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C-5

Real Gas Equation of State for Methane

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Methane is one of the most wide spread fuels and raw materials for chemical industry used for production of synthetic gas, acetylene, black carbon, etc. Despite its thermochemical and physical properties are in general well investigated, its numerous novel applications, in particular in transportation engines, require the knowledge of accurate thermal and calorific equations of state (EOS). The aim of this communication is to develop the thermal EOS for methane in a supercritical parametric domain at $250 \le T \le 1000$ K and $0.1 \le P \le 100$ MPa.

Figure 1 is the phase equilibrium diagram for methane obtained using the data of [1]. The shaded area in Fig. 1 is the supercritical parametric domain of our interest here.

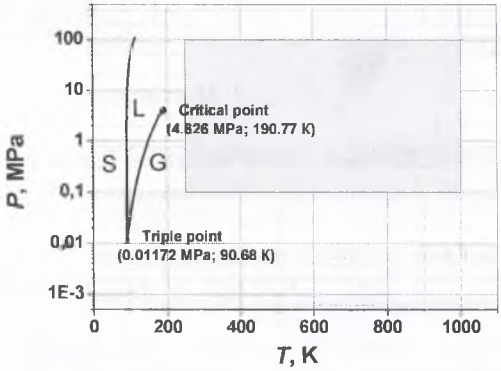

Fig. 1. Phase diagram for methane.

As is known from the solid state physics, at relatively low temperatures the pressure of solid matter can be decomposed into two parts: $P = P_c + P_t$, where P_c is the elastic ("cold") pressure component associated only with the interaction forces between atoms in the solid (this component depends only on solid volume) and P_t is the thermal pressure component associated with heating of the solid (this component depends on both solid volume and temperature). According to [2], a similar decomposition can be formally applied to dense gases, however the validity of such an approximation should be checked against experimental data.

Applying the approach of [2] to methane one can approximate the thermal EOS as:

$$P(\rho,T) = P_c(\rho) + \frac{\rho RT}{\mu} f(\rho) \qquad (1)$$

where ρ is the density, μ = 16.0426 g/mol is the molecular mass of methane, R = 8.314 J/(mol K) is the universal gas constant, and $f(\rho)$ is the (unknown) function of density. The EOS of Eq. (1) is automatically valid for the ideal gas since for such a gas $P_c(\rho)$=0 and $f(\rho)$=1. According to [2], the terms $P_c(\rho)$ and $f(\rho)$ are given by:

$$P_c(\rho) = \sum(\rho) - \frac{\rho R T_r}{\mu}[f(\rho) - 1] \tag{2}$$

$$\sum(\rho) = a\rho^2 + b\rho^3 + c\rho^4 + d\rho^5 \tag{3}$$

$$f(\rho) = \frac{1 + A\rho + B\rho^2 + C\rho^6}{1 + \frac{C}{6.69}\rho^6} \tag{4}$$

where T_r is the reference temperature and a, b, c, d, A, B, C are the coefficients. The values of these coefficients are:

$a = -641.7869$; $b = 3738.295$; $c = -14431.11$; $d = 31213.21$;
$A = 3.41409$; $B = 8.62367$; $C = 566.69609$

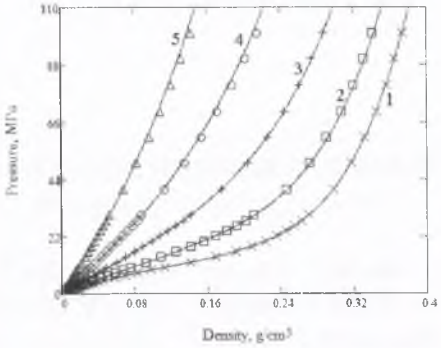

Fig. 2. Comparison of predicted (curves) and measured (points [1]) dependencies of pressure on density for five isotherms: $T = 250$ K (curve 1), 300 (2), 400 (3), 600 (4) and 1000 K (5) for methane

(units of a, b, c, d are in MPa, cm, g; units of A, B, C are in cm, g). These values were obtained by fitting Eqs. (1) and (2) with the experimental data [1] at reference temperature $T_r = 250$ K. The accuracy of the new EOS for methane thus derived is illustrated in Fig. 2. Figure 2 compares predicted (curves) and measured (points) dependencies of pressure on density for five isotherms: $T = 250$, 300, 400, 600 and 1000 K at $0.1 \le P \le 100$ MPa. The approximation error in terms of pressure is in average less than 1.5 %. The maximum approximation error of 4.2 % is attained at $T = 1000$ K and $P = 100$ MPa.

Thus, we have developed a new analytical thermal EOS for methane providing a good accuracy of $P-\rho-T$ data approximation at $250 \le T \le 1000$ K and $0.1 \le P \le 100$ MPa. Due to simplicity this EOS can be readily used in CFD simulations of operation processes in various energy conversion plants.

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C-6

To Non-Selfmaintained Discharge Impact on Lean Propane-Air Mixtures

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A goal of the present report is analysis of the electron-beam in external electric field impact on ignition of dry lean flammable propane-air mixture. Works on modeling of electron-molecule processes in propane-air mixture in external electric field and E-beam at different values of stoichiometricity have been realized.

As the basic we have chosen a simplified system of chemical reactions with added reverse reactions — 74 reactions: Hydrogen-Oxygen chain, Hydroperoxyl and Hydrogen Peroxide reactions, Propane reactions, I-Propyl, N-Propyl and Propene reactions, Ethylene, Ethyl, Vinyl, Vinoxy and Ketene reactions, Methyl, Methoxy, Formaldehyde, Formyl reactions), standard energy equation