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Development of a CFD real gas flow solver for hybrid grid

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SUMMARY

This paper describes the development and the testing of a CFD real gas flow solver. In the first part of the paper is the description of the analysis performed to define the best approach to a real gas flow solver and the various solution considered. In the second part the various solution adopted are described, in the last part of the paper the CFD solver tests are presented together with results. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: real gas; hybrid grid; LDFSS

1. INTRODUCTION

Aerodynamic analyses of turbine components are currently used by turbine manufacturers to improve the performance of their products. CFD simulations are nowadays a common practise in the design stage of a modern gas turbine. These numerical methods allow accurate investigations of the complex aerodynamic problems of gas turbine components at reasonable costs and also provide the designer with important details on the flow patterns. It is the authors opinion that further optimization of existing gas turbines efficiency cannot be achieved without the use of such detailed 3D aerodynamic investigations.

The demand for a reliable tool to study the aerodynamic behaviour of the component is growing amongst steam turbine designers too. Nevertheless, the application of CFD to the steam turbine area is still less widely spread than in the gas turbine field.

Undeniably, one of the main reasons for this delay is the lack of a proper model for the steam physical properties since solvers are developed in most of the cases under the limiting conditions of the perfect gas behaviour.

The aim of the present work is to provide an approach addressing this lack and a method is presented for implementing a real gas model in a perfect gas Reynolds averaged Navier–

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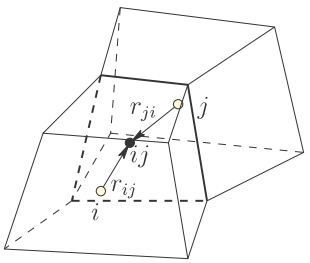
Stokes (RANS) flow solver. The solver considered is based on a 3D upwind unstructured finite volume method (FVM) with implicit time-marching for steady state flow. In the following, the real gas flow solver will be described considering the modifications in the discretization method, the implementation of the real fluid model and the treatment of boundary conditions as well.

2. DISCRETIZATION METHOD

In the present work the real gas solver is developed from an existing and well-tested 3D Navier–Stokes code for hybrid grids [1]. The spatial discretization is based on a cell centred FVM that integrates the equations over the volume Ω_i of every cell embodying the computational mesh:

$$\frac{\partial Q}{\partial t}+\frac{\partial F_k}{\partial x_k}=\frac{\partial G_k}{\partial x_k}\rightarrow\frac{\Delta Q}{\Delta t}\approx\frac{1}{\Omega_i}\int_{\partial\Omega_i}(G-F)\cdot\mathbf{n}\,\mathrm{d}s\rightarrow\frac{\Delta Q}{\Delta t}\approx\sum_{j\in\mathrm{neigh}(i)}(G-F)_{ij}\cdot\mathbf{n}\Delta A_{ij}\qquad(1)$$

Here F and G are the convective and diffusive fluxes of the equations, $Q=\{\rho,\rho V,\rho(e+V^2/2)\}$ the conservative variables, ΔA_{ij} the face area. The pointer neigh(i) represents the group of elements neighbouring the element i. The convective flux of mass, momentum and energy over the cell surfaces is computed numerically using an upwind scheme that consists of a reconstruction, an evaluation and a limiting phase [2]. In the reconstruction phase (or projection step) the solution on both sides of a face (*left* and *right*) is computed from the known average values of the two neighbouring elements. Second order accuracy of the discretization method is ensured when the solution is linearly interpolated onto the face midpoint (ij) from both the adjacent cell centres



$$Q_{ij,\mathrm{L}}=Q_i+\nabla Q_i\cdot\mathbf{r},\quad Q_{ij,\mathrm{R}}=Q_j+\nabla Q_j\cdot\mathbf{r}\qquad(2)$$

The gradient ∇Q_i is evaluated by means of a least-squares approximation using a computation molecule constituted by the element i, the elements $j\in\mathrm{neigh}(i)$ and the elements $k\in\mathrm{neigh}(j)$. The least-squares approximation enables a uniform second order approximation of the solution gradients throughout the whole grid despite the local cell type and shape [1]. The evolution phase computes the actual integral of convective flux for mass, momentum end energy across each face through a midpoint quadrature. The midpoint average convective flux is consistent with the interaction of the two left and right states computed by (2) according to a 1D Riemann problem. This step is carried out using the approximate Riemann solver suggested by Roe. A nonlinear slope limiting of the solution gradients is imposed on the projection phase as suggested by Reference [2]. The whole discretization scheme is second

order accurate in space and satisfies the monotonicity TVD requirements of the physical flow. The viscous flux term is discretized by a conventional unbiased centred scheme. The steady state time-marching approach is based on an implicit relaxed Newton method using an ILU(0) preconditioned GMRes iterative scheme as linear solver [3]. The turbulence model is the linear k–ω two equation model by Wilcox improved with some recent developments concerning the turbulence physical realizability [4].

2.1. Limits of the upwind method

When considering real gases, the main limit of the actual discretization scheme is represented by the evaluation phase. In fact, by definition, the Roe's scheme requires a linear relationship among pressure, density and internal energy. Accordingly, an attempt to solve real gases through this scheme is inconsistent and shows poor stability features arising as a consequence of the actual nonlinear relation linking pressure, density and internal energy. In order to overcome this problem a different and more general upwinding approach has been selected in the family of hybrid schemes.

The advantage of such hybrid schemes over the earlier Godunov-type approximate Riemann solvers (as the Roe's method) is the use of a separate treatment for the pressure waves and for the convective fluxes. This separation let the scheme to be more general and insensitive to the specific relationship linking the thermodynamic state variables (i.e. pressure, density and energy). The hybrid schemes from the AUSM + (advection upstream splitting method) family [5, 6] possess the necessary blend of robustness and accuracy required to be used with a real gas equation. The AUSM schemes are based on the acoustic propagation of pressure terms while a nonlinear law of the local Mach number is used for blending the left and right convection terms. More precisely, the AUSM version named LDFSS(2) (low diffusion flux-splitting scheme) from Edwards [7] was chosen for the present application. This version has the main advantage of a more stable resolution of shocks and flow gradients even for non-aligned grids. This last feature suggests the LDFSS(2) as the most suitable and promising approach to be used with general unstructured grids.

The original LDFSS(2) has been reviewed for the present application assuming a quasi-1D approximation normal to the faces allowing a straightforward implementation in the existing FVM method. In this regard, the conserved variables are projected from adjacent cells onto the face midpoint using the same linear reconstruction phase with slope limiting.

2.2. Flux evaluation: LDFSS(2)

The flux evaluation is based on the splitting of the flux (F) into pressure and convective terms

$$F = F^c + F^p = \rho a M_n \tilde{F}^c + p\tilde{F}^p \tag{3}$$

$$\tilde{F}^c = [1,\ u_x,\ u_y,\ u_z,\ H]^{\mathrm{T}}, \quad \tilde{F}^p = [0,\ n_x,\ n_y,\ n_z,\ 0]^{\mathrm{T}} \tag{4}$$

where ρ is the density, a the sound speed, u_x, u_y and u_z are the three components of the velocity vector and n_x, n_y and n_z are the three components of the inter-element face normal. In Equation (3), M_n is the normal Mach number. According to the proposed splitting the final

convective and pressure fluxes on the interface ij between elements i and j take the form

$$F_{ij}^{c} = a_{ij}(\rho_{ij,\mathrm{L}} C^{+} F_{ij,\mathrm{L}}^{\tilde{c}} + \rho_{ij,\mathrm{R}} C^{-} F_{ij,\mathrm{R}}^{\tilde{c}}) \tag{5}$$

$$F_{ij}^{p} = \tilde{F}_{ij}^{p}(D_{\mathrm{L}}^{+} p_{ij,\mathrm{L}} + D_{\mathrm{R}}^{-} p_{ij,\mathrm{R}}) \tag{6}$$

where the subscript L and R refer to the value projected on the face ij from left and right, respectively. The coefficients C^{+}, C^{-}, D^{+} and D^{-} are nonlinear functions of the Mach number whose values are defined in Reference [7]. In Equation (5) a_{ij} represents the mean value of the sound speed: $a_{ij} = (a_{ij,\mathrm{L}} + a_{ij,\mathrm{R}})/2$. The Mach number and pressure in Equations (5) and (6) are evaluated from the equation of state for the gas.

The modified upwind has been tested with the perfect gas model on transonic turbine stages providing the same accuracy and robustness with respect to the original Roe's scheme. Nevertheless, the explicit presence of Mach number and pressure in the formulation of LDFSS(2) eases the implementation of the real fluid model and, unlike the Roe's scheme, which strongly relies on the linearity of pressure and energy relation, it turns out to be actually independent of the perfect gas law.

3. REAL GAS EVALUATION METHOD

The method for the evaluation of the real gas state equation represents a relevant issue of the solver. The main problem is to find a suitable method that has to be fast, accurate enough for CFD computations and flexible for the use with general state equations. To the authors knowledge (see for example References [8–10]) the possible approaches to this problem may be grouped as: (a) direct function representation, (b) parametric general representation and (c) *look-up* table algorithms. Benefits and main drawback for each of those will be briefly introduced in the following.

3.1. Direct function representation

It is the most straightforward approach and, being analytical, has the advantage of the greatest numerical accuracy. It is actually an extension of the perfect gas model and therefore requires little effort for the implementation in the solver.

The main drawback of this method is the low computational efficiency and the very low flexibility when changing the gas nature. The computational efficiency may also be of great concern since, depending on the actual law used, the computational effort added to compute the gas state easily overwhelms the rest of the CFD solver. For example the number of required 'calls' to the state equation may be as follows: 2 'calls' for the flux and 20 'calls' for the Jacobian evaluation giving a total of 22 'calls' for each internal face at every iteration. The evaluation of pressure from density and temperature for steam using the relation given in [11] needs to perform a summation over 56 powers and products. This approach undeniably requires an extraordinary effort and in general cannot be accepted especially if compared to the single product necessary for the perfect gas equation.

3.2. *Parametric general representation*

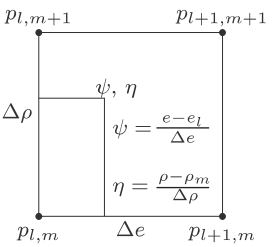
In this approach the state equation is replaced by means of a parametric representation (for example van der Waals equation) capable of approximating the real function up the desired extent. This kind of approximation has the same advantages of the former solution, but solves only partially the flexibility problems. Increasing the complexity of the representation to achieve a more general approach may again lead to high CPU costs.

3.3. *Look-up table* (*LUT*)

The LUT method is based on the discretization of the actual state equation onto a structured mesh. This kind of approach allows us to use any real gas state equation or thermodynamic database while cutting down the computational effort in the solver. The method is very flexible and general at the price of a loss of accuracy and of higher memory storage.

The LUT method here considered is obtained mapping the thermodynamic plane onto an evenly spaced grid in the conservative variables ρ (density) and e (internal static energy). Using a piecewise bi-linear interpolation, all the gas state variables can be retrieved continuously from the LUT for any combination of the primitive variables ρ and e. With this approach, given a couple (ρ, e), the number of operations required to locate the proper cell in the LUT is reduced to a couple of divisions and a rounding to integer: $l = \text{int}((e - e_{\min})/(\Delta e))$, $m = \text{int}((\rho - \rho_{\min})/(\Delta\rho))$.

The bi-linear interpolation defines the target state in terms of the local cell co-ordinate ψ, η: $p = (p_{l+1,m} - p_{l,m})\psi + (p_{l,m+1} - p_{l,m})\eta + (p_{l+1,m+1} - p_{l+1,m} - p_{l,m+1} + p_{l,m})\psi\eta + p_{l,m}$.



The primitive variable ρ and e are selected for mapping the LUT since these are directly available in the vector Q from the integration of the Navier–Stokes equations. The accuracy loss using the LUT depends mainly on the grid dimensions used for the table and on the interpolation algorithm. The bi-linear interpolation, proving to be efficient and flexible, should be kept. Accordingly, the accuracy can be raised up to the desired extent simply incrementing the number of divisions used in each primitive variable when mapping the LUT. In this case it is worthwhile considering that the CPU cost of the gas model remains unaffected while only the memory requirement increases for storing a larger table. This is a reasonable cost and, for example, a steam table consisting of 1000×1000 points has a total memory usage of 22.8 Mb. For these reasons, the LUT approach has been implemented into the real gas solver.

4. ISSUES ON BOUNDARY CONDITIONS

Despite the higher computational efficiency achieved by the LUT, this method has the main drawback of a more complex implementation for the *inverse evaluation*. An example of inverse evaluation occurs to retrieve ρ and e from the LUT given p (static pressure) and s (entropy) as known quantities. Having defined the LUT by ρ and e, the greatest part of the computational effort regarding the state equation is involved into the so-called *direct evaluation*, but several situations still require an *inverse evaluation*: these situations are mainly in the boundary conditions. The *inverse evaluation* can be performed iteratively starting from a *guessed* state as: $\rho^{n+1} = \rho^n + \Delta\rho^n$, $e^{n+1} = e^n + \Delta e^n$. In the present work a Newton's algorithm has been adopted; $\hat{p}$ and $\hat{s}$ being the variable defining the target gas state, the following linear system is solved at each iteration to get $\Delta\rho$ and Δe:

$$\begin{Bmatrix} \hat{p} - p^n \\ \hat{s} - s^n \end{Bmatrix} = [J] \cdot \begin{Bmatrix} \Delta\rho^n \\ \Delta e^n \end{Bmatrix} \tag{7}$$

The gradients in the Jacobian are readily known from the linear interpolation inside the cell. Convergence is usually achieved within $3/4$ iterations to a relative error of 10^{-4}. The undoubtedly higher cost for the *inverse evaluation* of LUT is limited to the boundary elements only and the global computational efficiency proved to be hardly affected. The boundary conditions are H_0, P_0 and angle α at inlet, T_{wall}, $V = 0$ at walls, the static pressure at outlet.

5. TEST AND RESULTS

The real gas code has been validated successfully for gaseous hydrogen in a test nozzle and it is routinely in use for the analysis of 3D steam turbine stages with satisfactory results. The main drawback observed from the applications is that the state equation is represented by a bounded range ρ–e in the thermodynamic plane. This has consequences on the convergence speed and stability. More precisely, using an implicit time-marching approach, the solution usually shows strong fluctuations before assessing on the convergence values as proved by the mass error in Figure 1(c). During those fluctuations the thermodynamic state related to the conservative variables can slip outside the prescribed range. This situation is unstable and can be avoided with a low time-step (i.e. CFL) during the numerical transitory. Furthermore, as shown in Figure 1(a), the shape of the LUT, being bounded by intervals of constant ρ and e, is not optimal in the (t,s) thermodynamic plane for describing a turbine expansion. This coverage of the thermodynamic plane is particularly prone to 'out of range' calls to the LUT for the late stages of a steam turbine especially if the expansion is not below the saturation curve. This is not a common working condition and the limitation of CFD usually satisfactorily. Anyway a proper treatment for handling out-of-range conditions is performs needed to avoid the occurrence of this type of instability at least for badly shaped or skewed cells of the grid. This has been achieved freezing the gas state of any point that is falling outside the table to the nearest boundary value available in the LUT. In case of a well-defined LUT table and using a stable transient time-step (i.e. CFL ~ 5) the convergence of the real gas code is very similar to that observed for the perfect gas case having the same Courant number. This is proved also for a practical application, as shown by Figure 1(b),

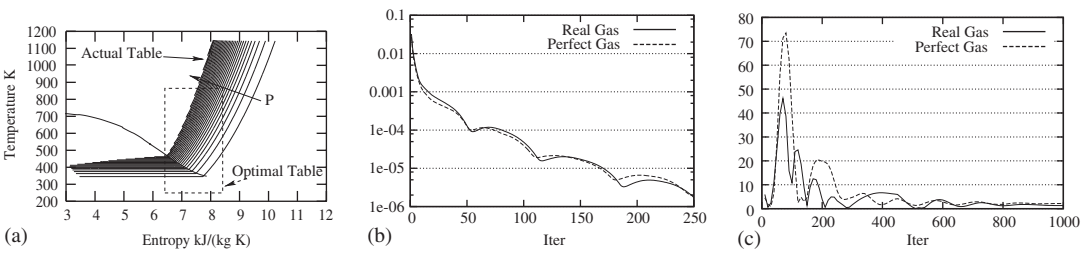


Figure 1. (a) Table in t–s plane; (b) residual convergence; and (c) mass convergence.

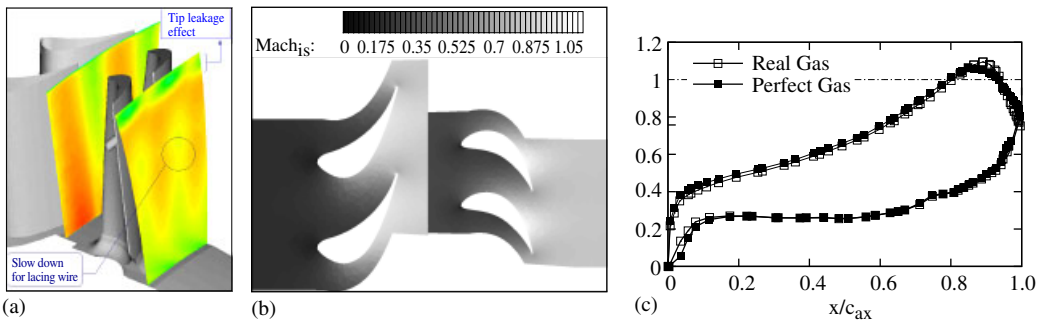


Figure 2. (a) Mach; (b) Mach$_{is}$ contours; and (c) isentropic Mach number profile.

considering the first turbine stage of a low pressure steam turbine for mechanical drive. In this example the code has a satisfactory performance despite the complex geometry that includes blade twist, lacing wire and tip leakage (Figure 2(a)). The stator is transonic and the expansion line crosses the saturation point. From isentropic Mach number at midspan (Figure 2(c)) it is also argued that the perfect gas model performs very similar to the real gas case delivering also the same massflow within an error less than 1%. In Figure 2(b) and (c) is shown the typical real gas midspan solution on the second LP turbine stage. Conversely from massflow and Mach profiles, computations using the real gas model allow a different prediction of stage efficiency with respect to the perfect gas on the same grids. For the turbine stage presented here, this difference is about 3% with the perfect gas underestimating the aerodynamic losses.

6. CONCLUSIONS

A real gas flow solver has been developed from an existing code for perfect gases. The upwind scheme LDFSS(2) has been implemented solving the stability problems observed for real gases computations using Godunov-type upwinding. A *look-up* table approach has been considered to represent the gas state equation showing it to be fast, flexible and accurate.

The whole approach maintains a good convergence rate although some concern of stability still remains. This has been attributed to the 'out of range' problem when accessing the LUT. Proposed remedies are the use of reduced Courant numbers and the clipping of variables outside the table. The boundary conditions require the use of *inverse evaluation algorithms* to work with the LUT. The real gas solver does not provide high differences in the aerodynamic flow pattern, at least in the example reported, but allows a better prediction of the stage loss. Improvements of the present approach should consider the phenomenon of steam condensation.

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