

**Extending an open source Python library:  *Computing ideal gas contributions for the calculation of thermodynamic properties***

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PyForFluids(Python-Fortran-Fluids) is a software package for the calculation of Phase-Equilibrium and Thermodynamic Properties of pure fluids and fluid mixtures by making use of equations of state. Three cubic equations of state ─the Redlich-Kwong-Soave (RKS), the Peng-Robinson (PR) and the so-called RKPR, which is essentially an algebraic combination between the two which incorporates a third parameter─ and the multiparametric equation of state, GERG-2008, have been implemented so far. Thermodynamic properties considered in *PyforFluids* are for example density, isothermal compressibility, speed of sound, Cp, Cv, enthalpy, entropy, etc. In terms of phase-equilibrium calculations, the tracing of two-phase envelopes (including dew and bubble points) as well as two-phase PT flash are already available, while other features involving three-phase separation in multicomponent fluids and also specific curves and diagrams for binary systems are in the list of extensions to incorporate in the near future.

Everything is calculated based on the residual Helmholtz Energy and its derivatives, that each equation of state provides, and organized following a modular approach as suggested by Michelsen and Mollerup in their book [1]. Taking advantage of that, the package is designed with a collaborative approach in mind.

While residual properties are obtained from the chosen equation of state, the ideal gas properties contributions are determined by the classic polynomial function of the absolute temperature and by a new technique that involves the de Broglie wavelength. Although temperature-dependent ideal gas contributions do not affect phase equilibrium calculations, they play a fundamental role in the estimation of important properties like enthalpy, specific heats and entropy, which find many important applications in Chemical Engineering. Models predictions are compared in this work with available experimental data for different systems and applications.

The calculation of thermodynamic properties of multicomponent mixtures can be a computational time demanding task, mostly due to the need of multiple iterative calculations and an increase of complexity with the addition of components. To assure fast calculationsll the computationally intensive procedures of PyForFluids are implemented in Modern Fortran, taking advantage of ’s higher computational performance in terms of speed and memory compared to to interpreted languages like Python [2]. These procedures are wrapped in a user-friendly way to be called from Python and used interactively.

Following high standards for the testing of codes, models predictions of properties for simple alkanes (methane, ethane, butane etc.) and their mixtures are checked on every code modification to assure reliability.

***References***

1. Michelsen, M. L.; Møllerup, J. Thermodynamic Models: Fundamentals & Computational Aspects, 2nd ed.; Stenby, E. H.,

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1. Laurence Kedward et al. The State of Fortran. Computing in Science & Engineering 2022, 24, 63-72.