat capacity, isentropic exponent and the JT coefficient can be implemented in object oriented paradigm, which enables its easy integration into the software projects. The interface to the software object $S$ is shown in Fig. 1. The input/output parameters and functions are accessible while the internal structure is hidden to the user. The function "Calculate" maps the input parameters (pressure, temperature and the molar fractions of natural gas components) into the output parameters (density, compression, molar heat capacity, isentropic exponent, JT coefficient, etc.).


Fig. 1. Interface to the software object, which implements the calculation of natural gas properties.

Table 2 depicts the calculation procedure. Prior to the calculation of the molar heat capacities, isentropic exponent and JT coefficient, the density and the compression factor of a natural gas must be calculated. The false position method is combined with the successive bisection method to calculate the roots of the equation of state [Starling \& Savidge, 1992].

## Input parameters - constant:

- molar gas constant $(R=8314.51 \mathrm{~J} /(\mathrm{kmol} \cdot \mathrm{K}))$
- natural gas equation of state parameters $\left(a_{n}, b_{n}, c_{n}, k_{n}, u_{n}, g_{n}, q_{n}, f_{n}, s_{n}, w_{n} ; n=1,2, \ldots, 58\right)$, characterization parameters $\left(M_{i}, E_{i}, K_{i}, G_{i}, Q_{i}, F_{i}, S_{i}, W_{i} ; i=1, \ldots, 21\right)$ and binary interaction parameters $\left(E_{i, j}^{*}, U_{i, j}, K_{i, j}, G_{i, j}^{*}\right)$ (see ISO 12213-2)
- DIPPR/AIChE gas heat capacity constants $\left(a_{j}, b_{j}, c_{j}, d_{j}, e_{j} ; j=1,2, \ldots, \mathrm{~N}\right)$

Input parameters - time varying:

- absolute pressure: $p$ [MPa]
- absolute temperature: $T[\mathrm{~K}]$
- molar fractions of the natural gas mixture: $y_{i} ; i=1,2, \ldots, \mathrm{~N}$


## Calculation procedure:

1. mixture size parameter $K$ (Eq. 13), second virial coefficient $B$ (Eq. 14) and temperature dependent coefficients $C_{n}^{*}$ (Eq. 18)
2. compression factor $Z$ (Eq. 8) (see ISO-12213-2 for details of calculation)
3. molar density $\rho_{m}=p / R T Z$, density $\rho=M \rho_{m}$, reduced density $\rho_{r}=K^{3} \rho_{m}$ and molar volume $v_{m}=1 / \rho_{m}$.
4. coefficients $D_{n}$ and $D_{1 n}$ (Eqs. 32 and 36)
5. $1^{\text {st }}$ and $2^{\text {nd }}$ derivative of the second virial coefficient $B: B^{\prime}$ (Eq. 23) and $B^{\prime \prime}$ (Eq. 24)
6. $1^{\text {st }}$ and $2^{\text {nd }}$ derivative of the coefficient $C_{n}^{*}: C_{n}^{*}$ (Eq. 25) and $C_{n}^{*}$ (Eq. 26)
7. $1^{\text {st }}$ derivative of the compression factor $\mathrm{Z}:(\partial Z / \partial T)_{p}$ (Eq. 33)
8. partial derivatives of pressure: $(\partial p / \partial T)_{v_{m}}$ (Eq. 29) and $\left(\partial p / \partial v_{m}\right)_{T}$ (Eq. 38)
9. ideal molar heat capacity of a gas mixture at constant pressure: $c_{m, p I}$ (Eq. 27)
10. molar heat capacity of a gas mixture at constant volume: $c_{m, v}$ (Eqs. 9)
11. molar heat capacity of a gas mixture at constant pressure: $c_{m, p}$ (Eqs. 4)
12. isentropic exponent $\kappa$ (Eq. 37)
13. Joule-Thomson coefficient $\mu_{J T}$ (Eq. 39)

Table 2. The input/output parameters and the procedure for the computation of the natural gas properties.

## 4. Comparison with experimental results

In order to compare the calculation results, for the specific heat capacity $c_{p}$ and the JT coefficient $\mu_{J T}$, with the corresponding high accuracy measurement data (Ernst et al., 2001), we assume the identical artificial natural gas mixture with the following mole fractions: $x_{\mathrm{CH} 4}=0.79942, x_{\mathrm{C} 2 \mathrm{H} 6}=0.05029, x_{\mathrm{C} 3 \mathrm{H} 8}=0.03000, x_{\mathrm{CO} 2}=0.02090$ and $x_{\mathrm{N} 2}=0.09939$. The results of the measurements (Ernst et al., 2001) and the results of the calculation of the specific heat capacity $c_{p}$ and the JT coefficient $\mu_{J T}$ of the natural gas mixture, for absolute pressure ranging from 0 MPa to 30 MPa in 0.5 MPa steps and for four upstream temperatures ( 250 K , $275 \mathrm{~K}, 300 \mathrm{~K}$ and 350 K ), are shown in Fig. 2 and 3, respectively. The differences between the calculated values and the corresponding measurement results (Ernst et al., 2001), for the $c_{p}$ and $\mu_{J T}$, are shown in Table 3 and 4, respectively.


Fig. 2. Calculated and measured molar heat capacity at constant pressure of the natural gas mixture.

From Table 3 it can be seen that the calculated values of $c_{p}$ are within $\pm 0.08 \mathrm{~J} /\left(\mathrm{g}^{*} \mathrm{~K}\right)$ with the measurement results for the pressures up to 12 MPa . At higher pressures, up to 30 MPa , the difference increases but never exceeds $\pm 0.2 \mathrm{~J} /\left(\mathrm{g}^{*} \mathrm{~K}\right)$. For pressures up to 12 MPa the relative difference between the calculated and experimentally obtained $c_{p}$ never exceeds $\pm 2.00 \%$.


Fig. 3. Calculated and measured JT coefficient of the natural gas mixture.

| $\mathrm{P}[\mathrm{MPa}: \mathrm{T}[\mathrm{K}]$ | 250 | 275 | 300 | 350 |
| ---: | ---: | ---: | ---: | ---: |
| 0.5 | -0.015 | $\left(c_{\left.\text {p_calculated }-c_{\text {p_measured }}\right)\left[\mathrm{J} /\left(\mathrm{g}^{*} \mathrm{~K}\right)\right]}\right.$ |  |  |
| 1.0 | -0.018 | -0.018 | -0.012 |  |
| 2.0 | -0.012 | -0.014 | -0.016 | -0.011 |
| 3.0 | -0.032 | -0.019 | -0.022 | -0.020 |
| 4.0 | -0.041 | -0.020 | -0.023 | -0.026 |
| 5.0 | -0.051 | -0.023 | -0.021 | -0.027 |
| 7.5 | -0.055 | -0.032 | -0.025 | -0.029 |
| 10.0 | -0.077 | -0.033 | - | - |
| 11.0 | -0.075 | - | -0.048 | -0.042 |
| 12.5 | -0.092 | -0.030 | - | - |
| 13.5 | -0.097 | -0.039 | - | - |
| 15.0 | -0.098 | -0.033 | - | - |
| 16.0 | - | -0.036 | -0.082 | -0.069 |
| 17.5 | - | -0.043 | - | - |
| 20.0 | -0.081 | -0.048 | -0.075 | - |
| 25.0 | -0.082 | -0.033 | -0.066 | -0.134 |
| 30.0 | -0.077 | -0.025 | -0.070 | -0.171 |

Table 3. Difference between the calculated and measured specific heat capacity at constant pressure of a natural gas.

| $\mathrm{P}[\mathrm{MPa}]: \mathrm{T}[\mathrm{K}]$ | 250 | 275 | 300 | 350 |
| ---: | ---: | ---: | ---: | ---: |
|  | $\left(\mu_{\text {JT_calculated }}-\mu_{\text {JT_measured }}[\mathrm{K} / \mathrm{MPa}]\right.$ |  |  |  |
| 0.5 | -0.014 | -0.023 | -0.075 | -0.059 |
| 1.0 | -0.032 | -0.024 | -0.068 | -0.053 |
| 2.0 | - | - | - | -0.051 |
| 3.0 | -0.092 | -0.032 | -0.069 | -0.049 |
| 5.0 | -0.022 | -0.036 | -0.044 | -0.026 |
| 7.5 | 0.043 | - | - | - |
| 10.0 | 0.060 | 0.096 | 0.019 | 0.030 |
| 12.5 | 0.034 | - | - | - |
| 15.0 | 0.113 | 0.093 | 0.050 | 0.061 |
| 20.0 | 0.029 | 0.084 | 0.009 | 0.047 |
| 25.0 | 0.025 | 0.059 | 0.002 | 0.043 |
| 30.0 | 0.031 | 0.052 | 0.005 | 0.012 |

Table 4. Difference between the calculated and measured JT coefficient of a natural gas.


Fig. 4. Calculated isentropic exponent of the natural gas mixture.
From Table 4 it can be seen that the calculated values of $\mu_{J T}$ are within $\pm 0.113 \mathrm{~K} / \mathrm{MPa}$ with the experimental results for the pressures up to 30 MPa . The relative difference increases with the increase of pressure but never exceeds $\pm 2.5 \%$ for the pressures up to 12 MPa . At higher pressures, when the values of $\mu_{J T}$ are close to zero, the relative difference may increase significantly. The calculation results obtained for pure methane and methaneethane mixture are in considerably better agreement with the corresponding experimental data (Ernst et al., 2001) than for the natural gas mixture shown above. We estimate that the relative uncertainty of the calculated $c_{p}$ and $\mu_{J T}$ of the AGA-8 natural gas mixtures in common industrial operating conditions (pressure range $0-12 \mathrm{MPa}$ and temperature range
$250-350 \mathrm{~K}$ ) is unlikely to exceed $\pm 3.00 \%$ and $\pm 4.00 \%$, respectively. Fig. 4 shows the results of the calculation of the isentropic exponent. Since the isentropic exponent is a theoretical parameter there exist no experimental data for its verification.

## 5. Flow rate measurement

Flow rate equations for differential pressure meters assume a constant fluid density of a fluid within the meter. This assumption applies only to incompressible flows. In the case of compressible flows, a correction must be made. This correction is known as adiabatic expansion factor, which depends on several parameters including differential pressure, absolute pressure, pipe inside diameter, differential device bore diameter and isentropic exponent. Isentropic exponent has a limited effect on the adiabatic correction factor but has to be calculated if accurate flow rate measurements are needed.


Fig. 5. The schematic diagram of the natural gas flow rate measurement using an orifice plate with corner taps.

When a gas expands through the restriction to a lower pressure it changes its temperature and density (Fig. 5). This process occurs under the conditions of constant enthalpy and is known as JT expansion (Shoemaker at al., 1996). It can also be considered as an adiabatic effect because the pressure change occurs too quickly for significant heat transfer to take place. The temperature change is related to pressure change and is characterized by the JT coefficient. The temperature change increases with the increase of the pressure drop and is proportional with the JT coefficient. According to (ISO5167, 2003) the upstream temperature is used for the calculation of flow rate but the temperature is preferably measured downstream of the differential device. The use of downstream instead of upstream temperature may cause a flow rate measurement error due to the difference in the gas density caused by the temperature change. Our objective is to derive the numerical procedure for the calculation of the natural gas specific heat capacity, isentropic exponent and JT coefficient that can be used for the compensation of flow rate error. In order to make the computationally intensive compensation procedure applicable to low computing power real-time measurement systems the low complexity surrogate models of original procedures will be derived using the computational intelligence methods: ANN and GMDH. The
surrogate models have to be tailored to meet the constraints imposed on the approximation accuracy and the complexity of the model, i.e. the execution time (ET).

## 6. Compensation of flow rate error

We investigated the combined effect of the JT coefficient and the isentropic exponent of a natural gas on the accuracy of flow rate measurements based on differential devices. The measurement of a natural gas (ISO-12213-2, 2006) flowing in a pipeline through orifice plate with corner taps (Fig. 5) is assumed to be completely in accordance with the international standard (ISO-5167, 2003). The detailed description of the flow rate equation with the corresponding iterative computation scheme is given in (ISO-5167, 2003). The calculation of the natural gas flow rate depends on multiple parameters:

$$
\begin{equation*}
q_{u}=q\left(P_{u}, T_{u}, \Delta p, \rho_{u}, \gamma_{u}, \kappa_{u}, D, d\right) \tag{40}
\end{equation*}
$$

where $q_{u}, \rho_{u}, \gamma_{u}$ and $\kappa_{u}$ represent the corresponding mass flowrate, density, viscosity and the isentropic exponent calculated at upstream pressure $P_{u}$ and temperature $T_{u}$, while $D$ and $d$ denote the internal diameters of the pipe and the orifice, respectively. In case of the upstream pressure and the downstream temperature measurement, as suggested by (ISO5167,2003 ), the flow rate equation, Eq. (40), changes to:

$$
\begin{equation*}
q_{d}=q\left(P_{u}, T_{d}, \Delta p, \rho_{d}, \gamma_{d}, \kappa_{d}, D, d\right) \tag{41}
\end{equation*}
$$

where $q_{d}, \rho_{d}, \gamma_{d}$ and $\kappa_{d}$ denote the corresponding mass flow rate, density, viscosity and the isentropic exponent calculated in "downstream conditions" i.e. at the upstream pressure $p_{u}$ and the downstream temperature $T_{d}$. For certain natural gas compositions and operating conditions the flow rate $q_{d}$ may differ significantly from $q_{u}$ and the corresponding compensation for the temperature drop effects, due to JT expansion, may be necessary in order to preserve the requested measurement accuracy (Maric \& Ivek, 2010).
The flow rate correction factor $K$ can be obtained by dividing the true flow rate $q_{u}$ calculated in the upstream conditions, Eq. (40), by the flow rate $q_{d}$ calculated in the "downstream conditions", Eq. (41):

$$
\begin{equation*}
K=\frac{q_{u}}{q_{d}} \tag{42}
\end{equation*}
$$

For the given correction factor Eq. (42), the flow rate at the upstream pressure and temperature can be calculated directly from the flow rate computed in the "downstream conditions", i.e. $q_{u}=K \cdot q_{d}$. Our objective is to derive the GMDH polynomial model of the flow rate correction factor. Given the surrogate model $\left(K_{S M}\right)$ for the flow rate correction factor Eq. (42), the true flow rate $q_{u}$ can be approximated by: $q_{S M}=K_{S M} \cdot q_{d}$, where $q_{S M}$ denotes the corrected flow rate.
The flow rate through orifice is proportional to the expansibility factor $\varepsilon$, which is related to the isentropic exponent $\kappa$ (ISO-5167, 2003):

$$
\begin{equation*}
\varepsilon=1-\left(0.351+0.256 \beta^{4}+0.93 \beta^{8}\right) \cdot\left[1-\left(p_{d} / p_{u}\right)^{1 / \kappa}\right], \tag{43}
\end{equation*}
$$

where $\beta$ denotes the ratio of the diameter of the orifice to the inside diameter of the pipe, while $p_{u}$ and $p_{d}$ are the absolute pressures upstream and downstream of the orifice plate, respectively. The corresponding temperature change $(\Delta T)$ of the gas for the orifice plate is defined by

$$
\begin{equation*}
\Delta T=T_{u}-T_{d} \approx \mu_{J T}\left(p_{u}, T_{d}\right) \Delta \omega, \tag{44}
\end{equation*}
$$

where $T_{u}$ and $T_{d}$ indicate the corresponding temperatures upstream and downstream of the orifice plate, $\mu_{J T}\left(p_{u}, T_{d}\right)$ is the JT coefficient at upstream pressure $p_{u}$ and downstream temperature $T_{d}$ and $\Delta \omega$ is the pressure loss across the orifice plate (Urner, 1997)

$$
\begin{equation*}
\Delta \omega=\frac{\sqrt{1-\beta^{4}\left(1-C^{2}\right)}-C \beta^{2}}{\sqrt{1-\beta^{4}\left(1-C^{2}\right)}+C \beta^{2}} \Delta p \tag{45}
\end{equation*}
$$

where $C$ denotes the coefficient of discharge for orifice plate with corner taps (ISO-5167, 2003) and $\Delta P$ is the pressure drop across the orifice plate. According to (ISO-5167, 2003), the temperature of the fluid shall preferably be measured downstream of the primary device but upstream temperature is to be used for the calculation of the flow rate. Within the limits of application of the international standard ISO-5167 it is generally assumed that the temperature drop across differential device can be neglected but it is also suggested to be taken into account if higher accuracies are required. It is also assumed that the isentropic exponent can be approximated by the ratio of the specific heat capacity at constant pressure to the specific heat capacity at constant volume of ideal gas. These approximations may produce a considerable measurement error. The relative flow measurement error $E_{r}$ is estimated by comparing the approximate $\left(q_{d}\right)$ and the corrected $\left(q_{u}\right)$ mass flow rate i.e.

$$
\begin{equation*}
E_{r}=\left(q_{d}-q_{u}\right) / q_{u} \tag{46}
\end{equation*}
$$

## Step Description

1 Calculate the natural gas properties ( $\rho_{d}, \mu_{J T}$ and $\kappa_{d}$ ) at $p_{u}$, and $T_{d,}$ (Table 2).
Calculate the dynamic viscosity $\gamma_{d}$ at $P_{u}$, and $T_{d}$, using e.g. the residual viscosity equation (Poling, 2000).
3 Calculate the mass flow rate $q_{d}$ and the discharge coefficient $C$ at $P_{u}, T_{d}$ and $\Delta p$ (ISO-5167, 2003).
4 Calculate the pressure loss $\Delta \omega$, Eq. (45).
5 Calculate the upstream temperature $T_{u}$ in accordance with Eq. (44).
6 Calculate the natural gas properties ( $\rho_{u}$ and $\kappa_{u}$ ) at $p_{u,}$ and $T_{u}$ (Table 2).
7 Calculate the dynamic viscosity $\gamma_{u}$ at $p_{u}$, and $T_{u}$, using e.g. the residual viscosity equation (Poling, 2000).
8 Calculate the mass flow rate $q_{u}$ at $p_{u}, T_{u}$ and $\Delta p$ (ISO-5167, 2003).
Table 5. Precise correction of the flow rate based on downstream temperature measurement and on the computation of natural gas properties.

The individual and the combined relative errors due to the approximations of the temperature drop and the isentropic exponent can be estimated by using the Eq. (46). The precise correction of the natural gas flow rate, based on upstream pressure and downstream temperature measurement and on the computation of the corresponding natural gas properties, is summarized in Table 5.

The procedure in Table 5 requires a double calculation of both the flow rate and the properties of the natural gas. To reduce the computational burden we aim to derive a lowcomplexity flow rate correction factor model that will enable direct compensation of the flow rate error caused by the measurement of the downstream temperature. The correction factor model has to be simple enough in order to be executable in real-time and accurate enough to ensure the acceptable measurement accuracy.

## 7. Results of flow rate measurement simulations

In order to simulate a flow rate measurement error caused by the non-compensated temperature drop, a natural gas mixture (Gas 3) from Annex C of (ISO-12213-2, 2006) is assumed to flow through orifice plate with corner taps (ISO-5167, 2003) as illustrated in Fig. 5. Following the recommendations (ISO-5167, 2003), the absolute pressure is assumed to be measured upstream $\left(p_{\mathrm{u}}\right)$ and the temperature downstream $\left(T_{\mathrm{d}}\right)$ of the primary device. Fig. 6


Fig. 6. Temperature drop due to JT effect $\Delta T=\mu_{J T} \Delta \omega$ when measuring flow rate of natural gas mixture through orifice plate with corner taps (ISO-5167, 2003). The upstream pressure varies from 1 MPa to 60 MPa in 1 MPa steps and upstream temperature from 245 K to 305 K in 20 K steps for each of the two differential pressures $\Delta p(20 \mathrm{kPa}$ and 100 kPa$)$. The internal diameters of orifice and pipe are: $d=120 \mathrm{~mm}$ and $D=200 \mathrm{~mm}$.

## Thank You for previewing this eBook

You can read the full version of this eBook in different formats:
> HTML (Free /Available to everyone)
$>$ PDF / TXT (Available to V.I.P. members. Free Standard members can access up to 5 PDF/TXT eBooks per month each month)
> Epub \& Mobipocket (Exclusive to V.I.P. members)
To download this full book, simply select the format you desire below

