Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 99 (2015) 713 – 722

Procedia Engineering

www.elsevier.com/locate/procedia

APISAT2014", 2014 Asia-Pacific International Symposium on Aerospace Technology, APISAT2014

Verification of a Chemical Nonequilibrium Flows Solver Using the Method of Manufactured Solutions

Li Wang*, Wei-jiang Zhou ,Chu-qun Ji

China Academy of Aerospace Aerodynamics, No.17 Yungang West Rd. Fengtai District Beijing,100074,China

Abstract

This paper presents code verification of a chemically nonequilibrium flows solver using the method of manufactured solutions.The Method of Manufactured Solutions(MMS) is a general approach for creating exact solutions to the governing equations and can be used in the code verification process. In the MMS, the analytical solutions for the flow variables are first constructed, then the governing equations are modified to satisfy these solutions by adding appropriate source terms which are generated by applying the governing equations to these solutions. After that, code verification process will start. The order of accuracy of the calculations will be computed and compared with theoretical order of accuracy to determine if the code passes the verification test. We created manufactured solutions for two different sets of Euler equations. One set includes the total density equation plus ns-1 species equations and the other contains only species continuity equations. The results show that the form of continuity equations has little influence on the behaviour of global conservative variable errors as the mesh is refined. Our study also indicates that a complete chemical reaction model is preferred to ensure the convergence of observed order of accuracy is smooth in the order of accuracy test.

Peer-review under responsibility of Chinese Society of Aeronautics and Astronautics (CSAA)

Keywords: method of manufactured solutions,code verification,chemical nonequilibrium flows

* Corresponding author. Tel.:+86- 010-68374390.
E-mail address: txwangli@yeah.net

Peer-review under responsibility of Chinese Society of Aeronautics and Astronautics (CSAA)
doi:10.1016/j.proeng.2014.12.593

1. Introduction

As Computational Fluid Dynamics(CFD) plays more and more important role in the field of aerospace, the evaluation of correctness of CFD predictions has received increasing attentions. The primary tools to build confidence in CFD results are verification and validation[1]. The verification and validation deal with different phases in the modeling and simulation activities. The verification process assesses the correctness of the numerical solutions to the mathematical equations. On the other hand, the validation process determines the degree to which a CFD model represents the real fluid physics from the perspective of the intended uses of the model. The verification of CFD simulations must be performed before validation.

The verification of CFD simulations can be further classified as code verification and solution verification[2]. Solution verification is the process of gathering evidence to demonstrate the calculation of particular case is correct. Solution verification usually involves the estimation of numerical solution error. Code verification is the process of eliminating coding mistakes in a computer code by comparing numerical solutions with prior known solutions to a given set of equations. The most critical criterion for code verification is order of accuracy test which checks if the order of calculations is approaching the formal order of accuracy as the mesh is refined. In order of accuracy test, the discretization error , defined as the difference between discrete solutions and the exact solutions, is required to compute the observed order of accuracy. However, the exact solutions to a specific partial differential equation rarely exist. Furthermore, most of the exact solutions are not appropriate for code verification because the simple form of these solutions makes them impossible to exercise all the terms in the equations being solved. In order to overcome this difficulty, Roache and Steinberg[3] proposed a new, general approach to generate exact solutions to a system of governing equations. This method is called the method of manufactured solutions(MMS). Instead of searching an exact solution to the governing equations with given initial and boundary conditions, the MMS modifies the governing equations to satisfy a priori chosen analytical solutions for flow variables. This method is rooted in the fundamental principle of code verification which emphasizes code verification only dealing with mathematical issues of a given problem. Thus, for code verification purpose, whether the manufactured solution be related to a realistic problem or not is inessential.

The MMS has been applied to code verification of several CFD solvers [4-6]. These works use the MMS to verify the solutions to Euler equations, N-S equations, or RANS equations. Relative little work has been done to perform verification for governing equations of nonequilibrium flows with the MMS. In this work, we present a code verification exercise of an inviscid, nonequilibrium reacting flows solver using the method of manufactured solutions. The chemical source term construction and alternative governing equations set are investigated to study their influence on the order of accuracy test.

2. Numerical Method

In this section, we will give a detailed description of the governing equations and present a brief description of the flow solver.

2.1. Governing Equations

The 2D Euler equations for a fluid flow in chemical nonequilibrium can be written in conservative form as follows

$$\frac{\partial \mathbf{Q}}{\partial t}+\frac{\partial \mathbf{E}}{\partial x}+\frac{\partial \mathbf{F}}{\partial y}=\mathbf{\Omega} \tag{1}$$

where the dependent variable vector $\mathbf{Q}$, x direction inviscid flux vector $\mathbf{E}$, y direction inviscid flux vector $\mathbf{F}$, and vector of chemical source terms $\mathbf{\Omega}$ are defined as:

$$\mathbf{Q}=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\\ \rho_1\\ \vdots\\ \rho_{ns-1}\end{bmatrix}\quad \mathbf{E}=\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ \rho uH\\ \rho uc_1\\ \vdots\\ \rho uc_{ns-1}\end{bmatrix}\quad \mathbf{F}=\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ \rho vH\\ \rho vc_1\\ \vdots\\ \rho vc_{ns-1}\end{bmatrix}\quad \mathbf{\Omega}=\begin{bmatrix}0\\ 0\\ 0\\ 0\\ \omega_1\\ \vdots\\ \omega_{ns-1}\end{bmatrix}$$

In the above, ρ , ρ_i , c_i ω_i , u , v , and p are total density, i[th] species density, i[th] species mass fraction, mass production rate of species i, x velocity component ,y velocity component and pressure respectively. ns is the number of species. The gas mixture is assumed to be perfect gas. Thus, the total pressure is given as the sum of the partial pressures of each species according to Dalton's Law:

$$p=\sum_{i=1}^{ns}p_i=\sum_{i=1}^{ns}\rho_i\frac{R_u}{M_i}T$$

Here R_u is universal gas constant and M_i is molecular weight of species i. $E=e+\left(u^2+v^2\right)/2$ represents total energy per unit mass and $H=h+\left(u^2+v^2\right)/2$ denotes total enthalpy. e and h are calculated from thermodynamic properties of individual species through the following relations. e_i is internal energy and h_i is enthalpy of species i.

$$h=\sum_{i=1}^{ns}c_ih_i,e=\sum_{i=1}^{ns}c_ie_i,e_i=h_i-\frac{R_u}{M_i}T$$

h_i is determined from polynomial curve fit relations[8]:

$$h_i=\frac{R_u}{W_i}T\left(a_1+\frac{a_2}{2}T+\frac{a_3}{3}T^2+\frac{a_4}{4}T^3+\frac{a_5}{5}T^4+a_6T^{-1}\right)$$

2.2. Flow Solver

The flow solver for inviscid, chemically reacting flows is based on finite volume framework. The AUSMPW scheme is used to construct the inviscid flux and MUSCL type interpolation incorporated with Vanalbada limiter is employed to reach second order accuracy in space. For time integration, LU-SGS method is used.

3. The Method of Manufactured Solutions

The method of manufactured solutions is a general approach to generate exact solutions to given equations. In this method, the solutions to slightly modified governing equations are first constructed in analytical form. Then differential operator for the governing equations is applied to the analytical solutions to generate source terms. This work can be done with symbolic manipulation software, such as Matlab or Mathematica. Finally we will obtain a system of new governing equations with additional analytical source terms. The analytical solutions that we created previously exactly satisfy the new governing equations. Thus, these manufactured solutions can be used in the code verification procedure.

Oberkampf and Roy have proposed 4 different acceptance criteria for code verifications with varying rigor[7]. Among these criteria, order of accuracy test is the most rigorous one. Order of accuracy test examines if the discretization error with respect to the manufactured solutions tends to zero at expected rate as the mesh is refined. This expected rate is called formal order of accuracy and it is usually found by performing a truncation error analysis of the numerical scheme. The actual rate at which the discretization error is reduced is called observed order of accuracy. The consistency of the observed order of accuracy and formal order of accuracy indicates that the code verification is passed. Once the order of accuracy mismatches each other, further investigation is needed to detect coding mistakes.

The observed order of accuracy is evaluated from the discretization errors on different mesh refinement levels. The discretization error is defined as the difference between the exact solution to the governing equations and the discrete solution obtained on given mesh level. In MMS, the exact solutions to the governing equations are known and only two successive refined meshes are required to compute the observed order of accuracy. Consider a series expansion of the discretization error ò in terms of h, where h is mesh spacing measurement[7].

$$\grave{o}_h = c_p h^p + O(h^{p+1}) \tag{2}$$

Now we can write the discretization errors on two different mesh levels as

$$\begin{aligned} \grave{o}_h &= c_h h^p + O(h^{p+1}) \\ \grave{o}_{rh} &= c_h (rh)^p + O\left((rh)^{p+1}\right) \end{aligned} \tag{3}$$

Here $r = h_c / h_f$ represents the ratio of coarse to fine grid mesh spacing. Note that c_h is independent of h and can be simply understood by recognizing that it is just the partial derivative of discrete solution u_h with respect to h in the limit as h tends 0. After some algebra, we can find the expression for the observed order of accuracy[7]:

$$\hat{p} = \frac{\ln\left(\frac{\grave{o}_{rh}}{\grave{o}_h}\right)}{\ln r} \tag{4}$$

In this study, the L2 norm of conservative variables error is used to compute the observed order of accuracy, which is defined as,

$$\varepsilon_{L_2} = \left\{ \frac{\sum_{i=1}^{N} \left(Q_{num,i} - Q_{mms,i}\right)^2}{N} \right\}^{1/2} \tag{5}$$

Mesh refinement study is essential in the order of accuracy test. The mesh size levels must be carefully chosen in order to reach the asymptotic range so that the discretization errors will be reduced at the theoretical rate associated with the discretization scheme. In our experience, the mesh levels required to reach the asymptotic range are highly dependent on the manufactured solutions. We use 6 mesh levels in this study, which are 9×9, 17×17, 33×33, 65×65,12 9×129 257×257. All the grids are uniformly spaced in each coordinate direction(fig.1).

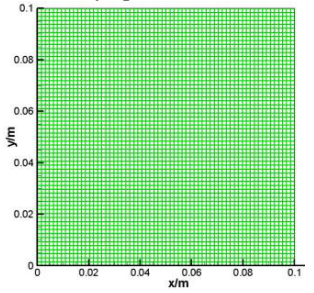

Fig. 1 Computational mesh(65×65)

4. Results

The verification of a nonequilibrium reacting flows solver using the method of manufactured solutions is tedious. Various factors can affect the final verification results. The unexpected results can be accounted for either wrongly application of the MMS method or coding mistakes. We should not contribute the MMS application mistakes to programming problems. Considering these concerns, the verification work is conducted in 2 exercises with increasing complexity. In the first exercise, we present verification results for Euler equations involving 4 species

without chemical source terms. After that, the chemical source terms computations are activated and the same manufactured solutions are used to carry out the verification. In this exercise, we encountered a serious problem. The observed order of accuracy shows relative large oscillations as the grid is refined although its value is very close to the theoretical value on the finest grid. We are not sure whether this behaviour is normal, so two attempts are made to address this problem.

4.1. Euler Equations Without Chemical Source Terms

As discussed in last section, analytical form solutions must be created to the governing equations. The manufactured solutions need not have physical implications, because the fundamental philosophy of code verification is to examine the correctness of the solutions to the governing equations. In this case, smoothness, differentiable, and general enough to exercise all the terms in the governing equations are more important. We choose to use trigonometric functions to construct the expressions for all the variables in the governing equations. In current work, 4 species, $O, N, O2$, and N_2 are assumed to present in the flow. Analytical solutions for p, ρ, u, v, O, N, and O_2, are expressed in the form shown below[4]:

$$\varphi = \varphi_0 + \varphi_1 f_1\left(\frac{\varphi_3 x}{L}\pi\right) + \varphi_2 f_2\left(\frac{\varphi_4 y}{L}\pi\right) \tag{6}$$

Where φ is a dummy variable representing p, ρ, u, v, O, N, and O_2, φ_i is constant and f represents cosine or sine functions. The form of these expressions will be given in the appendix. The constants in manufactured solutions for p, ρ, u, v are directly taken from the work of Roy[4]. However, the forms of expressions for individual species are created ourselves. These constants are carefully chosen through numbers of numerical tests. Ill-defined constants may require more grids to perform order of accuracy test. The solutions for O and N are presented in fig. 2. The analytical source terms are generated with the help of Matlab software. Distributions of source terms for x-direction momentum equation and continuity equation for O are shown graphically in fig. 3.

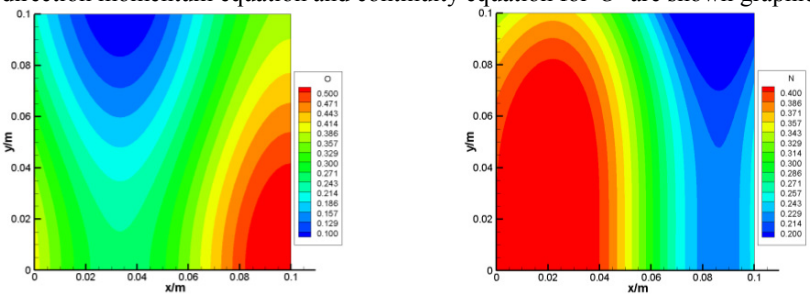

Fig. 2 Manufactured solutions for O(left) and N(right)

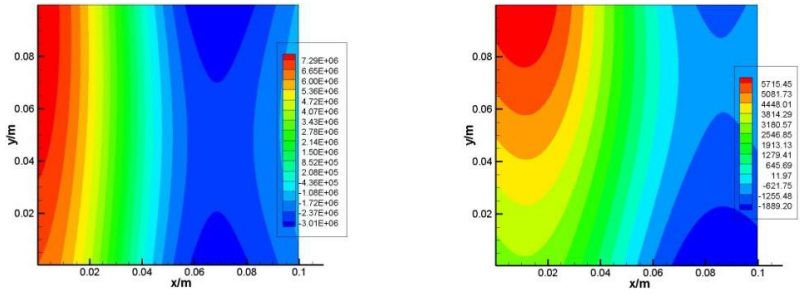

Fig. 3 Source terms for x-momentum equation(left) and O continuity equation(right)

The boundary conditions are enforced by directly specifying the boundary values with Dirichlet values from manufactured solutions. The reason of using such type of boundary conditions is that the main goal of current work is the verification of interior equations. The way of boundary conditions enforcement has no adverse influence on the order of accuracy test[7].

Fig. 4 shows the behaviour of density discretization error norm as the mesh is refined. The other variables error norms exhibit similar behavior. As can be seen, all the conservative variables error norms are reduced at the theoretical order in the vicinity of finest grid. Fig. 5 plots the observed order of accuracy of all the conservative variables, which confirms the previous observations in fig. 4.

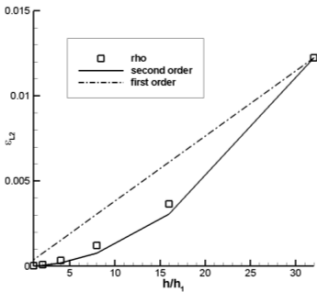

Fig. 4. Behavior of L2 norm of density error as the mesh is refined

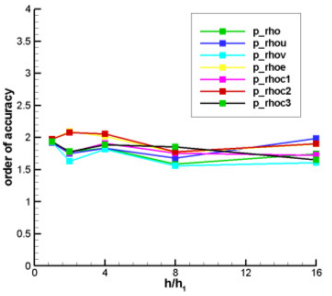

Fig. 5. Observed order of accuracy

4.2. Euler Equations With Chemical Source Terms

The results obtained in last section establish great confidence in the code resolving Euler equations without chemical source terms. Based on the previous work, the verification of Euler equations with chemical source terms is performed in this exercise. Because only 4 species are included in the governing equations, a sub set of Gupta's chemical reaction model[8] is employed. The sub reaction mechanism takes into account only dissociation processes of O_2 and N_2. The chemical reaction rate coefficients are given in the appendix. Note that the pre-exponential factor A_b in the backward rate constants is specified 3 orders less than the original value in Gupta's model. The chemical source terms computed with the original reaction rate constants are so large that the simulation will not be successfully completed.

Fig. 6 gives the numerical solution and manufactured solution for pressure on grid 257×257. In this figure, we can see that the numerical solution shows slight oscillations near the top right corner. Further examination of the observed order of accuracy is conducted and the result is shown in fig. 7. The order of accuracy of the calculations is approximate the same as formal order of accuracy on the grid 257×257, but the overall convergence of the calculations exhibits large oscillations. It is not defendable to draw the conclusion that the code is verified based on these results. Note that the only difference between the two tests is the species source terms calculation. It is reasonable to suspect that some coding mistakes may reside in that portion of the code. The chemical source terms are a function of ρ, T ,and ρ_i and all the operations are algebraic. For clarity sake, it is important to distinguish two types of chemical source terms in the code. One is computed in the code to be verified and the other is calculated in the code generated by Matlab. We will refer to the two source terms as numerical chemical source terms and manufactured chemical source terms. If ρ, T ,and ρ_i takes the same value as the manufactured solutions and the code contains no coding mistakes, the numerical chemical source terms will be identical with the manufactured chemical source terms. To confirm this assertion, rather than specifying values from actual calculation, we directly set the values of ρ, T , and ρ_i in the chemical source terms calculation from manufactured solutions. Fig. 8 presents the observed order of accuracy. This figure shows no difference from fig. 5, which indicates there is no coding mistakes in the chemical source terms computation.

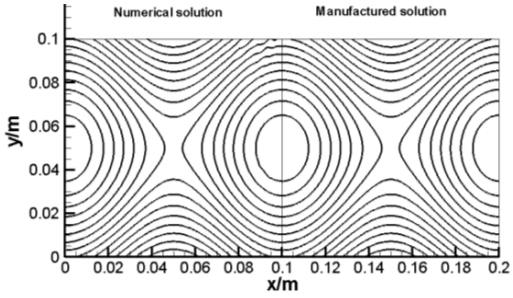

Fig. 6. Comparison of numerical solution and manufactured solution for pressure

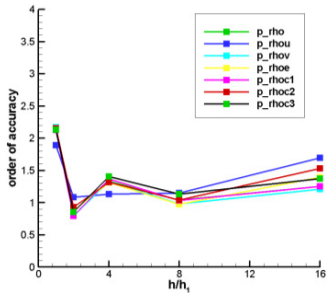

Fig. 7. Observed order of accuracy

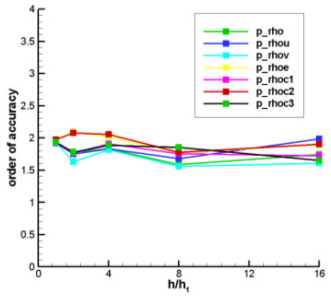

Fig. 8. Observed order of accuracy （using manufactured solution in the chemical source calculation）

It is very confusing that the chemical source terms calculation affects the behaviour of discretization error. Some possibilities exist to explain the observations. In current case, we solve the total density and $ns-1$ species equations. This will cause all the numerical errors in $ns-1$ species accumulate to the ns-th species. This error again will affect the species source terms calculation. This interaction between the relative large species density error and chemical source terms leads to the oscillation of flow field. Another possibility is that a sub set of chemistry model maybe not appropriate. Considering the maximum temperature of the manufactured solutions is no more than 400K， the dissociation rates of O_2 and N_2 are almost negligible. The chemical source terms are mostly resulted from the recombination of O and N, which makes them more sensitive to the mixture composition.

In order to investigate the first guess, we re-implement the solver to be capable of solving the two sets of governing equations, i.e., the governing equations containing total mass conservation equation plus $ns-1$ species conservation equations (set 1) and the governing equations including ns species equations (set 2). The new solver is verified with previous proposed manufactured solutions for solving the first set of Euler equations and identical results were obtained as before. Then the second set of governing equations is solved using the solver. The observed

order of accuracy obtained by the new solver is presented in fig. 9. This result is very similar with fig.7. Different sets of equations implemented in the solver have little influence on the observed order of accuracy when same numerical technique is employed.

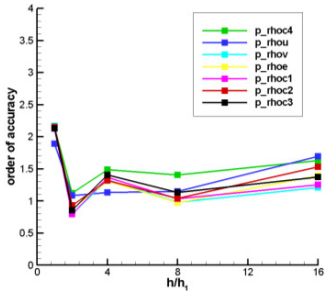

Fig. 9. Observed order of accuracy by solving all ns species equations

After elimination of the first possibility, we construct new manufactured solutions. In this case, the gas mixture is consist of 5 species of $O, N, O2, N_2$, and NO. The analytical expressions for them are given in the appendix. The 5 species air reaction model of Gupta is used and all the reaction rate coefficients are kept unchanged. Fig. 10 and fig. 11 give the observed order of accuracy by solving equations set 1 and 2 respectively. It can be seen that, the order of accuracy of both calculations matches the theoretical order of accuracy and the convergence curves are smooth.

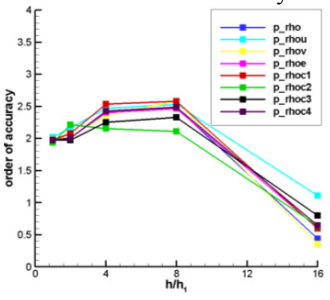

Fig. 10. Observed order of accuracy by solving governing equations set 1

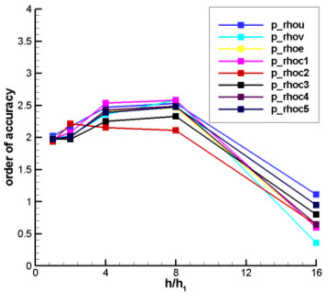

Fig. 11. Observed order of accuracy by solving governing equations set 2

5. Conclusions

The MMS was used in the code verification of an inviscid, nonequilibrium flows solver. When the same manufactured solutions are used to verify Euler equations with or without chemical source terms, significant difference is observed in the behavior of the observed order of accuracy as the mesh is refined. Formal order of

accuracy is easily obtained with the chemical source terms disabled, while observed order of accuracy shows large oscillation with the chemical source terms activated. In order to find the reasons, the solver is re-implemented to be capable of solving two sets of continuity equations: total density equation plus ns-1 species equations and all ns species equations. Different chemistry models, one is composed of only dissociations of O_2 and N_2 while the other is consist of both dissociation and recombination reactions, are also studied. Results show that the form of continuity equations has no influence on the overall order of accuracy test. Comparing to a sub set of chemistry model, the complete chemistry model is more appropriate to use in the order of accuracy test.

Appendix A. Manufactured solutions for Euler equations including 4 species equations

A.1. Form of manufactured solutions

$$\begin{aligned}
\rho(x,y) &= \rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right) \\
u(x,y) &= u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) + u_y \cos\left(\frac{a_{uy}\pi y}{L}\right) \\
v(x,y) &= v_0 + v_x \cos\left(\frac{a_{vx}\pi x}{L}\right) + v_y \sin\left(\frac{a_{vy}\pi y}{L}\right) \\
p(x,y) &= p_0 + p_x \cos\left(\frac{a_{px}\pi x}{L}\right) + p_y \sin\left(\frac{a_{py}\pi y}{L}\right) \\
c_i(x,y) &= c_{i0} + c_{ix} \sin\left(\frac{a_{c_{ix}}\pi x}{L}\right) + c_{iy} \cos\left(\frac{a_{c_{iy}}\pi y}{L}\right)
\end{aligned} \tag{7}$$

A.2. Constants for manufactured solutions

Table 1.Constants for manufactured solutions expressed by Eq. (7).

Flow variable	φ_0	φ_x	φ_y	a_{φ_x}	a_{φ_y}
$\rho(kg/m^3)$	1.0	0.15	-0.1	1.0	0.5
$u(m/s)$	800	50	-30	1.5	0.6
$v(m/s)$	800	-75	40	0.5	1.5
$p(pa)$	1.e5	0.2e5	0.5e5	2/3	1.0
c_O	0.25	0.1	-0.15	1.0	0.5
c_N	0.3	-0.15	0.1	1.5	0.8
c_{O_2}	0.2	0.05	-0.1	1.0	0.5

A.3. Reaction coefficients

Table 2.Reaction coefficients.

Reaction	A_f	β_f	B_f	A_b	β_b	B_b
$N_2 + M = 2N + M$	1.92E17	-0.5	113100	1.09E13	-0.5	0
$O_2 + M = 2O + M$	3.61E18	-1.0	59400	3.01E12	-0.5	0
Third body efficiencies for reaction 1	$O/1/, N/1/, O_2/1/, N_2/2.5/$					
Third body efficiencies for reaction 2	$O/25/, N/1/, O_2/9/, N_2/2/$					

The forward and backward reaction rates are computed through

$$k_j = A_j T^{\beta_j} \exp\left(-\frac{B_j}{T}\right).$$

Appendix B. Manufactured solutions for Euler equations including 5 species equations

Table 3. Constants for manufactured solutions expressed by Eq. (7).

Flow variable	φ_0	φ_x	φ_y	a_{φ_x}	a_{φ_y}
$\rho(kg/m^3)$	1.0	0.15	-0.1	1.0	0.5
$u(m/s)$	800	50	-30	1.5	0.6
$v(m/s)$	800	-75	40	0.5	1.5
$p(pa)$	1.e5	0.2e5	0.5e5	2/3	1.0
c_O	0.15	-0.05	0.06	1.5	0.8
c_N	0.2	0.07	-0.02	1.1	0.4
c_{O_2}	0.2	0.03	-0.09	1.1	0.6
c_{N_2}	0.2	0.05	-0.08	0.7	0.8

References

[1]W.L. Oberkampf, T.G. Trucano, Verification and Validation in Computational Fluid Dynamics, SAND2002-0529.
[2]P.J. Roache, Verification of Codes and Calculations, AIAA Journal, 1998, 36(5) 696-702.
[3] P.J. Roache, S. Steinberg, Symbolic manipulation and computational fluid dynamics, AIAA Journal, 1984, 22(10) 1390-1394.
[4] C.J. Roy, T.M. Smith, C.C. Ober, Verification of a Compressible CFD Code Using the Method of Manufactured Solutions, AIAA 2002-3110.
[5]L. Eca, M. Hoekstra, A. Hay, D. Pelletier. Verification of RANS Solvers with Manufactured Solutions. Engineering with Computers, 2007, 23:253~270
[6]S.P. Veluri, C.J. Roy, E.A. Luke, Comprehensive Code Verification for an Unstructured Finite Volume CFD Code, AIAA 2010-0127.
[7]W. L. Oberkampf, C. J. Roy, Verification and Validation in Scientific Computing, Cambridge University Press, 2010.
[8] R.N. Gupta, J.M. Yos, R.A. Thompson, K.-P. Lee, A Review of Reaction Rates and Thermodynamic and Transport Properties for an 11-Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30000K, NASA-RP-1232.