

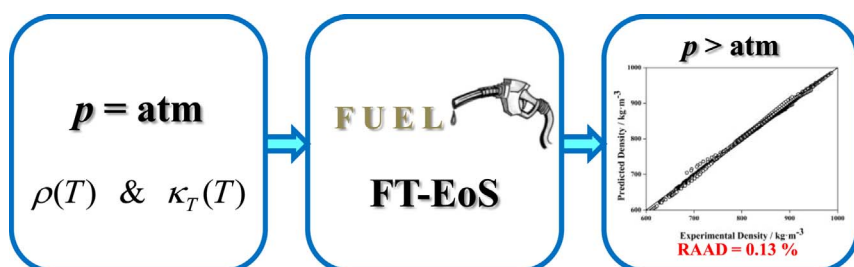


## Full Length Article

# The prediction of high-pressure densities of different fuels using fluctuation theory-based Tait-like equation of state

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## GRAPHICAL ABSTRACT



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## ABSTRACT

We demonstrate that the Fluctuation Theory-based Tait-like Equation of State (FT-EoS) allows an accurate prediction of the fuel density at high pressures using their density and isothermal compressibility data determined at atmospheric pressure only. The experimental data for 38 different fuels, given in literature as a function of temperature and pressure, were used for the comparison and its analysis, which supports this conclusion. We also describe the calculation algorithm and the procedure of testing for a range of applicability and accuracy of the reference data at ambient conditions, which assures the application of FT-EoS.

## 1. Introduction

Thermophysical property data over a wide range of temperatures and pressures are critically important for the design engineering of combustion engines. One of them is the density, which can be determined experimentally with high precision and accuracy in a wide range of temperatures and pressures and is related to other thermodynamic properties, which are required for the design and the optimization of many industrial processes. These density data are used to derive very important properties, for example, the isothermal compressibility,  $\kappa_T$ , the isobaric thermal expansivity,  $\alpha_p$ , the thermal pressure coefficient,  $\gamma$ , the internal pressure,  $P_{int}$ , and the difference between specific heat capacity at constant pressure,  $c_p$ , and specific heat

capacity at constant volume,  $c_v$ .

Fuels are one of the most commonly used fluids for engineering applications and home use. They are used in aircraft, military, agriculture and automotive industry, for example. Their properties are strictly described in the standards, which are applied worldwide (MIL-DTL-83133, EN 590, EN 14214, ASTM D6751, Shell Normafluid ISO 4113).

The wide application of fuels are found in the literature with many different implementations, i.e. commercial gas turbine fuels [1–3], rocket propellants and aviation fuels [4–6], jet fuels [7,8], biodiesels [9–18], petroleum diesel oils [19,20], automotive engines [21] etc. Other than fuels, in the literature, the applications include biodiesel components [22–24], fuel additives [21,25,26], fuels used for testing

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and calibrating diesel injection systems [27], aviation fuels which are interesting as potential add-ins or substitutes for traditional turbine fuels [3].

The density is one of the most important of fuel properties, due to its important impact on the operation of fuel injection systems [28], provides proper combustion while minimizing greenhouse emissions [19], improves biodiesel fuel properties [23]. Moreover provide the data necessary to formulate EoS to correlate the fluid properties, and to optimize new fuels for military applications [1], design of new rocket propellants [4] related to aircraft range. The models can provide a framework to predict properties fuels that have not yet been measured [8]. These models will aide in optimizing the combustion of fuels used in modern diesel engines injection systems to help control the pressure wave, the total mass of fuel injected for efficient fuel combustion while minimizing NO<sub>x</sub> emissions as well as model the composition of exhaust gases [22]. This information can help in improving engine performance [29] and reducing greenhouse gas emissions.

Different methods have been reported in the literature to correlate, evaluate and/or predict the volumetric properties of fuels [15,22]. These methods are i) CPA-EoS [22], and ii) the GCVOL group contribution method, the Halvorsen's model and the Zong's fragment-based approach model [15].

All proposed methods display good predictive capability, but they were developed using density data over a wide range of temperature and pressure. We want to show a model, which is based on only on the density and the isothermal compressibility at atmospheric pressure to predict accurately the fuels densities as a function of temperature and pressure – the FT-EoS. Its high accuracy was already appraised on a wide range of pure substances including halogenated and polar liquids [30–32] and ionic liquids [33]. However, in this work, the final version of the FT-EoS applies a novel approach, by excluding the molar mass which reflects in higher applicability.

During this work, we decided to further assess its predictive capability for the high-pressure density of 38 different fuels using experimental data available in the literature as a function of temperature and pressure (see Supplementary Table S1) [1,3–6,8–11,15,16,19,20,22,27,34–36].

## 2. Theory

To predict fuel densities at high pressures,  $P$ , basing the thermodynamic parameters measured at the atmospheric pressure  $P_0$  only, we will use the FT-EoS,

$$\rho = \rho_0 + \frac{1}{k} \log \left[ \frac{kM}{\nu RT} (P - P_0) + 1 \right], \quad (1)$$

where  $\rho$ ,  $\rho_0$ ,  $k$ ,  $M$ ,  $R$ ,  $T$  are the density under elevated pressure, the density at atmospheric pressure, the main control parameter, the molar mass, the gas constant and the temperature, respectively, and has been proposed [37] based on the study of the inverse reduced volume fluctuations defined as an inverse ratio of relative volume fluctuations in liquids with combined values for the hypothetical ideal gas at the same PVT thermodynamic conditions:

$$\nu = \left[ \frac{\langle (\Delta V)^2 \rangle}{V} \frac{V_{ig}}{\langle (\Delta V)_{ig}^2 \rangle} \right]^{-1} = \frac{M}{RT} \frac{1}{\rho \kappa_T} \quad (2)$$

Here  $\kappa_T$  is the isothermal compressibility.

It has been found that this parameters  $\nu$  satisfies the exponential dependence on the density

$$\nu = \exp(k\rho + b) \quad (3)$$

along the coexistence curve  $\rho = \rho_0(T)$  well below the critical point curve for a very wide range of organic liquids including normal and halogenated alkanes [30,31,37,38], 1-alcohols [32] and even ionic liquids [33]. The coefficients  $k$  and  $b$  have a very weak dependence on

the temperature and could be considered, within reasonable accuracy, as constant for the single phase region up to sufficiently high pressures, at which a dense packing (a kind of the contact percolation limit) of molecules will be reached [39]. This provides an opportunity to use (1) as an isothermal equation of state.

At the same time, Eq. (1), which uses definitions (2) and (3) to determine its coefficients, requires the molar mass of a substance can increase the complexity of use in the case of liquid mixtures such as industrial fuels.

For this reason, we modify it in this work noting, that the parameter of inverse ratio of relative volume fluctuation (2) could be also expressed through the isothermal compressibility as follows

$$\kappa_T^{-1} = \nu \frac{RT}{M} \rho = \left( \frac{\partial P}{\partial \rho} \right)_T \rho. \quad (4)$$

As a result, integration of Eq. (4) respectively to the exponential function (3) and using again the equality (4) along isotherms  $T = \text{const}$  leads to the expression

$$\rho = \rho_0 + \frac{1}{k} \log [k\rho_0 \kappa_T^0 (P - P_0) + 1], \quad (5)$$

which contains the density  $\rho_0$  and the isothermal compressibility  $\kappa_T^0$  determined at atmospheric pressure  $P_0$  as well as the main control parameter  $k$ , which is defined by two letters quantities for each temperature as

$$k = -\frac{1}{\rho_0} \left( \frac{d\rho_0}{dT} \right)^{-1} \left[ \frac{1}{T} + \frac{d \log \kappa_T^0}{dT} \right]. \quad (6)$$

To determine its value numerically from experimental data at the atmospheric pressure we follow the algorithm proposed in [33] fitting temperature dependent quadratic polynomials to the density and the logarithm of the isothermal compressibility

$$\begin{aligned} \rho_0 &= a_2 T^2 + a_1 T + a_0 \\ \log \kappa_T^0 &= a_2' T^2 + a_1' T + a_0' \end{aligned} \quad (7)$$

where  $a_i$  are the coefficients of the quadratic polynomial for density and  $a_i'$  are the coefficients for isothermal compressibility at atmospheric pressure.

Consequently, Eq. (6) could be written as

$$k = -\frac{1}{a_2 T^2 + a_1 T + a_0} \frac{1 + T(2a_2' T + a_1')}{T(2a_2 T + a_1)}. \quad (8)$$

As well,  $\rho_0$  and  $\kappa_T^0$  will be substituted into Eq. (6) using the fitting expressions (7) too.

It should be pointed out that the quadric polynomials of Eq. (7) are sufficient for all considered substances independently of their composition since the considered temperature interval is sufficiently far from the critical conditions (as it assumed by FT-EoS range of applicability). Whence, functions representing both the density and the logarithm of the isothermal compressibility have a quite small curvature. Fig. 1 shows the typical fits of experimental values of density and isothermal compressibility, where two chosen fuels i) RP-1 [4] and ii) EuroDiesel [20] are chosen as examples. The correlation coefficient between experimental and approximated data is over 0.99 and the average absolute deviation is much more less than the experimental uncertainties. Other substances demonstrate the same picture as well.

## 3. Results

During this work, various density and isothermal compressibility datasets at atmospheric pressure were used to predict volumetric properties of 38 selected industrial fuels. Normally these liquids are mixtures of petrochemicals and additives so the molar mass is not available, due to patent protection, or difficult to calculate [1,4,8]. Hence in our analysis we will show that we can accurately predict the

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