Consistent look-up table interpolation method for real-gas flow simulations

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ABSTRACT

Nowadays the reliable modeling of real fluid flows is of paramount importance in many industrial applications, especially in the energy field with the growing diffusion of Organic Rankine Cycles, supercritical CO_2 compressors, and advanced refrigeration systems. In these applications the assumption of flow ideality is profoundly inaccurate and may lead to erroneous physical interpretations. As a consequence thereof, various thermodynamic models have been recently developed for real gases and a number of tools are by now available to accurately predict the thermodynamic properties of fluids in presence of relevant non-ideal effects. However, these thermodynamic libraries are frequently computationally inefficient when coupled with existing simulation codes, such as in process modeling and computational fluid-dynamics (CFD).

An effective alternative is proposed in this paper. The equations of state embedded in the thermodynamic programs are used, at preliminary level, to construct a grid of nodes storing a subset of thermo-physical properties, i.e. v, s, e, k, μ, required by the method for a given region of interest. Then, an interpolation-based method is conceived for determining the remaining properties in any other point. A key feature is as follows: the nodal values of the basic thermodynamic quantities are used to locally construct, i.e., within each cell of the table, a model of the fundamental relation, assuming a differentiable functional form of at least C^2 class.

The presented Look-up Table (LuT) approach is intrinsically consistent and guarantees thermodynamic stability, with inherent high accuracy and very limited computational costs, as demonstrated by the quantitative examples reported in the paper. As a final step, the LuT method is coupled with two in-house flow solvers and applied to simulate real gas transonic flow in Organic Rankine Cycle turbines; a comprehensive assessment of the approach is provided by comparison with direct equations of state implementation.

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1. Introduction

The accurate modeling of thermodynamic and transport properties of fluids exhibiting non-negligible real-gas behavior is crucial in many technical applications; in energy-conversion systems fluids are often employed far from ideal gas conditions, and the availability of proper thermodynamic models is a necessary prerequisite for the accurate estimate of both component and whole-system performance. The prediction of real-gas thermodynamic properties can be achieved by determining analytical expressions for the fundamental relation or, more commonly, by resorting to Equations of State (EoS) and their derivatives. Several formulations of the EoS and of transport properties correlations are

available [24,20,12,14,4,3,6], but their use through thermodynamic libraries [7] is computational expensive in case of numerical studies, when a set of governing equations is iteratively solved, e.g., detailed Computational Fluid Dynamic (CFD) calculations [10], dynamic plant simulations [18].

As an alternative, Look-up Tables (LuT) can be adopted to represent the thermo-physical behavior of the fluid. The LuT concept is fairly simple; in the thermodynamic region of interest, a grid of nodal points (storing all thermodynamic and transport properties) is preliminary built and the properties at any other point are computed using fast interpolation methods, with a dramatic reduction in computational time [11,13,2,22]. However, standard LuT approaches do not automatically satisfy thermodynamic consistency, as it is guaranteed by the use of analytical EoS. Referring to a pure substance or to a mixture of given composition, thermodynamic consistency implies that, given a triple of thermodynamic

properties, e.g. P, T, ρ, if $T = g(P, \rho)$ and $P = f(T, \rho)$, then $P \equiv f(g(P, \rho), \rho)$. Generally, most of the LuT approaches substitute the functions f, g with their approximate counterparts $\tilde{f}, \tilde{g}$ and this finally leads to $P \not\equiv f(g(P, \rho), \rho)$. The consistency error $\epsilon = P - \tilde{f}(\tilde{g}(P, \rho), \rho)$ can be minimized by increasing the accuracy of the LuT, improving either the number of mesh nodes or the order of the interpolation scheme. This can be usually done at the expense of a greater computational cost. On the other hand, consistency errors may induce significant non-smooth perturbations over CFD code iterations, which may even prevent the solver to converge.

This paper presents a novel interpolation method for property calculation of real gases using LuT. At first, the values of specific internal energy e, expressed in terms of specific entropy s and specific volume v, are calculated for each node of the grid by exploiting the accurate EoS implemented in the software *FluidProp* [7]. Then, the nodal values are utilized to construct, once assigned a certain functional dependency, a fundamental relation in the energy form $e = e(v, s)$, one for each cell of the thermodynamic domain. More specifically, the set of closure coefficients pertaining to a single fundamental relation is determined by interpolation on the closest grid data, according to the order of the function. Lastly, the algorithm provides the thermodynamic properties by conveniently combining the derivatives of the fundamental relation. The method results to be compactly supported, i.e. it has local nature, it can be retained semi-analytical, and primarily guarantees that any thermodynamic property of any internal point is consistently calculated. Nevertheless, to avoid failures during property calculation, the functional form chosen for e needs to exhibit a sufficient regularity (derivatives up to second order are usual for process or fluid-dynamic calculations) and must fulfill the thermodynamic stability within the cell.

A similar approach is adopted for obtaining the transport properties. Two different functional forms are prescribed for the dynamic viscosity μ and for the thermal conductivity k; coherently with the thermodynamic table, also the transport properties are expressed as functions of the specific volume and of the specific entropy $\mu = \mu(v, s)$, $k = k(v, s)$. Correspondingly, the set of coefficients of the two interpolating functions is resolved at any cell on the basis of the transport properties stored inside the grid points. Since such values are computed (starting from two independent thermodynamic properties) by resorting to semi-empirical relations, no consistency issues have to be taken into account, providing that positive values are achieved.

The paper is structured as follows: the theoretical background of the novel LuT methodology is initially outlined in Section 2. Issues concerning thermodynamic stability, accuracy and computational cost are discussed in Section 3, in which the LuT method is applied to the siloxane MDM and the carbon dioxide; both single

and two-phase regions close to the vapor saturation line are explored, for reduced temperatures ranging between $T_r \simeq 0.6$ and $T_r \simeq 1.05$. To conclude, two examples of LuT application in combination with CFD simulation are extensively presented in the latest Section 4.

2. Look-up Table approach (LuT)

The standard computational scheme of any interpolation based method for the calculation of thermo-physical properties consists of a two-step procedure. As a first step, the thermodynamic mesh is generated based on the data provided by an existing database (tables of experimental data or even Equations of State and transport properties correlations). The whole set of properties is computed afterwards on the basis of the data stored in each node of the grid. The key aspects of a LuT algorithm, namely its efficiency and its accuracy, are then related to the methodologies introduced to resolve either steps. This section presents the methods developed in this work to achieve an optimal compromise between accuracy and computational cost, given that the thermodynamic consistency is intrinsically satisfied.

Differently from current LuT approaches, the present method allows to compute the thermodynamic quantities on physical basis, i.e. the properties stored in the nodes of the table are used to construct (by proper interpolation) local fundamental relations, which are analytically differentiated to retrieve the properties of interest –P, T, c, ...– in a straightforward manner. Each step of the procedure is separately described in the following.

2.1. Generation of the thermodynamic mesh

The construction of the thermodynamic mesh is based on the discretization of the saturation line according to a given temperature interval. The points can be uniformly or variably spaced through a spline-based reconstruction method, allowing also a refinement as the critical point is approached; an example of discretized vapor saturation line for siloxane *MDM* is given in Fig. 1. The resulting saturation grid represents the support line on which the LuT is constructed by proceeding along directions locally orthogonal to the line.

The normal spacing may be, in principle, specified using a generic pair of states (e.g. ρ, e), however, this choice strongly affects the shape and the thermodynamic regions covered by the resulting grid. Fig. 2 depicts three different thermodynamic meshes generated starting from the same basis points and specifying the normal spacing as a function of $log(v)$, s, $log(T)$, s, and $log(v)$, e. As well visible, the third grid extends in regions far from the critical point, while the former two also include the supercritical zone; this represents a crucial advantage in processes that occur, at least
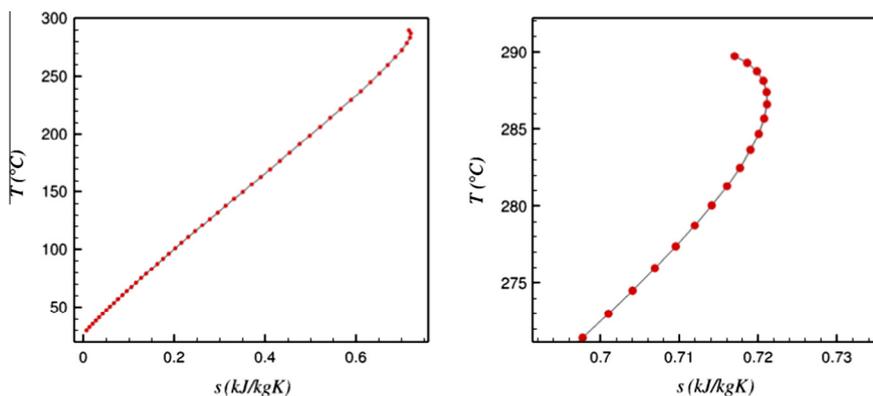
Fig. 1. Left: Discretized MDM vapor saturation line in the *T–s* plane. Right: Discretized MDM vapor saturation line in the critical region of the *T–s* plane.