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LOCALLY OPTIMIZED VIRIAL EQUATION FOR CFD SIMULATIONS OF REAL GAS FLOWS

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Abstract

The contribution proposes a simple virial-like equation of state (EOS) suitable for CFD simulations of real gas flows through turbines or compressors. The virial coefficients are locally optimized using the idealized isentropic flow through the machine. The resulting equation combined with a simple polynomial fit for the ideal part of the heat capacity provides a better approximation of the full EOS than standard cubic EOS such as Aungier-Redlich-Kwong.

Keywords: CFD, equation of state, real gas.

1 Introduction

The current work is motivated by the needs of an efficient approximation to the real gas equation of state for numerical simulations of flows of nitrogen in the secondary loop of a gas-cooled nuclear reactor. The secondary loop operates at pressures between 7 MPa to 20 MPa and temperatures between 330 K to 800 K. The thermodynamic properties of nitrogen in this temperature and pressure range no longer satisfy the equation of state of an ideal gas with constant heat capacities, and therefore one has to consider a real gas model.

The simplest approach is based on the concept of the so-called pseudoperfect gas model proposed e.g. in [1] where an ideal gas EOS and constant heat capacities are used with parameters set to some nonphysical average values. This approach leads to a very simple model that is, moreover, fully compatible with most simulation software packages. However, the precision of this approach is very limited and is generally not recommended for the simulation of flows through turbines or multistage compressors [1].

The more accurate models of the behavior of real gas are usually based on the Van der Waals cubic equation of state or on its modifications such as the Redlich-Kwong EOS [2], Peng-Robinson EOS [3], or Aungier-Redlich-Kwong EOS [1]. These models, combined with the polynomial fit for the ideal part of the specific heat capacity, generally provide a very good approximation of gas properties in a wide range of pressures and temperatures. Moreover, some of them have already been implemented in commercial and open-source simulation software packages [4]. The main drawback of the cubic equation of state is that the correct evaluation of thermodynamic properties such as internal energy, enthalpy, entropy, etc. becomes rather complicated, and therefore the CFD simulations of flows become much more computationally expensive than for the case of ideal or pseudoperfect gas models.

The complete real gas model of nitrogen according to [5] is formulated using free Helmholtz energy, which is approximated by a combination of 45 terms including exponentials, logarithms and powers of reduced density and reduced temperature. The other thermodynamic quantities are then obtained using appropriate partial derivatives of the Helmholtz energy. The evaluation of thermodynamic properties is computationally extremely demanding, and this model is therefore unsuitable for larger-scale CFD simulations of flow fields. Certain improvements in computational time can be achieved by the labeled variant of the model which has been successfully applied in [6] for superheated steam flows. Note that both the full real gas model and the labeled form are available in the open source CoolProp thermodynamic library [7].

The goal of this work is to develop a simple real gas model of pure nitrogen, which will be formulated using the pressure and temperature as independent variables in order to be able to use it in the framework of the OpenFOAM package. The proposed model will be based on a modified virial equation of state with compressibility expressed as a linear function of pressure. The parameters of the equation will be specifically fitted to a given flow regime to achieve good accuracy at very low computational costs.

2 Real gas model for turbomachinery applications

The cubic equations of state usually provide a very good overall accuracy in a wide range of pressures and temperatures. Nevertheless, for specific regimes, one can obtain better accuracy and lower computational expenses by employing locally optimized EOS in virial form.

2.1 p-virial equation of state

The proposed virial equation of state is based on the standard real gas equation of state in the form

$$pv = zrT, \tag{1}$$

where z is the compressibility factor. The compressibility factor z is usually expanded as a power series in specific volume, i.e.

$$z \approx z(v) = 1 + \frac{B}{v} + \frac{C}{v^2} + ..., \tag{2}$$

where b, C, ... are the so-called virial coefficients. The virial EOS can be expressed also as a power series in pressure as

$$z \approx z(p) = 1 + B'p + C'p^2 + ... \tag{3}$$

The first variant is usually preferred due to its faster convergence [2]. Nevertheless, our model uses the pressure-based variant of the EOS, keeping only the linear part of the expansion

$$z \approx z(p) = z_0 + z_1 p. \tag{4}$$

The coefficients z_0 and z_1 are then set to match the expansion line as closely as possible to the diagram in $p - v$.

The proposed EOS is then

$$pv = (z_0 + z_1 p)rT. \tag{5}$$

Note that it can be equivalently rewritten in the "standard" pressure-based virial form as $pv = (1 + z_1' p)r'T$ with $z_1' = z_1/z_0$ and the modified specific gas constant $r' = z_0 r$.

2.2 Thermophysical properties

The real gas specific enthalpy at a given pressure and temperature is evaluated using

$$dh = c_p dT + \left[v - T \left(\frac{\partial v}{\partial T} \right)_p \right] dp. \tag{6}$$

One can see from the proposed EOS that

$$\left(\frac{\partial v}{\partial T} \right)_p = \frac{(z_0 + z_1 p)r}{p} = \frac{v}{T}, \tag{7}$$

and therefore the second term on the right-hand side disappears. Therefore

$$dh = c_p dT. \tag{8}$$

Moreover, from the conditions of the total differential we have $\partial c_p / \partial p = 0$ and therefore c_p depends only on the temperature. Therefore

$$h(p, T) = h(T) = \int_{T_{ref}}^{T} c_p(\theta)\, d\theta + h_{ref}, \tag{9}$$

where T_{ref} and h_{ref} are some reference values.

The expression for specific entropy is obtained from

$$ds = \frac{c_p}{T} dT - \left(\frac{\partial v}{\partial T} \right)_p dp = \frac{c_p(T)}{T} dT - \frac{(z_0 + z_1 p)r}{p} dp. \tag{10}$$

Integrating this relation from a reference state denoted by subscript ref one gets

$$s(p,T) = \int_{T_{ref}}^{T} \frac{c_p(\theta)}{\theta}\, d\theta - r z_0 \ln\left(\frac{p}{p_{ref}}\right) - r z_1 (p - p_{ref}) + s_{ref}. \tag{11}$$

The specific internal energy ε is calculated from

$$\begin{aligned} d\varepsilon &= \left[c_p(T) - p\left(\frac{\partial v}{\partial T}\right)_p\right] dT - \left[p\left(\frac{\partial v}{\partial p}\right)_T + T\left(\frac{\partial v}{\partial T}\right)_p\right] dp = \\ &= \left[c_p(T) - (z_0 + z_1 p) r\right] dT - \left[-\frac{z_0}{p} r T + (z_0 + z_1 p)\frac{rT}{p}\right] dp = \\ &= \left[c_p(T) - (z_0 + z_1 p) r\right] dT - z_1 r T dp, \end{aligned} \tag{12}$$

which gives

$$\begin{aligned} \varepsilon(p,T) &= \int_{T_{ref}}^{T} c_p(\theta)\, d\theta - (z_0 + z_1 p_{ref}) r (T - T_{ref}) - z_1 r T (p - p_{ref}) = \\ &= h(p,T) - pv - h_{ref} + p_{ref} v_{ref} + u_{ref}. \end{aligned} \tag{13}$$

The specific heat capacity at constant volume is then

$$c_v(p,T) = \left(\frac{\partial \varepsilon}{\partial T}\right)_v = c_p(T) - r\frac{(z_0 + z_1 p)^2}{z_0}. \tag{14}$$

3 Numerical method

The real gas model has been implemented in a finite-volume solver in house *myLusgsFoam* [8] available at [9]. The is built on top of the OpenFOAM software package. In contrast to the segregated pressure correction method implemented in standard OpenFOAM solvers, the *myLusgsFoam* uses the so-called coupled approach where the inviscid fluxes are evaluated using approximate Riemann solvers and the viscous fluxes are approximated using central schemes. The spatial approximation is improved by piecewise linear reconstructions with the Barth-Jespersen or Venkatakrishnan limiter [10]. The implicit discretization in time is achieved using the matrix-free lower-upper symmetric Gauss-Seidel (LU-SGS) method [11]. In the case of steady-state problems, the method uses the local time-stepping acceleration method. In the case of transient simulations, the LU-SGS with local time-stepping is employed in dual time.

The method is formulated in the so-called conservative variables (ie ρ, $\rho\vec{u}$, and ρE where ρ is the density, $\vec{u}$ is the velocity vector and E is the total energy). However, the solver internally uses different sets of variables, namely p, $\vec{u}$, and h. The reason for choosing $(p, \vec{u}, h)$ as the independent variables for the solver is to keep compatibility with other parts of the OpenFOAM package, namely, with the turbulence models, boundary conditions, additional sources, online postprocessing tools, etc.

Each step of the solver therefore requires:

1. Convert from (p,h) to (ρ,ε) pair.
2. Make one LU-SGS step that gives new values of ρ, $\vec{u}$, and $E = \varepsilon + ||\vec{u}||^2/2$.
3. Convert from (ρ,ε) to (p,h) pair.

Moreover, the solver requires also a calculation of $T = T(p,h)$, and, especially for input boundary conditions based on total quantities, also the evaluation of pressure and temperature of the (h,s) pair.

The conversion from (p,h) to (ρ,ε) can be done by solving the scalar nonlinear problem for enthalpy, see eq. (9):

$$h(\mathbf{p}, T) = \mathbf{h} \tag{15}$$

for unknown temperature T. The bold symbols represent given values of pressure and enthalpy. The solution is obtained by using Newton-Raphson iterations. The initial estimate for the temperature is taken, e.g. from the last time step. The density and internal energy are then directly evaluated using (5) and (13).

The conversion from (ρ, ε) to (p, h) is achieved by the solution of the energy relation combined with the equation of state, see (13):

$$\varepsilon(p(\boldsymbol{\rho}, T), T) = \boldsymbol{\varepsilon}. \tag{16}$$

This is again a scalar non-linear equation for the temperature which can be solved using the Newton-Raphson method. The pressure is then evaluated using the equation of state (5) and finally, the enthalpy is directly evaluated from the temperature.

Evaluation of thermodynamic quantities from the pair (h, s) usually requires the solution of a system of two non-linear equations, which is computationally more expensive. Nevertheless, we usually use those functions only at the inlet boundary, and therefore the overall computation time is not affected too much by these calculations.

4 Results

The performance of the proposed thermodynamic model is investigated by the solution of a 2D inviscid transonic flow through a channel, 3D turbulent flow through a model of a 5-stage axial compressor, and through a model of a 2-stage axial turbine. The results obtained with the proposed model are compared to the results employing the model of pseudoperfect gas, cubic EOS, and the tabelated full real gas model from CoolProp library.

4.1 2D inviscid flow through a channel

The first case considered here is the 2D inviscid flow through a channel with a circular arc bump on the lower wall. The inlet boundary conditions were set to total pressure $p_{tot,1} = 10\,\mathrm{MPa}$, total temperature $T_{tot,1} = 400\,\mathrm{K}$, and the inlet velocity direction parallel to the channel length. The outlet static pressure was set to the value corresponding to the outlet isentropic Mach number $M_{2i} = 0.675$ considering the corresponding thermodynamic model.

In order to calibrate the thermodynamic model, the isentropic expansion from the total inlet values to sonic conditions has been calculated for a full real gas model using the CoolProp library. Then z_0 and z_1 have been obtained by a least-square fit of the true value of z along this expansion line. The $c_p(T)$ was approximated by the fourth order polynomial fit to the values of c_p along the expansion. The locally optimized EOS is then (in SI units)

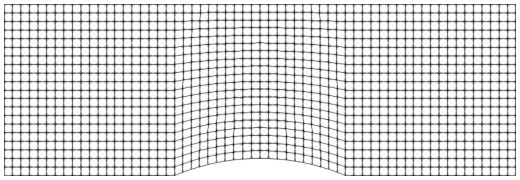
$$pv = (0.945149 + 7.402\,86 \times 10^{-9} p) rT \tag{17}$$

with

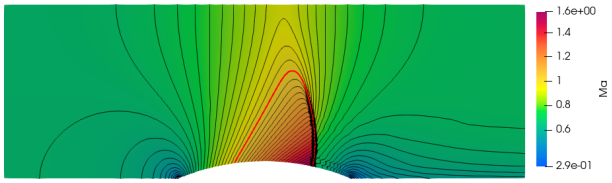
$$c_p(T) = 1012.1 + 0.73661T - 5.7491 \times 10^{-4} T^2 - 1.4646 \times 10^{-6} T^3 + 2.1026 \times 10^{-9} T^4. \tag{18}$$

The results obtained with the proposed thermodynamic model have been compared to the pseudoperfect gas model calibrated according to [1]. The constant compressibility factor was in this case set as $z = 1.073$, the heat capacity $c_p = 1092.82\,\mathrm{J/kg/K}$ and the c_p/c_v ratio was 1.411. The cubic Aungier-Redlich-Kwong EOS parameters were taken from [1] and the polynomial representation of c_p was taken from [12].

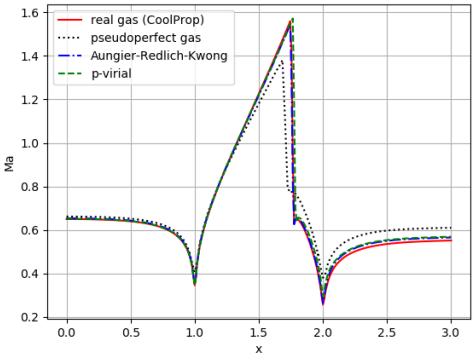
Calculations have been carried out using a structured mesh with 300×100 cells without any mesh refinement. Figure 1 shows the sketch of the computational mesh and the distribution of the Mach number in the channel obtained using the proposed thermodynamic model. One can see there the acceleration of the flow that reaches supersonic speed over the bump. The supersonic region is closed by a shock wave. Figure 1c compares the distribution of the mach number along the lower wall. One can see that the pseudoperfect gas model does not agree well with the full real gas results obtained with the CoolProp library. However, both the cubic Aungier-Redlich-Kwong EOS and the current model denoted here as p-virial agree very well with the full real gas simulation.



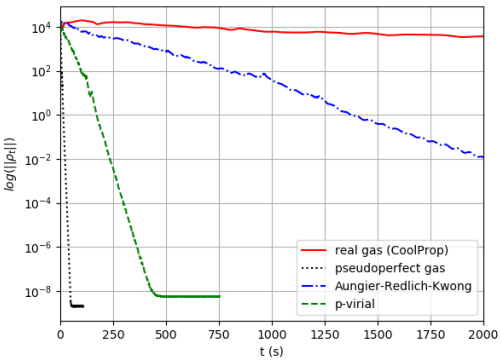
(a) Computational mesh (every 5th line shown)



(b) Distribution of Mach number in the channel



(c) Distribution of the Mach number along lower wall



(d) Convergence to steady state w.r. to computational time

Figure 1: Inviscid flow through a 2D channel.

Finally, figure 1c compares the convergence history with respect to computational time for all four models. All calculations were carried out using a single core of Intel i5-12600 at 4.8 GHz CPU. Although all simulations converged very well to a steady state, the computational times were very different. The fastest pseudoperfect gas model required approximately 5.5 ms per iteration, the proposed p-virial model needed 37.6 ms, which is about 7 times more than the pseudoperfect gas model. The Aungier-Reglich-Kwong model required 303 ms and the full real gas model via the tabelated CoolProp 3056 ms.

4.2 3D turbulent flow through 5-stage axial compressor

The second case deals with the simulation of turbulent flows through a 5-stage axial compressor model designed within the framework of a project Kobra supported by the Czech Republic Technology Agency. The compressor should drive nitrogen into the secondary loop of the gas-cooled nuclear reactor. The design mass flow rate is 274 kg/s at 1750 rpm with the total inlet pressure $p_{tot,1} = 7.5$ MPa and the total temperature $T_{tot,1} = 333.15$ K.

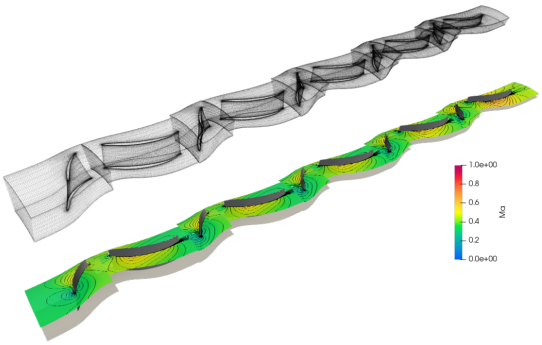
The calibration of the thermodynamic model has been performed in the same way as before, i.e. fitting z and c_p to an isentropic expansion between the inlet total and sonic states. The least-square fit gives in this case

$$pv = (0.962184 + 6.761\,31 \times 10^{-9} p) rT, \tag{19}$$

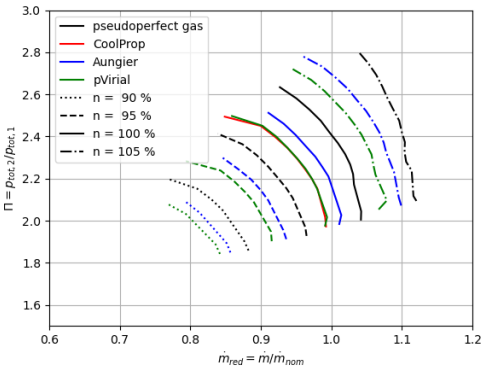
$$c_p(T) = 1031.6 - 0.273\,54T - 0.632 \times 10^{-3} T^2 + 5.0538 \times 10^{-6} T^3 - 2.5729 \times 10^{-9} T^4. \tag{20}$$

Calculations have been performed in two configurations. In the first case, a steady-state calculation has been performed using the so-called mixing plane approach. In this case, a single channel has been simulated, see Figure 2a. The mesh contains approximately 1×10^6 hexahedral cells. The near wall refinement was chosen in such a way that the first cell was located at $y^+ \approx 300$. The effects of turbulence were modeled using the RANS approach with the $k - \omega$ SST model [13] combined with wall functions.

Figure 2b shows the part of the compressor map obtained for different thermodynamic models at compressor 90 % to 105 % of nominal speed of the compressor. Note that, because of high computational time, only the nominal speed was considered for full gas model. Figure 2b clearly

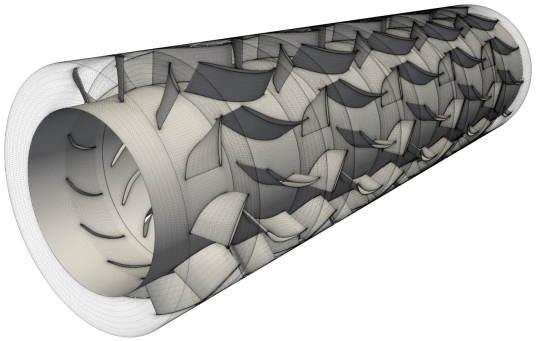


(a) Computational mesh and the distribution of Mach number in a cylindrical cut.

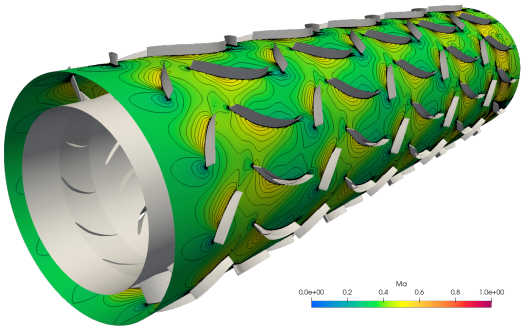


(b) Compressor map obtained with different models.

Figure 2: Steady state flows through a model of 5-stage axial compressor using mixing-plane



(a) Computational mesh.



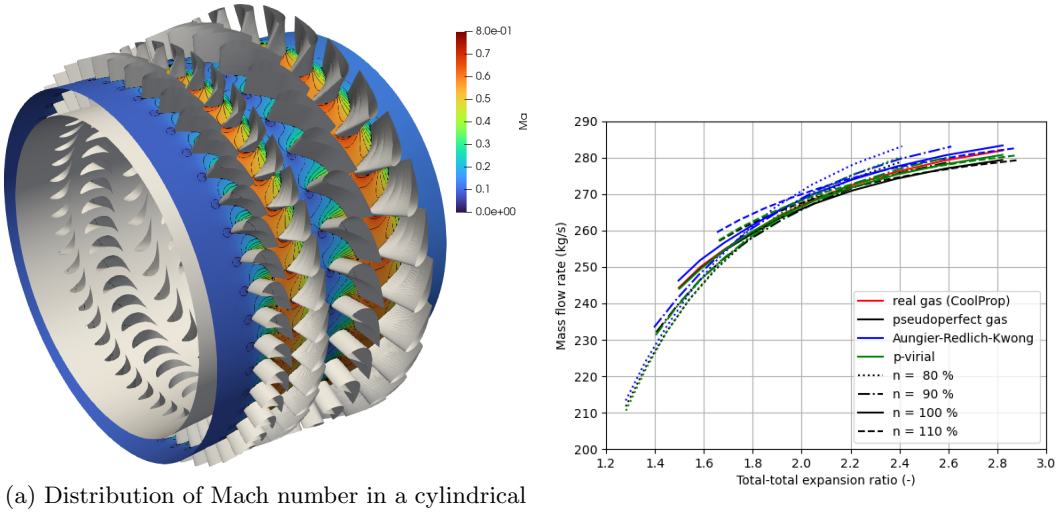
(b) Distribution of Mach number in a cylindrical cut.

Figure 3: Transient flows through a full model of 5-stage axial compressor

shows that the pseudo-perfect model significantly overestimates the flow rate and/or compression ratio compared to all other models. The proposed p-virial model corresponds very well to the full real gas model (at least for nominal speed), and the correspondence is even better than for the Aungier-Redlich-Kwong EOS.

The second setup corresponds to the full model of the compressor with sliding mesh interfaces between the stators and the rotors. The mesh consists of approximately 11×10^6 hexahedral cells with the same near wall refinement as in the previous case. Due to the extremely high computational costs of full and cubic EOS models, only pseudoperfect gas and p-virial simulations have been performed in the nominal regime. The total-total compression ratio obtained with the pseudoperfect gas was evaluated $\Pi = 2.6$ while the p-virial model gives only $\Pi = 2.2$. Similarly, the thermodynamic efficiency evaluated from the simulation with pseudo-perfect gas was $\eta = 92\,\%$ whereas for the p-virial model we got only $\eta = 86\,\%$.

These calculations indicate that the pseudoperfect gas model is not suitable for multistage compressors. This is in accordance to [1] where the author recommends this model, but for the case of multi-stage configuration, he assumes calibration of the model for each of the stages separately. On the other hand, the p-virial model corresponds very well to the full real gas model and the computational demands are still acceptable.



(a) Distribution of Mach number in a cylindrical cut.

(b) Turbine map.

Figure 4: Flows through a full model of 2-stage axial turbine

4.3 3D turbulent flow through 2-stage axial turbine

Another case considered in this work is a flow through a model of a two-stage turbine. The inlet boundary conditions were set to $p_{tot,1} = 20\,\text{MPa}$ and $T_{tot,1} = 1103.2\,\text{K}$. The nominal speed was 17 500 rpm. The computational mesh has approximately 400 000 and 14×10^6 hexahedral cells for steady-state single-channel mixing plane and full transient configurations, respectively. The near-wall refinement was $y^+ \approx$100 to 200.

The p-virial model parameters fitted to isentropic expansion from inlet state to nominal outlet pressure are

$$pv = (1.008383 + 2.920\,928 \times 10^{-9} p) rT, \tag{21}$$

$$c_p(T) = 1039.9 - 0.3050T + 0.9220 \times 10^{-3} T^2 - 0.6079 \times 10^{-6} T^3 + 0.176\,58 \times 10^{-9} T^4 \tag{22}$$

Figure 4a shows the complete turbine model with a distribution of the absolute Mach number in a cylindrical cut near the mean radius. The turbine map calculated for different thermodynamic models using a one-channel mixing plane configuration is shown in Fig. 4b. One can see that in this case, all models predict similar mass flow rates for a given expansion ratio.

5 Conclusions

The main contribution of the work is the design and testing of a simple thermodynamic model that allows for complex simulations of the flow fields in turbines and compressors. The key point is the assumption of a simple linear dependence of the compressibility coefficient only on the pressure. The consequence is, among other things, that enthalpy is only a function of temperature. Thanks to this, conversions between some pairs of state variables are realizable by solving a scalar nonlinear problem, which significantly reduces the computational effort.

Numerical simulations then show that the fitted model approximates the full real gas model very well. On the other hand, it should be noted that the fitted model, unlike the cubic equation of state, is only applicable in the vicinity of the parameter to which it has been calibrated.

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