20th International Conference
ENGINEERING MECHANICS 2014
Svratka, Czech Republic, 12 – 15 May 2014

NUMERICAL SOLUTION OF INVISCID TRANSONIC FLOW IN A CHANNEL WITH COMPLEX EQUATION OF STATE

V. Hric, J. Halama, J. Fürst*

Abstract: *The presented paper deals with the incorporation of complex (non-ideal) equation of state into the Euler model which describes dynamics of inviscid fluid. We have performed numerical experiments for the steady transonic flow of steam in the 2D GAMM channel (channel with the 10% thick circular arc bump on the lower wall). The using of complex equation of state allows the more accurate prediction of thermodynamic quantities, mainly in the regions where compressibility factor differs from unity. The results achieved by the van der Waals, Redlich-Kwong-Aungier, one-coefficient virial and special gas IAPWS equation of state are compared with the traditional perfect gas model. All of these models are implemented into in-house CFD code based on the finite volume method in 2D along with the AUSM+ flux scheme. The results confirmed the necessity of using more complex equations of state, especially when higher pressures are considered.*

Keywords: Real gas, Euler inviscid model, GAMM channel, Finite volume method.

1. Introduction

Major part of CFD codes frequently limit attention to the perfect gas model (PG). This approach is justified only if thermodynamic quantity ranges are relatively narrow and the compressibility factors do not differ too much from unity. It is usually true if pressures are relatively low and (or) temperatures are higher. It yields significantly reductions in computational times. However, not negligible errors can be occured in some non-ideal state regions. To remedy this, more complex equations of state must be used.

2. Flow Model and Equations of State

The dynamics of inviscid fluid flow in 2D is described by the system of time dependent Euler equations

$$\boldsymbol{W}_t + \boldsymbol{F}_x + \boldsymbol{G}_y = \boldsymbol{0},$$

where $\boldsymbol{W}(t,x,y) = (\rho, \rho u, \rho v, \rho E)^T$ is vector of conservative variables, $\boldsymbol{F}(\boldsymbol{W}) = (\rho u, \rho u^2 + p, \rho uv, \rho uH)^T$, $\boldsymbol{G}(\boldsymbol{W}) = (\rho v, \rho uv, \rho v^2 + p, \rho vH)^T$ are vectors of fluxes in which ρ, u, v, E, p, H is density, x- and y-component of velocity, specific total (internal) energy, static pressure and specific total enthalpy, respectively. This system of equation must be closed by the relation for pressure $p = p(\boldsymbol{W})$. Analytical form of the pressure equation exists only in the case of PG model. In cases where more complex equations of state are used we obtain the pressure value only by some iterative procedure. In this paper we adopted the Newton-Raphson method (NR) which solves firstly nonlinear algebraic equation for temperature $T = T(\rho, e) = T(\boldsymbol{W})$ from known values of density $\rho(\boldsymbol{W})$ and internal energy $e(\boldsymbol{W})$. Static pressure is then evaluated from relation $p = R\rho_c T_c (1 + \delta\phi_\delta^{res})\, \delta/\tau$.

In the following we briefly summarize one of the possible techniques for evaluation of thermodynamic quantities in the case of non-ideal gases. The value of certain thermodynamic quantity $Q(\rho, T)$ is given as the contribution of its ideal part $Q^{id}(\rho, T)$ computed with the means of PG model from the known value of density and temperature. This ideal value is then corrected by the residual correction $Q^{res}(\rho, T)$, cf. Fig. 1, for which the following integral formula reads (Novák, 2007)

* Ing. Vladimír Hric (vladimir.hric@gmail.com), Assoc. Prof. Ing. Jan Halama, PhD, Assoc. Prof. Ing. Jiří Fürst: Department of Technical Mathematics, Faculty of Mechanical Engineering, CTU Prague, Karlovo náměstí 13, 121 35 Prague, CZ

$$Q^{res} = Q - Q^{id} = \int_0^{\rho} \left(\frac{\partial Q}{\partial \rho} - \frac{\partial Q^{id}}{\partial \rho} \right) d\rho.$$

There are actually two equations required for evaluation of all thermodynamic quantities. The first is the thermal equation of state typically in the form $p = p(\rho, T)$. It is the so-called incomplete equation of state since it lacks caloric description. The second is the temperature dependent relation for specific isobaric heat capacity in the ideal gas state $c_p^{id} = c_p^{id}(T)$. However, in the last decades the approach with so-called fundamental equations of state became popular. In this paper we use the form with non-dimensional Helmholtz (free) energy $\phi(\delta, \tau)$, where $\delta = \rho/\rho_c, \tau = T_c/T$ and $(\cdot)_c$ designates critical state. This function has two parts. The first part is the ideal contribution ϕ^{id} only stemmed from the ideal specific internal energy e and the ideal specific entropy s along with some supplied equation for $c_p^{id}(T)$. In the case of steam we adopted the relation from (Wagner & Pruss, 2002). The second part is the residual correction ϕ^{res} stemmed from some non-ideal equation of state. In the paper all of the used traditional equations of state in the form $p = p(\rho, T)$ are transformed to its corresponding residual Helmholtz energy part via the relation borrowed from (Novák, 2007)[†]

$$\phi^{res}(\rho, T) = \int_0^{\rho} \frac{z - 1}{\rho} \, d\rho,$$

where $z = p/\rho RT$ is the compressibility factor and R is the specific gas constant. All thermodynamic properties can be derived by using the appropriate combinations of ϕ^{id} and ϕ^{res} and their first and second derivatives. Details can be found e. g. in (Wagner & Pruss, 2002).

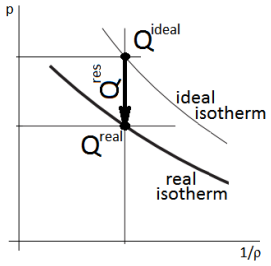

Fig. 1: Residual correction.

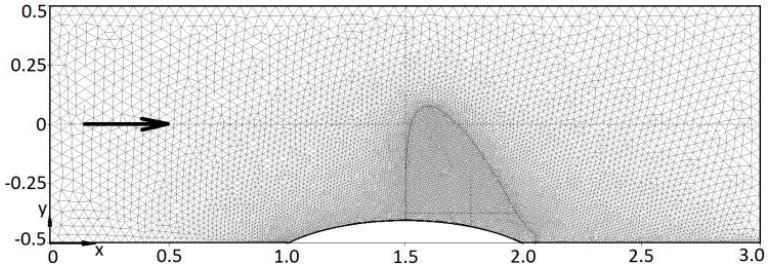

Fig. 2: Computational mesh of GAMM channel.

PG model is both thermally and calorically perfect. This model predicts constant value of compressibility factor which consequences in validity of Mayer's relation. Furthermore, the specific isobaric heat capacity is constant too. This limitation naturally causes vanishing of residual part ϕ^{res}, and so reduces thermodynamic concept to simple analytical form. The residual part relation for others used equations of state along with their coefficients which were computed in this paper are briefly summarized in the following part where e. g. in the case of vdW model for its coefficients holds $n = -a\rho_c/RT_c$, $d = b\rho_c$ where a, b are classical coefficients of this model.

- **Van der Waals (vdW)**

  $\phi^{res}(\delta, \tau) = n\delta\tau - \ln(1 - d\delta)$ $n = -1.838708$, $d = 0.544802$

- **Redlich-Kwong-Aungier (RKA)**

  $\phi^{res}(\delta, \tau) = n\tau^t \ln(1 - d_1\delta) - \ln(1 - d_2\delta)$

  $n = -4.933962$, $t = 1.958391$, $d_1 = -0.377615$, $d_2 = 0.367840$

- **One-coefficient virial (1-VIR)**

  $\phi^{res}(\delta, \tau) = \delta \sum_{i=1}^{4} n_i \tau^{t_i}$ t_i given in (Harvey & Lemmon, 2004)

- **Special gas equation IAPWS-95 (GE-IAPWS-95)**

  $\phi^{res}(\delta, \tau) = \sum_{i=1}^{7} n_i \delta^{d_i} \tau^{t_i}$ n_i, d_i, t_i given in (Wagner & Pruss, 2002)

[†] Owing to consistency and comparison with the special gas equation provided by IAPWS

3. Numerical Method

The computational domain of the test GAMM channel is discretized by using Gmsh mesh generator (Geuzaine & Remacle, 2009). The mesh is unstructured triangular (set frontal meshing algorithm) and contains 9247 nodes, 18144 cells and 27390 interfaces, cf. Fig. 2. The cell-centered finite volume method with piece-wise constant reconstruction of cell data is used for discretization of spatial derivatives. Fluxes through common cell interfaces are computed applying AUSM+ scheme. The resulting system of ordinary differential equations is solved by 3-stage low-storage Runge-Kutta method with $CFL = 1.5$. Time step for this method is estimated by the relation borrowed from (Blazek, 2006). Subsonic inlet flow is considered, and so we prescribed stagnant pressure $p_{stg} = 12\ MPa$, stagnant temperature $T_{stg} = 675\ K$ and zero y-component of velocity at the inlet boundary. Prescription of high pressure is due to effort to simulate flow in non-ideal state region. The value of stagnant entropy along with extrapolated static pressure from interior is used for calculation of density and temperature in ghost cells where the system of two nonlinear algebraic equations must be solved (NR method applied). Considering outlet flow in subsonic regime, we prescribed back pressure p_{out}, via the pressure ratio $p_{out}/p_{stg} = 0.7463$; density and velocity components are extrapolated from interior. NR method is applied for evaluation of temperature from known density and pressure. At the inviscid wall boundary zero normal velocity component is prescribed. Initial estimates for all NR calculations are taken from previous time level.

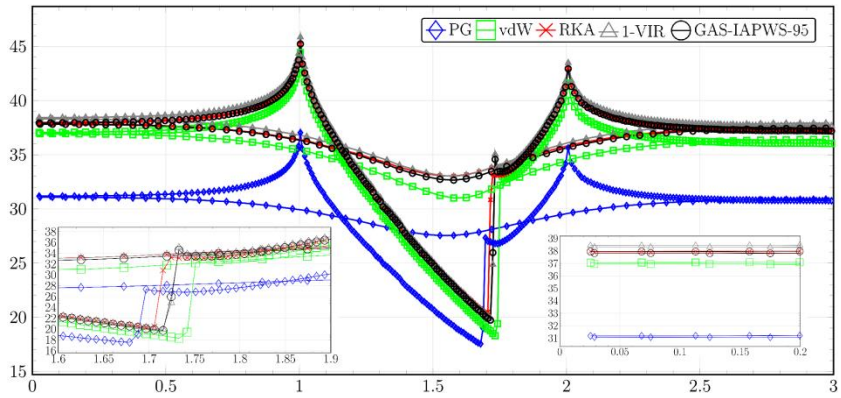

Fig. 3: Lower and upper wall density [kg m^{-3}] distribution.

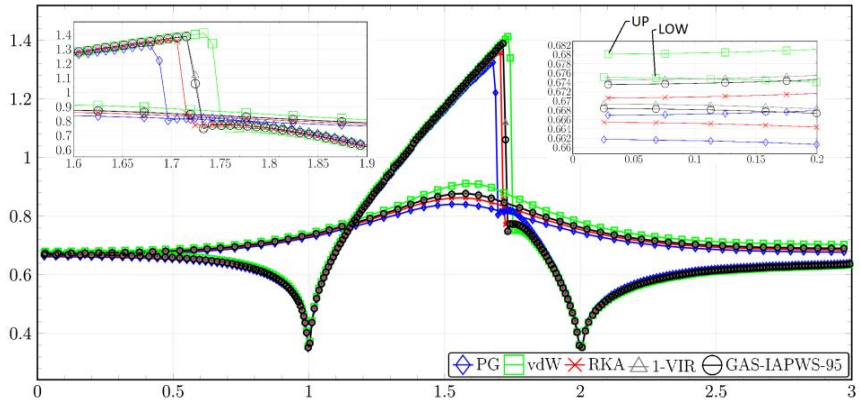

Fig. 4: Lower and upper wall Mach number [-] distribution.

4. Results

Fig. 3 shows distribution of density along the upper and the lower wall. Real gas models give significantly higher values and they shift location of shock wave downstream. Fig. 4 presents distribution of Mach number. Deviations from PG model are on either walls relatively small. However, this is not true in the vicinity of shock wave along the lower wall and in the middle of the upper wall. Shifting of shock wave location on the lower wall resulted in higher peak values of Mach number (PG 1.32, vdW 1.41, RKA 1.36, 1-VIR and GE-IAPWS-95 1.39) and in lower values in the location of so-called Zierep's singularity (= stronger shock waves). Maximum Mach number values on the upper wall are as follows, PG 0.84, vdW 0.91, RKA 0.86, 1-VIR and GE-IAPWS-95 0.88.

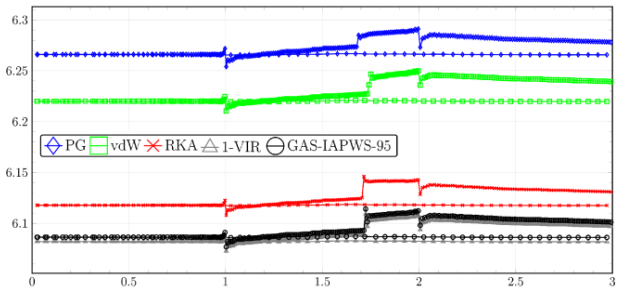

Fig. 5: Entropy [kJ kg^{-1} K^{-1}] distribution.

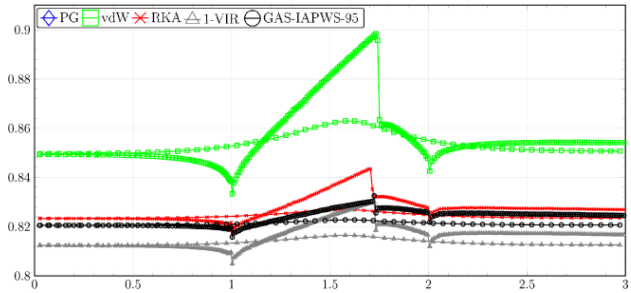

Fig. 6: Compressibility factor [-] distribution.

Fig. 5 depicts distribution of entropy. Real gas models give lower values. From physical point of view it is known that in the case of inviscid fluid flow entropy should grow only as a result of shock wave formation. Non-physical entropy increase and decrease on the bump surface up to the shock wave location and wiggles at the bump inlet and outlet in our results are caused by imperfection and numerical viscosity of used flux scheme. Fig. 6 shows distribution of the compressibility factor. All real gas models give substantially lower values and range between 0.805 and 0.845 (except vdW model). The comparison of real gas total CPU time per one cell and per one time step related to the same quantity in the case of PG model is summarized in Tab. 1. The most CPU time consuming operation (relative to the real gas model implementation) is repeated numerical solution of temperature from known internal energy and density (temperature is required for evaluation of pressure and other quantities like e. g. sound speed). In this case the average number of iterations in NR method ranges between 1.55 and 2.15. The maximum values are in the vicinity of shock wave.

Tab. 1: Relative CPU time comparison

EQUATION OF STATE	PG	vdW	RKA	1-VIR	GE-IAPWS-95
RELATIVE CPU TIME	1.00	2.08	3.04	4.37	6.13

5. Conclusion Remarks

Results confirmed necessity of using more complex equations of state when flow simulations include non-ideal state regions. It was presented on distributions of selected parameters. Drawbacks of this augmentation are loss of explicitness in thermodynamic concept and higher CPU time demands.

Acknowledgement

This work was supported by the grant No. SGS13/174/OHK2/3T/12 of the Grant Agency of the Czech Technical University in Prague.

References

Aungier, R. H. (1994) A fast, accurate real gas equation of state for fluid dynamic analysis applications. J. Fluids Eng., 117, 2, pp. 277-281.

Blazek, J. (2006) Computational fluid dynamics – principles and applications. Elsevier, Amsterdam.

Geuzaine, Ch. & Remacle, J. F. (2009) Gmsh – a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities. International Journal for Numerical Methods in Engineering, 79, 11, pp. 1309-1331.

Harvey, A. H. & Lemmon, E. W. (2004) Correlation for the second virial coefficient of water. J. Phys. Chem. Ref. Data, 33, 1, pp. 369-376.

Novák, J. P. (2007) Thermodynamic properties of gases. ICT Press, Prague, (in Czech).

Wagner, W. & Pruß, A. (2002) The IAPWS formulation 1995 for the thermodynamic properties of ordinary water substance for general and scientific use. J. Phys. Chem. Ref. Data, 31, 2, pp. 387-535.