Nitrogen (N_2) equation of state in pressure up to 10 kbar – molecular dynamic simulation

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Molecular dynamic simulation program using N_2-N_2 interaction potential, obtained be van der Avoird et al [1], has been used to determine nitrogen equation of state. Using this potential the pressure temperature dependence has been obtained by intensive molecular dynamic simulation. The temperature range spans from 1000K to 2000K while the pressure range extends from 1 bar to 10 kbar.

For low pressures the obtained pressure-temperature-density dependence follows that of ideal gas. The pressure range depends on the temperature, but generally ideal gas-like behavior is observed for pressure below 1 kbar. For these pressures the MD data are in very good agreement with the data of Jacobsen et al [2].

For higher pressure significant deviation from the ideal gas law, stems from strong molecule-molecule repulsion. This has been accounted for in the revised version of equation of state of nitrogen by Jacobsen et al [2]. The MD simulation were used to recover p-T-ρ dependence for the pressures, up to 10 kbar. For high pressure range i.e. from 1 to 10 kbar, the deviation from Jacobsen data was much larger, about 10%, which is larger that estimated standard error [2]. The possible sources of discrepancy are the approximate accounting of the vibrational motion and also the finite size of the simulation domain.

References:

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