

A New Fundamental Equation of State for 3,3,3-Trifluoroprop-1-ene (R-1243zf)

Ryo Akasaka^{1, S, C} and Eric W. Lemmon²

¹*Department of Mechanical Engineering, Kyushu Sangyo University, Fukuoka, Japan*

²*Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO, U.S.A.
ryo-a@ip.kyusan-u.ac.jp*

A new fundamental equation of state is presented for 3,3,3-trifluoroprop-1-ene (R-1243zf). The first equation for this fluid, developed in 2016 and consisting of only polynomial and exponential terms, was an interim model based on limited experimental data. It was then refitted to a functional form including Gaussian bell-shaped terms (second equation) in 2019 to reproduce reasonable behavior of the virial coefficients over a wide range of temperatures; nevertheless, there are a few regions where the second equation shows deviations larger than experimental uncertainties for recently published data, particularly those for liquid densities and vapor-phase sound speeds. The new equation of state (third equation) was developed with more sophisticated and highly optimized fitting techniques acquired from our recent works. The terms used in the new equation are less intercorrelated compared to previously developed equations, and thus exhibit reasonable extrapolation behavior at extremely low and high temperatures and at high pressures. This third equation is valid at temperatures from the triple point (122.35 K) to 430 K and pressures up to 35 MPa, where the consistent experimental datasets are represented within their uncertainties. Expected uncertainties at the 95 % confidence interval ($k = 2$) in properties calculated from the third equation are 0.1 % for vapor pressures, 0.3 % for saturated liquid densities, 1 % for saturated vapor densities, 0.1 % for liquid densities, 1 % for vapor densities, and 0.06 % for vapor-phase sound speeds. This is the best equation of state currently available for property representation for R-1243zf and will soon be published in a scientific journal.