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COMPUTATIONALLY EFFICIENT MODELS FOR THE NUMERICAL SIMULATION OF THERMODYNAMICALLY COMPLEX FLOWS

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ABSTRACT

In recent years, compressible flows of thermodynamically complex gases have found considerable attention among the scientific community. Actually, many problems in physics and engineering are characterized by thermodynamic conditions where the perfect gas approximation is no longer valid. Advances in computational fluid dynamics as a fundamental design tool both in aerodynamics and in energy engineering have promoted the development of fluid dynamic solvers characterized by a more accurate thermodynamic modeling for non-reacting flows of gases in special thermodynamic conditions, for instance close to saturation, or in the supercritical region, or in the two-phase regime [1-3]. Crucial issues for the numerical simulation of compressible flows with complex thermodynamic behavior are, on the one hand, the choice of a suitable model that accurately describes the fluid thermodynamic response; on the other one, its implementation complexity and computational cost. With regard to the first point, there are essentially two ways: the first one is the use of an equation of state (EOS), i.e. a mathematical model representing the fluid behavior within a given range of conditions; the second one is the numerical interpolation of a suitable database of thermodynamic properties. About the first approach, a wealth of literature exists, diversified according to the substance to be modeled. Equations of state based on theoretical and analytical criteria require only a few thermodynamic inputs and may be applied to potentially any substance. On the other hand, it is possible to develop semi-empirical equations of state, very accurate for specific classes of substances, by means of suitable regression techniques applied to experimental data sets (see, e.g. [1]). In general, the more accurate an EOS is, the more complex its mathematical form. For this reason, most of the computational studies about non reacting flows of real gases are actually based on simple thermodynamic models. A special case is represented by studies about dense gas flows, i.e. flows of molecularly complex gases close to saturation conditions. Most of these works are intended to qualitatively study the flow physics more then to provide quantitative results and adopt the simple the van der Waals model [3]. More recent works have utilized more realistic models, such as the Peng-Robinson, Stryjek-Vera and Martin-Hou ones [1,5]. Recently, an equation of the Span-Wagner type has been proposed for some classes of organic fluids [6]; this equation however has a quite cumbersome mathematical form and it is not easy to implement it within a fluid dynamic solver. A possible alternative to the use of an analytical equation of state is interpolation on a database of thermodynamic properties. This avoids in part numerical complexities related to the use of analytical models, but requires some caution about interpolation errors in regions characterized by large variations of thermodynamic properties. The computational load varies according to the chosen interpolation procedure. In the past, methods for the interpolation of thermodynamic properties have been developed for some common fluids of industrial interest, like air and water (e.g. [7]). Polynomial interpolation methods for fluid flow simulations in turbomachinery are proposed in [3]. The present research aims at the development of accurate thermodynamic models for dense gas flows. Such models should be, at the same time, computationally sustainable, in order to be implemented within computational fluid dynamics (CFD) codes, possibly coupled with optimizers. Remark that the target accuracy of the thermodynamic model is obviously limited by the confidence interval on the experimental calibration data. In particular, for many dense gases, and namely heavy fluorocarbons, accurate experimental data are not available. Anyway, even in such unfavorable case, the construction of a thermodynamic model still represents an advantage for CFD simulations over direct interpolations on the experimental database. In this work, two strategies are considered. The first one is the development of an analytic EOS of the Span-Wagner type, characterized by an innovative choice of the independent thermodynamic variables, which greatly

simplifies its implementation within numerical solvers and drastically reduces computational costs. The second strategy employs neural networks of the multi-layer-perceptron type to perform a regression from available thermodynamic data. Both approaches will be validated a priori, through detailed comparisons with well-known thermodynamic models and experimental data available in the literature, and a posteriori, by means of suitable dense-gas-flow test cases.

Analytical equation of State

We look for a functional relationship written in the form proposed by Span-Wagner [4], but with a different choice of the independent thermodynamic variables. The proposed equation is of the form:

$$T = \sum_{l=0}^{L} c_l \left| \frac{\rho}{\rho_{c,ref}} - a \right|^{\bar{i}_l} \left| \frac{\rho e}{(\rho e)_{c,ref}} - b \right|^{\bar{j}_l} \tag{1}$$

where p_c, T_c, Zc, T_e, n, $c_{v\infty}$, are fluid-dependent properties. For a given substance the parameters c_l , $\bar{i}_l$, and $\bar{j}_l$ are fixed for every *l*. The quantities denoted as "ref" are reference quantities used to normalize each variable. A minmax regression is performed to compute the equation coefficients: the search for the coefficients of the new equation is formulated as an optimization problem which minimizes the maximum error between the approximating function (EOS) and a reference thermodynamic database. The minimization is performed by means of a hybrid genetic/gradient-based optimization method.. This procedure is applied to find an equation of state of the form (1) for a class of substances (heavy fluorocarbons) used as working fluids in heat transfer and energy generation applications. In order to check the equation accuracy, the calibration database is derived by applying the classical Martin-Hou equation of state: thus, the model accuracy can be tested outside the range of conditions for which it has been optimized by direct comparison with the "exact" baseline equation. The computed maximal error in this enlarged region is found to be about 0.3%, which remains acceptable. The new equation, however, allows saving 30% of the computational cost while ensuring almost the same accuracy. This gain concerns a single evaluation: when the equations are implemented within a CFD code, where several evaluations are required for each iteration and each grid point, the CPU savings are even more relevant.

Multilayer Perceptron Neural Network

In this paper, the fluid thermodynamic properties at a given point are also computed by means of a neural network of the multi-layer-perceptron (MLP) type, used to perform a regression from available thermodynamic data. We build an MLP with a single internal layer. The network is trained over a subset of the training data available, such that the resulting MLP weights provide the minimum error when applied to the remaining data (test set). The MLP is then implemented within a CFD code, and several dense gas flow simulations are performed.

Conclusions

In the presentation the full details of the analytical equation of state and the multi-layer perceptron neural network will be presented. Both the procedures will be compared, in terms of accuracy and computational cost, with the analytical approach for a variety of dense gas flow problems.

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