

ThermoLibrary: an Open-source Library for the Evaluation of Fundamental Helmholtz Equations of State

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Thermophysical properties of fluids are very important for fluids' industrial applications, and many high-precision models have been developed to satisfy this demand, such as Helmholtz equation of state, PC-SAFT equations, ePC-SAFT equations, etc. However, the implementation of these models are very difficult, seriously hindering their technical application.

Many high-precision models belong to fundamental Helmholtz equation of state, which can evaluate all thermodynamic properties just using corresponding partial derivatives, and no integrals were needed. Because of this excellent feature, many repetitive works can be avoided, and the implementation complexity of those models can be reduced significantly. The evaluation formula for specific thermodynamic properties is universal for fundamental Helmholtz equations of state, the only difference is the evaluation formula for corresponding partial derivatives. Thus, the universal part of the evaluation can be implemented in a universal library. For a specific model, after the implementation of corresponding partial derivatives is done, all thermodynamic properties can be evaluated easily.

In this present work, an open-source library named ThermoLibrary was developed to make the evaluation of fundamental Helmholtz equations of state easy; many universal evaluation formulas of specific thermodynamic properties have been implemented. ThermoLibrary was written using C++, but wrappers for other programming languages and platforms are also available. So far, only pure and pseudo-pure component models are implemented; mixture models will be added in the future.

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