APPROXIMATION OF THE THERMODYNAMIC PROPERTIES OF ACETYLENE

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Abstract: Acetylene (C_2H_2) is the individual unsaturated hydrocarbon widely used in various chemical technologies, particularly, in the manufacture of explosives. Recently, interest has grown to acetylene in connection with its possible use as a liquid propellant in a mixture with ammonia. Derived in the paper are the thermal and caloric equations of state (EOS) of acetylene in the single- and two-phase regions of thermodynamic parameters. Thermal EOS of acetylene is presented in the form of two components — the "cold" component, which depends only on the density, and "thermal" component proportional to temperature. This form of EOS is theoretically justified for solids and holds asymptotically for an ideal gas. With respect to the dense gas and liquid, such an EOS is the approximation, the accuracy of which is estimated by comparing the calculations with the available reference data. The EOS are represented by mathematical formulae and are accurate enough for gasdynamic applications.

Keywords: acetylene; thermal equation of state; caloric equation of state; single-phase region; two-phase region

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References

1. http://community.sk.ru/press/events/april2012/popechitelsky_sovet/p/energomash_akademika_glushko.aspx (accessed February 5, 2105).

2. Dubrovskii, A. V., V. V. Kozynda, and S. M. Frolov. 2012. Termicheskoe uravnenie sostoyaniya ammiaka [Thermal equation of state of ammonia]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 5:120−124.

3. Basevich, V. Ya., A. A. Belyaev, and S. M. Frolov. 2013. Kineticheskiy mekhanism khimicheskikh prevrashcheniy v gazovykh smesyakh atsetilena i ammiaka [Kinetic mechanism of chemical transformations in gaseous mixtures of acetylene and ammonia]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 6:26−30.

4. Dubrovskii, A. V., N. M. Kuznetsov, and S. M. Frolov. 2015. Approksimatsiya termodinamiche-skikh svoystv ammiaka [Approximation of the thermodynamic properties of ammonia]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 8(1):198–214.

5. Kuznetsov, N. M., A. V. Dubrovsky, and S. M. Frolov. 2011. Analytical approximation of the thermal and caloric equations of state for real gases over a wide density and temperature range. *Russ. J. Phys. Chem. B* 5(7):1084–1105.

6. Kuznetsov, N. M., A. V. Dubrovsky, and S. M. Frolov. 2011. Analiticheskaya approksimatsiya uravneniy sostoyaniya real'nykh gazov v rasshirennom diapazone davleniya i plotnosti [Analytical approximation of the thermal and caloric equations of state for real gases over a wide pressure and density range]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 4:68–74.

7. Miller, S. A. 1969. *Atsetilen, ego svoystva, poluchenie i primenenie* [Acetylene, its properties, production, and application]. Vol. 1. — Leningrad: Khimiya. 681 p.

8. Vargaftik, N. B. 1972. *Spravochnik po teplofizicheskim svoistvam gazov i zhidkostei* [Textbook on thermophysical properties of gases and liquids]. Moscow: Nauka. 721 p.

9. Landau, L. D., and E. M. Lifshitz. 1951. *Statisticheskaya fizika* [Statistical physics]. Moscow: Gostekhizdat. 480 p.

10. Teranishi, H. 1955. On the thermodynamic properties of acetylene under high pressures. *Rev. Phys. Chem. Japan* 25(1):25–33.

11. Kuznetsov, N. M. 1981. Dvukhfaznaya smes' voda–par. Uravnenie sostoyaniya, skorost' zvuka, izentropy [Two-phase water–steam mixture. Equation of state, sound velocity, isentropes]. *Dokl. Akad. Nauk SSSR* [Dokl. Phys.] 257(4):858–860.

12. Kuznetsov, N. M. 1982. Uravnenie sostoyaniya i krivaya fazovogo ravnovesiya system zhidkost'–par [Equations of state and phase equilibrium curve for liquid–vapor systems]. *Dokl. Akad. Nauk SSSR* [Dokl. Phys.] 266(3):613–616.

13. Kuznetsov, N. M., E. N. Aleksandrov, and O. N. Davydova. 2002. Analiticheskoe predstavlenie krivykh fazovogo ravnovesiya zhidkost'–par dlya nasyshchennykh uglevodorodov [Analytical representation of the curves of phase equilibrium liquid–vapor for saturated hydrocarbons]. *Teplofizika Vysokikh Temperature* [High Temp.] 40(3):359–363.

14. Gurvitch, L. V., I. V. Vetz, and V. A. Medvedev. 1979. Termodinamicheskie svoystva individu-al'nykh veshchestv [Thermodynamic properties of individual substances]. Vol. 2. Bk. 1. Moscow: Nauka. 440 p.

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