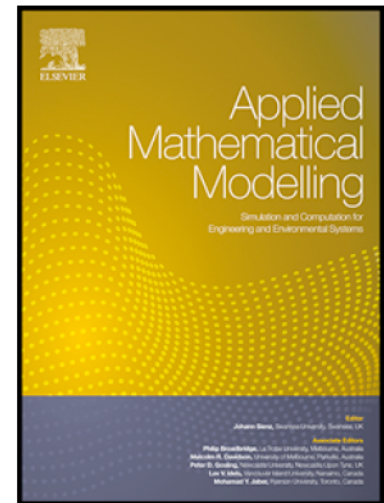


Journal Pre-proof

A Novel Combination of Mathematical Modelling Approaches for Simulating Nearly Hypersonic, Viscous, Reacting Magnetogasdynamical Flows

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PII: S0307-904X(22)00104-4
DOI: <https://doi.org/10.1016/j.apm.2022.02.041>
Reference: APM 14436



To appear in: *Applied Mathematical Modelling*

Received date: 14 October 2021
Revised date: 19 February 2022
Accepted date: 24 February 2022

Please cite this article as: Hrishabh Chaudhary, László Könözy, Zeeshan A. Rana, A Novel Combination of Mathematical Modelling Approaches for Simulating Nearly Hypersonic, Viscous, Reacting Magnetogasdynamical Flows, *Applied Mathematical Modelling* (2022), doi: <https://doi.org/10.1016/j.apm.2022.02.041>

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Highlights

- Chemical- and magnetogasdynamic models are coupled using high-order WENO schemes and the HLLC Riemann solver
- Numerical and physical models are thoroughly analysed for stability
- Highly resolved bow shock structures around a cube are observed and discussed
- Shock interactions of bow shocks in different arrangements are investigated
- Shock standoff distance dependences are analysed at different conditions

A Novel Combination of Mathematical Modelling Approaches for Simulating Nearly Hypersonic, Viscous, Reacting Magnetogasdynamic Flows

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Abstract

This work focuses on the mathematical combination of magnetogasdynamics (MGD) and the Dunn and Kang chemical kinetic model with a multi-component Harten–Lax–van Leer Contact (HLLC) local Riemann solver using high-order interpolation schemes. Due to the nature of nearly hypersonic, unsteady, viscous, reacting MGD flows, the gas dissociates which is taken into account with 11 species and 26 chemical reactions along with the temperature dependent transport properties through the Wilke model. In the present work, the electromagnetic effects are considered by solving a Poisson equation simultaneously with the chemical reaction equations. The non-linear convective terms are treated numerically with third-, fifth- and seventh-order Weighted Essentially Non-Oscillatory (WENO) interpolation schemes along with second-, fourth- and sixth-order central finite difference schemes for the viscous terms. The combination of these numerical and physical models are analysed for stability and validated for benchmark problems such as a) Hartmann flow as MGD validation test case and b) the shock-tube problem for testing the chemical reaction model in which case the reaction rate controlling temperature suggested by Park has also been taken into account. Furthermore, a complex physical problem of an external aerodynamic flow over the cube for the Mach number varying from 1.25 to 3 have also been investigated, because a limited number of studies is available for understanding the flow behaviour of sharp cornered blunt bodies such as cubes. The knowledge of shock structures of these objects has become imperative to predict the atmospheric re-entry trajectories of de-orbiting CubeSats, space debris or fragments of launch vehicles. The main physical finding is that the shock structures are observed to be much more resolved compared to previous works, especially in the wake region. The knowledge gap is bridged by detailing the shock structures and showing the dependence of the shock standoff distance on total enthalpy of the flow.

Keywords: Magnetogasdynamics, Hypersonics, Chemical reactions, High-order schemes, Shock interactions

1. Introduction

The ability to manipulate the fluid flow field plays a pivotal role in the design of an aerospace vehicle and is one of the most researched areas in fluid mechanics. The advancements in magnetic technologies and arising demand on hypersonic and space travel have led to an increasing interest in utilising the magnetic field as a flow control technique for alleviating blackouts and mitigating material ablation. The experimental studies for hypersonic flow based on the ground testing include testing in different wind tunnels which cannot fully generate the realistic flow conditions and the flight-testing is extremely expensive, complex and utilise a tremendous amount of resources. Thus, for the optimisation studies, the best alternative available is to use Computational Fluid Dynamics (CFD), which comes with its

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own challenges and over many years several authors worked in the development of computational techniques to correctly simulate hypersonic flows and simultaneously study the magnetogasdynamic (MGD) flow control. Previously, authors have proposed a variety of techniques for the resolution of the same but were hampered by the computational requirements. The first numerical demonstration of MGD was employed by Brio and Wu [1] in 1994, where they implemented an upwind differencing scheme for the governing equations of ideal magnetogasdynamics. Furthermore, Hughes et al. [2] analysed simple parabolic and elliptic MGD flows. Powell [3] extended their work to multi-dimensions through the implementation of an approximate Riemann solver in ideal magnetogasdynamics equations. Gaitonde [4], Agarwal and Augustinus [5], MacCormack [6], Damevien and Hoffmann [7] and others, further developed MGD flow solvers. Nowadays, many authors such as Evans et al. [8, 9], Yang et al. [10], Bao et al. [11], Qiu et al. [12] and others, are focusing on developing particle-based methods, which are appropriate for Knudsen number above 0.1 and altitude above 90 km. For Knudsen number below 0.1, where most of the hypersonic applications occur, the particle-based methods are susceptible to random walks and utilise a lot of computational resources and time. Lofthouse et al. [13–15] showed the comparison between the continuum model and particle-based methods for hypersonic flow, and they concluded that a) particle-based methods are more accurate above Knudsen number 0.01; b) for Knudsen number between 0.01 and 0.002, the accuracy of continuum model based methods are comparable to particle-based approaches; and c) for Knudsen number below 0.002 continuum model based methods are more accurate and take less computational time. Vehicles such as hypersonic cruise missile usually fly between altitude of 15–30 km from Mach number of 3 to 6 and beyond, where the Knudsen number varies from 10^{-6} to 10^{-4} . In this work, the Mach number ranges from 3 to 8, therefore, a continuum model approach has been employed.

In hypersonic flows, the temperature due to shocks becomes high enough that flow dissociates, ionises and becomes chemically reacting. This results in a sheath of a weakly ionised plasma layer surrounding the hypersonic flight or re-entry vehicle. The behaviour of this weakly ionised plasma layer can be controlled to some extent by imposing a magnetic field using a control system within the vehicle. The application of the imposed magnetic field to the weakly ionised plasma flow induces electric current in shock layer. The interaction of the electric current and the magnetic field generates the Lorentz force, which decelerates the plasma flow in the shock layer. The deceleration of the plasma flow causes the expansion of the shock layer and the mitigation of the convective heat flux [16]. The weakly ionised plasma produced in hypersonic flows is a poor electrical conductor, consequently, the electrical current density induced in plasma is small. It means that the induced magnetic field generated by this plasma current will be much smaller than any imposed magnetic field. In the years of 1958–59, Meyer [17], Bush [18] and Ziemer [19] proposed the idea of MGD flow control as an active flow control and active heat shield for re-entry vehicles. In the 1960s, Lykoudis [20], Wu [21], Ericson et al. [22] and others dealt with more theoretical, semi-analytical and empirical studies on magnetic flow control for hypersonic flows. These theoretical studies concluded that effective magnetic control requires a strong magnetic field and the technology is not yet feasible enough to make MGD flow control effective.

Since that time, considerable technological advancements in the field of semiconductors, superconducting magnets and artificial ionisation have been made, which makes MGD flow control feasible. Damevien and Hoffmann [23] compared the full solution of MGD governing equations including air chemistry with the small magnetic Reynolds number approach for flows over a hemisphere and a cylinder, and showed excellent agreement with existing theoretical solutions. Khan et al. [24] used a full MGD model to treat flows with zero electric field around a flat plate and a blunt body, and tested for agreement between the solutions of the full MGD model and the small magnetic Reynolds number approximation. They obtained good agreement for values of magnetic Reynolds number of less than 0.125. Imamura et al. [25], Otsu et al. [26], and others, have used the small magnetic Reynolds number approach for MGD flow control in hypersonic flight and showed results similar to those generated by Gaitonde [4], MacCormack [27], Gaitnode et al. [28], and others, who used the full MGD models. Papadopoulos et al. [29] in 1999, highlighted the significance of the grid generation techniques required for the computational analysis of hypersonic flows. Papadopoulos et al. [29] compared the experimental results of the aeroheating environment experienced by the X-38 vehicle with the numerical investigation on a structured grid, and based on the results provided a detailed approach of the grid generation for simulating hypersonic flows. In 2002, Mack et al. [30] showed, relying on the validation of DLR-Tau solver, that unstructured grids achieves good accuracy and produces results for the cases that could only be solved with a large effort by structured grids. In 2006, Scalabrin et al. [31] developed a CFD solver which was used for an unstructured grid with a line implicit solver to simulate hypersonic flows. In 2011, Prakash et al. [32] developed a fifth-order shock-fitting method for hypersonic flows and highlighted the importance of high-order methods for capturing hypersonic flow features with high accuracy. Bonfiglioli et al. [33] in 2013 and Pepe et al. [34] in 2015, developed an unstructured

shock-fitting solver for hypersonic plasma flows and showed that the shock fitting approach outperforms the shock-capturing approach in terms of accuracy of the numerical solution. Furthermore, Casseau et al. [35, 36] in 2016, developed a two-temperature open-source CFD model for hypersonic reacting flows using the OpenFOAM software.

Due to high speed and relatively low density as compared to sea level, the turbulent time scale has approximately the same order as that of chemical and energy transfer time scale. This leads to thermal and chemical non-equilibrium inside the shock layer and it requires separate models for simulating non-equilibrium conditions. Moreover, the high temperature and ionised flow result in the shock layer emitting radiation which is partly absorbed by the spacecraft as radiative heating. Various models were proposed over the past 50 years to simulate the finite rate chemistry involved in the case of hypersonic flows. Blottner (1969) [37], Dunn and Kang (1973) [38] and Gupta et al. (1990) [39] dealt with one-temperature models, and Park (1987) [40], Gnoffo et al. (1989) [41], Park et al. (1991, 2000) [42, 43] proposed different versions of two-temperature models in conjunction with chemically reacting flows. Dunn and Kang [38] proposed a one-temperature model based on the standard finite rate chemistry model, in which air is made up of eleven species, and the interaction of these species with each other are represented by twenty-six chemical reactions. Further experimental studies showed that the temperatures during the re-entry process reach high enough values to excite vibrational energy of the molecules. Therefore, Park [42, 43] proposed a two-temperature model, in which rotational and translational energies are defined by a particular temperature, and vibrational and electronic energies are defined by a single different temperature. Similarly, researchers were investigating the potential benefits of three-temperature (Imamura and Fujino [25]), and four temperature models (Kim [44]). For the investigation of hypersonic flows, Gupta et al. [39], Capitelli et al. [45], D'Angola et al. [46, 47] and Colonna et al. [48] highlighted that the thermodynamic and transport properties of the weakly ionised plasma are paramount to the model. According to Gupta et al. [39], for multi-species flows, the heat ratios of the mixture can be computed by taking weighted average of the heat ratio of each species with respect to mixture density. Colonna et al. [48] and D'Angola et al. [46, 47] proposed models employing partition functions, therefore, much more accurate in predicting the thermodynamic properties of multi-species plasma. Furthermore, the numerical investigation of multi-species flows requires a mixing model for the calculation of transport properties. Researchers have a strong preference to use either the mixing model of Wilke [49] or Gupta-Yos collision model [39]. The mixing model of Wilke [49] is suitable for velocities up to 8–10 km/s and for the maximum temperature of around 10000 K. The Gupta-Yos collision model [39] is a simplification of the first-order approximation of Chapman-Enskog and more detailed, however, it is computationally expensive. The model of Capitelli et al. [45] used for the perturbation of Chapman-Enskog method to compute the transport coefficients for the temperature range 50–100000 K.

In the present work, an in-house high fidelity fully coupled CFD code is developed for the chemically reacting turbulent magnetogasdynamics (MGD) problems in the supersonic and nearly hypersonic fluid applications. After validating and verifying the code, numerical investigations have been performed on a cube placed in a supersonic flow. The supersonic aerodynamic characteristics of bluff bodies have been adequately studied, because there is a lack of understanding in the fluid flow behaviour of sharp cornered blunt bodies, e.g., cubic objects. The knowledge of shock structures of such bodies has become imperative to predict the atmospheric re-entry trajectories of de-orbiting CubeSats, space debris or fragments of launch vehicles. In this work, the observed shock structures for supersonic cases for a cube are much more resolved than any previously reported results in the literature, especially in the wake region. These results were not apparent in previous studies [50, 51] where the CFD was carried out using Reynolds-Averaged Navier-Stokes (RANS) turbulence modelling approaches with $k-\epsilon$ and $k-\omega$ models. Furthermore, these studies were carried out with the use of commercial solvers which have limited accuracy at very high Mach numbers. Moreover, the results provided in experimental studies by Hansche et al. [52] and Seltner et al. [53] are hampered by the measuring instruments and the experimental results provided by Rees [54] are limited to Schlieren images. The discussions of the numerical and experimental results in previous papers are limited to the investigation of drag coefficient and pitching moment. It is important to note that the analytical solution of standoff distance is limited to two-dimensional flows (see, e.g., Askari [55] and Olivier [56]). Furthermore, for three-dimensional flows, one has to rely on semi-empirical relations, which may not represent its dependence on actual physical parameters. In this paper, the knowledge gap is bridged by detailing the shock structures and showing the dependence of the shock standoff distance on total enthalpy of the flow. Further studies have been carried out on the shock interactions of the bow shock generated by two bodies flying in side-by-side and staggered formation.

2. Governing Equations of Magneto-Gas-Dynamics for Multi-Species Flows

To take into account the effects of Magneto-Gas-Dynamics (MGD) for unsteady, viscous, chemically reacting multi-species flows, a partial differential equation for the magnetic induction vector derived from the set of Maxwell equations has to be considered coupled with fully compressible Navier–Stokes equations. Two assumptions are required when the partial differential equation for the magnetic induction vector is derived [57] as follows:

$$\frac{\epsilon_o \omega}{\sigma} \ll 1, \quad \text{and} \quad \left(\frac{|\vec{u}|}{c} \right)^2 \ll 1. \quad (2.1)$$

The first of these two assumptions allows the simplification of the Ampere–Maxwell law (2.5) where the displacement current term $[\partial(\epsilon_o \vec{E})/\partial t]$ can be neglected. Therefore, the set of Maxwell equations can be written as

$$\nabla \cdot \vec{E} = \frac{\rho_e}{\epsilon_o}, \quad (2.2)$$

$$\nabla \cdot \vec{B} = 0, \quad (2.3)$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad (2.4)$$

$$\nabla \times \vec{B} = \underbrace{\frac{\partial(\epsilon_o \vec{E})}{\partial t}}_{=0} + \frac{\vec{j}}{\epsilon_o c^2}, \quad (2.5)$$

$$\vec{j} = \sigma(\vec{E} + \vec{u} \times \vec{B}). \quad (2.6)$$

The second assumption in Eq. (2.1) allows the relativistic effects to be neglected in the present case as well. Therefore, the electric field vector $\vec{E}$ can be expressed from Ohm's law (2.6) and the current density $\vec{j}$ can be obtained from Ampere's law (2.5), and combining them with Faraday's law (2.4) (see Appendix A), the equation of the magnetic induction field $\vec{B}$ can be given by

$$\frac{\partial \vec{B}}{\partial t} + \nabla \cdot (\vec{u} \otimes \vec{B} - \vec{B} \otimes \vec{u}) + \nabla \times \left[\frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right) \right] = 0. \quad (2.7)$$

For nearly hypersonic, unsteady, viscous, reacting multi-species flows, the governing equations of MGD is obtained by coupling the continuity equation, the fully compressible Navier–Stokes momentum equations, the total energy equation and the species transport equations with the pre-Maxwellian equations as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \quad (2.8)$$

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla \cdot \left[\rho(\vec{u} \otimes \vec{u}) + \left(p + \frac{\vec{B} \cdot \vec{B}}{2\mu_e} \right) \underline{\underline{I}} - \frac{\vec{B}}{\mu_e} \otimes \vec{B} \right] = \nabla \cdot \underline{\underline{\tau}}, \quad (2.9)$$

$$\frac{\partial \vec{B}}{\partial t} + \nabla \cdot (\vec{u} \otimes \vec{B} - \vec{B} \otimes \vec{u}) + \nabla \times \left[\frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right) \right] = 0, \quad (2.10)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\vec{B} \cdot \vec{B}}{2\mu_e} \right) \vec{u} - \frac{\vec{B}}{\mu_e} (\vec{u} \cdot \vec{B}) \right] = \frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right)^2 - \nabla \cdot \vec{q} + \nabla \cdot \left[(\vec{u} \cdot \underline{\underline{\tau}}) + \sum_{s=1}^{N_s} (\vec{J}_s h_s) \right], \quad (2.11)$$

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \vec{u}) + \nabla \cdot \vec{J}_s = \dot{\omega}_s, \quad s = 1, \dots, N_s, \quad (2.12)$$

where N_s is the number of species which is equal to 11 in this work. The different species will be described in the next section. However, it is important to mention that in the present case, when $N_s = 11$ ($s = N_s = e$), the electron transport equation has been considered when the transport Eq. (2.12) is solved numerically. It means that in the transport Eq. (2.12), ρ_s and $\vec{J}_s$ must be replaced with ρ_e and $\vec{J}_e$, respectively. The Eqs. (2.8) to (2.12) represent the full set of equations that are needed to simulate the hypersonic or chemically reacting flow with magnetogasdynamic effects. The weakly ionised plasma produced in hypersonic flows is a poor electrical conductor, consequently, the electrical current density induced in plasma is small, which means that the induced magnetic field generated by this plasma current will be much smaller than any imposed magnetic field. As an example, a returning command module like Dragon or Apollo, which has a characteristic length of roughly 3.5 m can have a Mach number of around 8 at an altitude of 60 km. As stated in the investigations of Shneider et al. [58], at a Mach number of 8, the electrical conductivity is between 5 S/m, which results in a magnetic Reynolds number of 0.055 ($R_m = \mu_e \bar{\sigma} \bar{u}$). Similarly, cases of hypersonic vehicles like X33 flying at an altitude of 30 km at Mach Number 8 will have a magnetic Reynolds number of 0.05. Consequently, the magnetic Reynolds number, which is also the ratio of the induced magnetic field to the imposed magnetic field, is a small value, thus the low magnetic Reynolds number approach is valid here. Moreover, Khan et al. [24] performed an in-depth analysis on the validity of the low magnetic Reynolds number formulation and concluded that when the ionization is confined between the body and the shock, the low magnetic Reynolds number approximation and full set of equations provided similar results. This allows the use of a low magnetic Reynolds number approximation, however, the imposed magnetic field must follow the following two initial conditions:

1. The divergence-free criterion:

$$\nabla \cdot \vec{B} = 0. \quad (2.13)$$

2. The normal to the wall derivative of the magnetic field component vanishes:

$$\frac{\partial \vec{B}}{\partial n} = 0. \quad (2.14)$$

Under this small magnetic Reynolds number approximation, the magnetogasdynamic (MGD) effects can be solely represented by source terms. These source terms correspond to the Lorentz force in the momentum equation, which generates the Maxwell stresses in the fluid resulting in the Joule heating, represented in the source term of the energy equation. Therefore, the governing equations in conservative form are then represented as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = \frac{\partial \mathbf{F}_v}{\partial x} + \frac{\partial \mathbf{G}_v}{\partial y} + \frac{\partial \mathbf{H}_v}{\partial z} + \mathbf{S}. \quad (2.15)$$

The vector of conservative variables $\mathbf{U}$, inviscid fluxes $\mathbf{F}$, $\mathbf{G}$ and $\mathbf{H}$, viscous and diffusion fluxes $\mathbf{F}_v$, $\mathbf{G}_v$ and $\mathbf{H}_v$ and source terms $\mathbf{S}$ are

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \\ \rho_1 \\ \vdots \\ \rho_{N_s} \end{bmatrix}, \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u(E + p) \\ \rho_1 u \\ \vdots \\ \rho_{N_s} u \end{bmatrix}, \mathbf{G} = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v(E + p) \\ \rho_1 v \\ \vdots \\ \rho_{N_s} v \end{bmatrix}, \mathbf{H} = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w(E + p) \\ \rho_1 w \\ \vdots \\ \rho_{N_s} w \end{bmatrix}, \mathbf{F}_v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ \tau_{xx}u + \tau_{xy}v + \tau_{xz}w - q_x - \sum_s J_{s,x}h_s \\ -J_{1,x} \\ \vdots \\ -J_{N_s,x} \end{bmatrix},$$

$$\mathbf{G}_v = \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ \tau_{yx}u + \tau_{yy}v + \tau_{yz}w - q_y - \sum_s J_{s,y}h_s \\ -J_{1,y} \\ \vdots \\ -J_{N_s,y} \end{bmatrix}, \mathbf{H}_v = \begin{bmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ \tau_{zx}u + \tau_{zy}v + \tau_{zz}w - q_z - \sum_s J_{s,z}h_s \\ -J_{1,z} \\ \vdots \\ -J_{N_s,z} \end{bmatrix}, \mathbf{S} = \begin{bmatrix} 0 \\ S_{MGD_x} \\ S_{MGD_y} \\ S_{MGD_z} \\ \vec{j} \cdot \vec{E} \\ \dot{\omega}_1 \\ \vdots \\ \dot{\omega}_{N_s} \end{bmatrix}.$$

Note that it is crucial which temperature model is used for modelling chemical reactions in terms of accuracy and computational time of the numerical simulations. To overcome the non-equilibrium radiation overshoot phenomenon and take into account the freezing of the vibrational temperature in expanding flows at high speeds, temperatures and altitudes, Park [42, 43] proposed a two-temperature model in which case two total energy transport equations have to be solved in addition to the chemical reaction equations. In each two-temperature model, the total energy is decomposed into the sum of the total energy of combined translational-rotational and combined vibrational-electronic degrees of freedom. It means that the total energy per unit volume of the gas mixture can be given as follows:

$$E = E_{tr} + E_{ve}, \quad (2.16)$$

where the total energy E on the left hand side of the decomposed total energy Eq. (2.16) can be obtained by the solution of the system of Eqs. (2.15). The total energy E_{ve} of the combined vibrational and electronic degrees of freedom in Eq. (2.16) can be computed simultaneously with the solution of an additional energy equation as

$$\frac{\partial E_{ve}}{\partial t} + \nabla \cdot (E_{ve}\vec{u}) = \nabla \cdot \left[\kappa \nabla T_{ve} - \sum_s^{N_s} (J_s e_{ev,s}) \right] + \sum_s^{N_s} \frac{C_{v,s}(T - T_{ve,s})}{\tau_s^*} + \sum_s^{N_s} (\dot{\omega}_s e_{v,s}), \quad (2.17)$$

where T_{ve} is the combined vibrational and electronic temperature which can be taken from the initial conditions in the first iteration step, and τ_s^* is the relaxation time which can be evaluated by the Landau–Teller model [41, 59]. The combined vibrational and electronic energy per unit mass of the species $e_{ev,s}$ can be given by

$$e_{ev,s} = \begin{cases} e_{v,s} + e_{e,s}, & \text{for molecules,} \\ \frac{3RT_{ve}}{2M_e}, & \text{for electrons,} \end{cases} \quad (2.18)$$

where $e_{v,s}$ and $e_{e,s}$ are the vibrational and the electronic energy per unit mass, respectively, which can be given by

$$e_{v,s} = \frac{R}{M_s} \frac{\theta_{v,s}}{\exp(\theta_{v,s}/T_{ve}) - 1}, \quad \text{and} \quad e_{e,s} = \frac{R}{M_s} \frac{\sum_{i=1}^{\infty} g_{i,s} \theta_{el,i,s} \exp(-\theta_{el,i,s}/T_{ve})}{\sum_{i=0}^{\infty} g_{i,s} \exp(-\theta_{el,i,s}/T_{ve})}, \quad (2.19)$$

where $\theta_{v,s}$ is the characteristic vibrational temperature, $g_{i,s}$ is degeneracy of the i^{th} energy level of a given species, and $\theta_{el,i,s}$ is the characteristic electronic temperature, respectively. The values of these coefficients are given in Appendix B. The vibrational part $e_{v,s}$ of Eq. (2.18) can be modelled as a harmonic oscillator [41, 60]. As can be seen from Eq. (2.16) that the total energy E_{tr} of the combined translational and rotational degrees of freedom can be expressed by

$$E_{tr} = E - E_{ve}. \quad (2.20)$$

At this point, it is important to emphasise that in order to compute the combined translational and rotational temperature T_{tr} and the combined vibrational and electronic temperature T_{ve} in each iteration step, a temperature model must be employed which will be discussed in the next subsection. Using Eq. (2.20), the relationship between the combined

translational-rotational energy E_{tr} and temperature T_{tr} can be written [60] as

$$E_{tr} = \sum_{s \neq e} \rho_s C_{v,ir,s} T_{tr} + \frac{1}{2} \rho (u^2 + v^2 + w^2) + \sum_{s \neq e} \rho_s h_s^0, \quad (2.21)$$

and using the solution of the vibrational energy transport Eq. (2.17), the relationship between the combined vibrational-electronic energy E_{ve} and temperature T_{ve} can be given [41] by

$$E_{ve} = \sum_{s \neq e} \rho_s \left[\frac{R}{M_s} \frac{\theta_{v,s}}{\exp(\theta_{v,s}/T_{ve}) - 1} + \frac{R}{M_s} \frac{\sum_{i=1}^{\infty} g_{i,s} \theta_{el,i,s} \exp(-\theta_{el,i,s}/T_{ve})}{\sum_{i=0}^{\infty} g_{i,s} \exp(-\theta_{el,i,s}/T_{ve})} \right] + \rho_e \frac{3RT_{ve}}{2M_e}. \quad (2.22)$$

For modelling compressible chemically reacting turbulent flows, due to the elaborate mathematical treatment of the physical behaviour of the total energy transport relying on Eqs. (2.15)–(2.22), e.g., Blottner (1969) [37], Dunn and Kang (1973) [38] and Gupta et al. (1990) [39] dealt with one-temperature models, and Park (1987) [40], Gnoffo et al. (1989) [41], Park et al. (1991, 2000) [42, 43] proposed variants of two-temperature models in conjunction with chemically reacting flows. The investigated chemical reactions occur due to the presence of shock waves in compressible turbulent flows, thus the numerical treatment of discontinuities is required through the solution of the local Riemann problem. In this work, the Harten–Lax–van Leer Contact (HLLC) [61] approximate Riemann solver has been employed and coupled with compressible multi-species reacting magnetogasdynamic turbulent flows. Further details about the mathematical treatment of the above discussed total energy transport Eqs. (2.15) and (2.17) can be found in the works of Nelson [60], Gnoffo et al. [41] and Park et al. [42, 43], respectively.

2.1. Chemical and temperature models

A standard finite rate chemistry model for 11 species ($N_s = 11$) reacting air is implemented in this work. The 11 species considered in the air model are N_2 , O_2 , NO , N , O , N_2^+ , O_2^+ , NO^+ , N^+ , O^+ and e^- , respectively. The reactions considered for the 11 species model are based on the chemical kinetic models of Dunn and Kang [38] and Park [40] which consist of 26 and 21 chemical reactions, respectively. The reason for using the Dunn and Kang [38] chemical kinetic model is discussed in this section. The reactions are mentioned in Appendix C which are represented generically by Eq. (2.23), where $[S]$ represents one of the 11 species, and α and β are the stoichiometric coefficients [41]. The right hand arrow notation in the description of chemical reactions represents exothermic reaction and vice versa, thus one can write

$$\sum \alpha_s [S] \rightleftharpoons \sum \beta_s [S]. \quad (2.23)$$

According to Gnoffo et al. [41], the chemical production rate of a species ‘s’ in a reaction ‘k’ can be predicted as

$$\dot{\omega}_{sk} = (\beta_{sk} - \alpha_{sk}) \left[10^3 k_{fk} \prod_j \left(10^{-3} \frac{\rho_j}{M_j} \right)^{\alpha_{jk}} - 10^3 k_{bk} \prod_j \left(10^{-3} \frac{\rho_j}{M_j} \right)^{\beta_{jk}} \right]. \quad (2.24)$$

Therefore, the source term in the species transport Eq. (2.12) can be given by

$$\dot{\omega}_s = M_s \sum_{k=1}^{N_k} \dot{\omega}_{sk}, \quad s = 1, \dots, N_s, \quad (2.25)$$

where N_k is the number of chemical reactions ($N_k = 26$). The forward reaction rate k_{fk} and the backward reaction rate k_{bk} in Eq. (2.24) are obtained from Arrhenius Eq. (2.26), and the reaction rates can be computed by

$$k_{(f,b)r} = C_{(f,b)r} T^{n_{(f,b)r}} \exp(-E_{(f,b)r}/kT), \quad (2.26)$$

where the numerical values of the coefficients $C_{(f,b)r}$, $n_{(f,b)r}$, $E_{(f,b)r}/k$ are taken from the chemical kinetic model of Dunn and Kang [38]. Further details on chemical reaction equations can be found in Appendix C. The choice of the temperature model in conjunction with the chemical kinetic model is crucial in terms of computational accuracy and efficiency. Therefore, details on how to select an appropriate temperature model has been discussed here. After solving

the system of Eqs. (2.15) when the one-temperature model of Dunn and Kang [38] is employed, the relationship between the total energy E and the temperature T can be used for predicting the single temperature value as

$$E = \sum_{s=1}^{N_s} \rho_s C_{v_s} T + \frac{1}{2} \rho (u^2 + v^2 + w^2) + \sum_{s=1}^{N_s} \rho_s h_s^o, \quad (2.27)$$

where h_s^o is the species enthalpy of formation and its numerical values can be found in Appendix B. However, in the case of the two-temperature model of Park [40] (see also the general Eqs. (2.15)–(2.22)), the temperature for the computation of forward and backward reaction rates can be given as follows:

$$T_P = T_{tr}^{a^*} \cdot T_{ve}^{1-a^*}, \quad (2.28)$$

where $a^* = 0.5$ in the present case which is a positive exponent value, and further calibrations on this exponent values were provided by Park [42, 43]. In this two-temperature model, the forward reaction rate is computed based on the Arrhenius curve fit Eq. (2.26), and the numerical values of the coefficients $C_{(f)r}$, $n_{(f)r}$, $E_{(f)r}$ are taken from the works of Park [40, 42, 43]. For modelling dissociation reactions, the forward and backward reaction rates have to be computed based on the temperature values of T_P and T_{tr} as controlling temperatures, respectively. For exchange and charge exchange reactions, T_{tr} must be used as a controlling temperature for the forward and backward reaction rates. For modelling associative recombination reactions, the forward and backward reaction rates have to be computed relying on the temperature values of T_{tr} and T_{ve} as controlling temperatures, respectively. Furthermore, for the electron impact ionisation reactions, T_{ve} must be used as a controlling temperature for the forward and backward reaction rates. According to Park [40, 42, 43], the backward reaction rate can be predicted as

$$k_{bk}(T_{bc}) = \frac{k_{fbk}(T_{bc})}{K_e(T_{bc})}, \quad (2.29)$$

where T_{bc} is the backward controlling temperature which is equal to T_{tr} for all chemical reactions, except for recombination ionization and impact ionization reactions in which cases T_{bc} is equal to T_{ve} . The numerical value of $K_e(T_{bc})$ in the denominator of Eq. (2.29) can be given by semi-empirical curve fitting as

$$K_e(T_{bc}) = e^{\left[A_1 \left(\frac{T_{bc}}{10000} \right) + A_2 + A_3 \ln \left(\frac{10000}{T_{bc}} \right) + A_4 \left(\frac{10000}{T_{bc}} \right) + A_5 \left(\frac{10000}{T_{bc}} \right)^2 \right]}, \quad (2.30)$$

where A_1, A_2, A_3, A_4, A_5 coefficients are different for each chemical reaction and can be taken from the tables published by Park [42, 43]. Relying on Eqs. (2.15)–(2.22) in comparison with Eqs. (2.26) and (2.27), one can see that the mathematical treatment of two-temperature models is more complex than one-temperature models. As a consequence of that, it would be expected that a two-temperature model should be more accurate than a one-temperature model. Therefore, Park (2010) [62] investigated the limitations of the two-temperature model proposed by himself in 1987 [40] in conjunction with its accuracy on the numerical solution. According to Park [62], two-temperature models, including the model proposed in 1987 [40], are acceptable for most practical applications, except for a) Martian and Titan entries, b) radio blackout, and c) rarefied rocket plume flows. Longo et al. (2007) [63] overviewed the challenges of simulating hypersonic flows and carried out a comparison between one-temperature models proposed by Dunn and Kang (1973) [38] and Gupta et al. (1990) [39] with the two-temperature model of Park et al. (1991) [42]. Longo et al. [63] found that the one-temperature model of Dunn and Kang [38] predicted the location of the bow shock slightly more accurately in comparison with the two-temperature model of Park et al. [42] against experimental data for a hypersonic flow at $Ma = 8.0$. Furthermore, in a recently published numerical study, Wang et al. (2017) [64] carried out a comparative assessment of different types of temperature models including a detailed comparison of one-temperature models with two-temperature models. Wang et al. [64] concluded that the two-temperature model proposed by Park (1987) [40] and the one-temperature model of Dunn and Kang (1973) [38] do not exhibit significant differences even at high speeds (i.e., $M = 20.5$). In this work, we focus on the physical investigation of nearly hypersonic flows up to Mach number of at around 10 in the radio blackout region which is within the altitude of 15 to 65 km depending on the speed and the size of the hypersonic vehicle. Therefore, to reduce the computational time, we have chosen and implemented the one-temperature model of Dunn and Kang [38] chemical model in conjunction with

Godunov-type high-resolution intercell flux interpolation schemes in the context of Finite Volume Method (FVM). This implementation and validation of the one-temperature model of Dunn and Kang [38] chemical model in conjunction with magnetogasdynamic turbulent flows is a novelty of this work. However, to assess the verification of the chemical reaction model, the reaction rate controlling temperature suggested by Park (1987) [40] has also been implemented and taken into account which is discussed subsequently.

2.2. Thermodynamic properties of multi-species compressible flows

In this subsection, numerical computations of the mixture pressure, specific heats at constant volume and pressure, specific heat ratio, speed of sound and species enthalpy are discussed. The mixture pressure of any one-temperature model can be computed from Dalton's law of partial pressure and ideal gas law for each species as

$$p = \sum_{s=1}^{N_s} \rho_s \frac{R}{M_s} T, \quad (2.31)$$

and the mixture pressure of any two-temperature model can be computed by

$$p = \left(\sum_{s \neq e} \rho_s \frac{R}{M_s} T_{tr} \right) + \rho_e \frac{R}{M_e} T_{ve}, \quad (2.32)$$

where the vibrational-electronic temperature T_{ve} is taken into account. Due to the fact that the transitional and the rotational energy modes are fully excited even at low temperatures, the specific heat at constant volume of a species is given by the sum of the transitional and the rotational specific heats at constant volume [39] as

$$C_{v,s} = \begin{cases} C_{vt,s} + C_{vr,s} = \frac{3}{2} \frac{R}{M_s} + \frac{R}{M_s} = \frac{5}{2} \frac{R}{M_s}, & \text{for molecules,} \\ C_{vt,s} + C_{vr,s} = \frac{3}{2} \frac{R}{M_s} + 0 = \frac{3}{2} \frac{R}{M_s}, & \text{for atoms and electrons,} \end{cases} \quad (2.33)$$

thus, the specific heat at constant pressure of a species can be given by

$$C_{p,s} = C_{v,s} + \frac{R}{M_s} = \begin{cases} \frac{7}{2} \frac{R}{M_s}, & \text{for molecules,} \\ \frac{5}{2} \frac{R}{M_s}, & \text{for atoms and electrons.} \end{cases} \quad (2.34)$$

The heat ratios of the mixture are given by taking weighted average of the heat ratio with respect to density [41] as

$$C_p = \frac{1}{\rho} \sum_{s=1}^{N_s} \rho_s C_{p,s}, \quad C_v = \frac{1}{\rho} \sum_{s=1}^{N_s} \rho_s C_{v,s}, \quad \gamma = \frac{C_p}{C_v}, \quad (2.35)$$

therefore, the speed of sound has to be known for the solution of the local Riemann problem and is computed by

$$a = \sqrt{\gamma R T}. \quad (2.36)$$

The species enthalpy is used in the viscous term of the total energy equation (2.11) which is given by

$$h_{f,s} = C_{p,s} T + h_{f,s}^0. \quad (2.37)$$

2.3. Transport properties for viscous, heat and mass diffusion fluxes

To obtain physically correct computational results, the mixture transport properties μ , κ , ρ , D of the viscous-, heat- and mass diffusion terms in the governing Eqs. (2.8)–(2.12) have to be considered as the function of the species molar fraction X_s , the dynamic viscosity coefficient of each species μ_s and the empirical function ϕ_s , respectively. In this

study, the transport properties are numerically predicted by using the Wilke model [49]. Therefore, let us consider the viscous stress tensor in the momentum Eq. (2.9) which is modelled through the Navier–Stokes hypothesis [65] as

$$\underline{\underline{\tau}} = \mu \left[\nabla \otimes \vec{u} + (\nabla \otimes \vec{u})^T \right] - \frac{2}{3} \mu (\nabla \cdot \vec{u}) \underline{\underline{I}}, \quad (2.38)$$

where the scalar components of the viscous stress tensor (2.38) can be written as

$$\tau_{xx} = 2\mu \frac{\partial u}{\partial x} - \frac{2}{3}\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) = \frac{4}{3}\mu \frac{\partial u}{\partial x} - \frac{2}{3}\mu \left(\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right), \quad (2.39)$$

$$\tau_{yy} = 2\mu \frac{\partial v}{\partial y} - \frac{2}{3}\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) = \frac{4}{3}\mu \frac{\partial v}{\partial y} - \frac{2}{3}\mu \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right), \quad (2.40)$$

$$\tau_{zz} = 2\mu \frac{\partial w}{\partial z} - \frac{2}{3}\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) = \frac{4}{3}\mu \frac{\partial w}{\partial z} - \frac{2}{3}\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right), \quad (2.41)$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \quad (2.42)$$

$$\tau_{yz} = \tau_{zy} = \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right), \quad (2.43)$$

$$\tau_{zx} = \tau_{xz} = \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right). \quad (2.44)$$

The heat flux vector in the total energy transport Eq. (2.11) is computed by using the Fourier law as

$$\vec{q} = -\kappa \nabla T. \quad (2.45)$$

According to the semi-empirical mixing rule of Wilke [49], the mixture dynamic viscosity μ and thermal conductivity κ depend on the species molar fraction X_s , the species dynamic viscosity μ_s and the empirical function ϕ_s as

$$\mu(X_s, \mu_s, \phi_s) = \sum_{s=1}^{N_s} \frac{X_s \mu_s}{\phi_s} \quad \text{and} \quad \kappa(X_s, \mu_s, \phi_s) = \sum_{s=1}^{N_s} \frac{X_s \kappa_s}{\phi_s}, \quad (2.46)$$

where the dimensionless empirical function ϕ_s in the denominator can be given [49] by

$$\phi_s = \sum_{r=1}^{N_s} X_r \left[1 + \sqrt{\frac{\mu_s}{\mu_r}} \left(\frac{M_r}{M_s} \right)^{1/4} \right]^2 \left[\sqrt{8 \left(1 + \frac{M_s}{M_r} \right)} \right]^{-1}. \quad (2.47)$$

The species coefficient of dynamic viscosity μ_s in Eqs. (2.46) and (2.47) are computed by using the curve fit formulations obtained from Gupta–Yos Collision model [39] as

$$\mu_s = \left(e^{C_{\mu,s}} \right) T^{(A_{\mu,s} \ln T + B_{\mu,s})}, \quad (2.48)$$

where $A_{\mu,s}$, $B_{\mu,s}$ and $C_{\mu,s}$ are constants determined for each species and their numerical values are listed in Appendix D. The species coefficient of thermal conductivity κ_s in Eq. (2.46) are also computed by using the curve fit formulations of the Gupta–Yos Collision model [39] as

$$\kappa_s = \left(e^{E_{\kappa,s}} \right) T^{[A_{\kappa,s} (\ln T)^3 + B_{\kappa,s} (\ln T)^2 + C_{\kappa,s} \ln T + D_{\kappa,s}]}, \quad (2.49)$$

where $A_{\kappa,s}$, $B_{\kappa,s}$, $C_{\kappa,s}$, $D_{\kappa,s}$ and $E_{\kappa,s}$ are constants determined for each species and their numerical values can be found in Appendix E. Note that the charged species coefficient values given in Appendix D and Appendix E are for the

limiting electron pressure. For different electron pressures, the numerical values of the species coefficients of dynamic viscosity μ_s and thermal conductivity κ_s should be corrected by the tile formula [39] as

$$\frac{\chi_s(p_e)}{\chi_s(p_m)} = \frac{2}{\ln \left[2.09 \cdot 10^{-2} \cdot \left(\frac{T}{1000 \cdot p_e^{0.25}} \right)^4 + 1.52 \cdot \left(\frac{T}{1000 \cdot p_e^{0.25}} \right)^{8/3} \right]}, \quad (2.50)$$

where χ_s represents the species dynamic viscosity μ_s or thermal conductivity κ_s when the expression (2.50) remains the same, p_e is the electron pressure, and p_m is the limiting value of the electron pressure which is taken [39] as

$$p_m = 0.0975 \cdot \left(\frac{T}{10^3} \right)^4. \quad (2.51)$$

It is important to note that Eqs. (2.48) and (2.49) are applicable for temperature range of 1000 K to 30000 K. For temperatures below 1000 K [39], the Sutherland law [66] of viscosity and thermal conductivity for air is used for all species, which can be expressed by

$$\mu(T) = 1.73 \cdot 10^{-5} \cdot \left(\frac{T}{273.16} \right)^{3/2} \cdot \left(\frac{373.16}{T + 110} \right), \quad (2.52)$$

$$\kappa(T) = 0.02364 \cdot \left(\frac{T}{273.16} \right)^{3/2} \cdot \left(\frac{373.16}{T + 110} \right). \quad (2.53)$$

The mass diffusion fluxes for individual species $\vec{J}_s$ in the species transport Eq. (2.12), except for the mass diffusion flux of electrons ($s \neq e$), are modelled through the Fick law [67] as

$$\vec{J}_{s \neq e} = -\rho D \nabla Y_s, \quad (2.54)$$

where Y_s is the ratio of species density ρ_s to mixture density ρ . The modified Fick law [67] requires the value of mass diffusion coefficient for each species D_s . A simple way to ensure that the sum of diffusion fluxes is equal to zero is to replace D_s by a single binary coefficient D , whose value can be obtained by

$$D = \frac{\kappa \cdot Le}{\rho \cdot C_p}, \quad (2.55)$$

where κ is the mixture thermal conductivity, C_p is the mixture specific heat at constant pressure, and Le is the Lewis number which is assumed to be constant and set to be equal to 1.4 [68]. This approach is accurate for the velocity up to 10 km/s [68]. Furthermore, the mass diffusion flux of electrons ($s = e$) in the transport Eq. (2.12), is computed by assuming ambipolar diffusion to ensure charge neutrality of the flow [69] which can be given by

$$\vec{J}_e = -\frac{1}{q_e} \sum_{s \neq e} q_s \vec{J}_s. \quad (2.56)$$

2.4. Lorentz force source terms in the momentum equation

To compute the magnetic (Lorentz force) source terms in the momentum Eq. (2.9), the electrical current density has to be computed by summing all the charge species ρ_i in the flow and multiplying it by the flow velocity vector $\vec{u}$ as

$$\vec{J} = \sum_{s=1}^{N_s} n_s q_s \vec{u} = \sum_{s=1}^{N_s} \frac{\rho_s}{M_s} N_A q_s \vec{u}, \quad (2.57)$$

where n_s is the number density of species, $N_A = 6.02214076 \cdot 10^{23} \text{ mol}^{-1}$ is the Avogadro number, M_s is the atomic or the molecular mass of species, and q_s is the charge of a particle [70]. The Lorentz force of MGD in the momentum

Eq. (2.9) can be given by the cross product of the current density $\vec{j}$ and the externally applied magnetic field $\vec{B}$ as

$$\vec{j} \times \vec{B} = \left[(vB_z - wB_y) \cdot \mathbf{e}_x + (wB_x - uB_z) \cdot \mathbf{e}_y + (uB_y - vB_x) \cdot \mathbf{e}_z \right] \cdot \sum_{s=1}^{N_s} \frac{\rho_s N_A}{M_s} q_s, \quad (2.58)$$

where e_x, e_y, e_z are unit vectors, and the MGD Lorentz force source terms in Eq. (2.9) can explicitly be written as

$$S_{MGD_x} = (vB_z - wB_y) \cdot \sum_{s=1}^{N_s} \frac{\rho_s q_s}{M_s} N_A, \quad (2.59)$$

$$S_{MGD_y} = (wB_x - uB_z) \cdot \sum_{s=1}^{N_s} \frac{\rho_s q_s}{M_s} N_A, \quad (2.60)$$

$$S_{MGD_z} = (uB_y - vB_x) \cdot \sum_{s=1}^{N_s} \frac{\rho_s q_s}{M_s} N_A. \quad (2.61)$$

2.5. Poisson equation for computing the induced electric potential

The Joule heating in the total energy transport Eq. (2.11) is computed by the dot product of the current density $\vec{j}$ and the induced electric field $\vec{E}$, where $\vec{E}$ can be obtained by using the conservation of charge in Ohm's law (2.6), which leads to a Poisson equation for computing the induced electric potential as

$$\nabla^2 \varphi = \nabla \cdot (\vec{u} \times \vec{B}). \quad (2.62)$$

The Poisson equation (2.62) is solved by applying the Successive Over-Relaxation (SOR) method yielding the induced electric potential φ which provides the electric field $\vec{E} = -\nabla \varphi$. Therefore, the Joule heating can be given by

$$\vec{j} \cdot \vec{E} = \vec{j} \cdot (-\nabla \varphi) = - \left(u \frac{\partial \varphi}{\partial x} + v \frac{\partial \varphi}{\partial y} + w \frac{\partial \varphi}{\partial z} \right) \cdot \sum_{s=1}^{N_s} \frac{\rho_s N_A}{M_s} q_s. \quad (2.63)$$

3. Numerical Schemes for Under-Resolved Direct Numerical Simulation Approach

In this section, the Under-Resolved Direct Numerical Simulation (DNS) approach is used for modelling viscous, compressible, chemically reacting magnetogasdynamic (MGD) turbulent flows. However, to resolve the smallest possible time and length scales with the traditional DNS technique would lead to an extremely long computational time for our numerical investigations. DNS solves the Navier-Stokes equations in the instantaneous (turbulent) velocity field using very high-order Finite Difference Method (FDM) or spectral schemes which can accurately capture the fluid flow physics when incompressible fluid flow is considered. However, for compressible MGD turbulent flows, due to the presence of shock waves and discontinuities in the fluid flow field, the local Riemann problem must be solved. It means that instead of using high-order finite difference schemes, high-order interpolation schemes in the context of Godunov-type Finite Volume Methods (FVM) have been employed here. This approach is often called "Implicit Large-Eddy Simulation" (ILES) technique in the literature [71–74], however, the expression ILES might be misleading, because in certain cases, the modelling of the dissipation has to be quantified in the context of dissipative/dispersive properties of numerical schemes used in the discretisation of the non-linear convective terms. As can be seen in the literature, according to other authors [75–78], it is more appropriate to call these types of compressible turbulent flow computations as "Under-Resolved DNS" approach, because this approach gives an overall accurate prediction of compressible turbulent flows due to the fact that the local Riemann problem is solved in each computational cell and in each iteration in conjunction with high-order cell-face interpolation schemes. Therefore, in the present work, the governing Eqs. (2.8)–(2.12) are solved based on that methodological approach, where the inviscid fluxes are computed by using a cell-centred Godunov-type FVM, and the viscous and source terms are discretised with high-order FDM using the cell-centred points. This approach can be considered as a type of Godunov-type Mixed

Method (GMM). The implemented computer code uses a structured grid for the cell-centred computations. Further details on this subject are discussed by Grinstein et al. [71], Drikakis [72], Ritos et al. [73], and Deng et al. [74].

3.1. Modelling of non-linear inviscid flux terms

Godunov-type schemes were developed to capture shock waves and provide an adequate numerical treatment of arising discontinuities by assuming a piece-wise distribution of the fluxes within each cell [79]. To discretise the non-linear convective/advection flux terms in the momentum Eq. (2.9), i.e., the Godunov-procedure of the computation of inviscid flux terms has been employed here. According to the order barrier theorem of Godunov [80], one can observe that linear numerical schemes preserve their monotonicity behaviour when the scheme is first-order accurate in terms of its truncation error. Godunov originally dealt with the mathematical behaviour of linear numerical schemes, however, the approach proposed by Godunov can also be used for the discretisation of non-linear convective flux terms in which case many practical evidences are available in the literature [71, 72, 81]. Therefore, the method of Godunov is widely used for simulating compressible turbulent flows in the context of the Under-Resolved DNS technique. Note that the Godunov discretisation procedure for the inviscid flux terms consists of three steps [71, 72, 81] which can be used for solving compressible and incompressible fluid flow problems as follows: 1) the use of a high-order interpolation scheme, e.g., MUSCL, ENO, WENO are widely used for predicting the 'Left' and 'Right' values of the inviscid flux variable at the cell interfaces, which can be called as high-order intercell flux interpolation, 2) the solution of the local Riemann problem to obtain inviscid flux values to capture discontinuous behaviour of the investigated physical problem, and 3) the computation of the inviscid flux term in each spatial direction relying on the solution of the local Riemann problem to compute cell-averaged values which is known as flux differentiation [81]. For the discretisation of inviscid flux terms in the momentum Eq. (2.9), the Godunov-procedure is briefly described here.

3.1.1. High-order intercell flux interpolation (reconstruction) schemes

In the present work, the high-order reconstruction of inviscid intercell flux values is carried out by MUSCL and WENO schemes which ensure that no new local extrema is generated. In this code, MUSCL scheme is implemented as piece-wise linear approach with three different limiters. As proposed by Bram van Leer [82, 83], the value of the inviscid flux $\phi \in U$ at the intercell face $i + \frac{1}{2}$ on the left 'L' and right 'R' sides of the control volume can be given by

$$\phi_{i+\frac{1}{2}}^L = \phi_i + \frac{1}{2}\bar{\Delta}_i, \quad \text{and} \quad \phi_{i+\frac{1}{2}}^R = \phi_{i+1} - \frac{1}{2}\bar{\Delta}_{i+1}, \quad \text{where} \quad \phi_{i+\frac{1}{2}}^L \in U_L \quad \text{and} \quad \phi_{i+\frac{1}{2}}^R \in U_R, \quad (3.1)$$

where $\bar{\Delta}_i$ is the limited slope which can be computed as

$$\bar{\Delta}_i = \xi_i \Delta_i, \quad (3.2)$$

where ξ_i is the slope limiter, and Δ_i is the non-limited slope given as

$$\Delta_i = \frac{1}{2}(1 + \omega_M)(\phi_i - \phi_{i-1}) + \frac{1}{2}(1 - \omega_M)(\phi_{i+1} - \phi_i), \quad (3.3)$$

where ω_M is the weight parameter which determines the contribution of the forward and backward slope to the reconstruction of inviscid fluxes. The slope limiter ξ_i is a function of the ratio of backward to forward differences. All implemented slope limiter functions are second-order and exhibit the symmetry property which ensures that the limiting actions for forward and backward gradients operate in the same way. These limiters are given as follows:

Minmod limiter [84]:

$$\xi_i(r_i) = \max[0, \min(1, r_i)], \quad \lim_{r \rightarrow \infty} \xi_i(r_i) = 1, \quad (3.4)$$

Van Leer limiter [82, 83]:

$$\xi_i(r_i) = \frac{r_i + |r_i|}{1 + |r_i|}, \quad \lim_{r \rightarrow \infty} \xi_i(r_i) = 2, \quad (3.5)$$

Van Albada limiter [85]:

$$\xi_i(r_i) = \frac{r_i^2 + r_i}{r_i^2 + 1}, \quad \lim_{r \rightarrow \infty} \xi_i(r_i) = 1. \quad (3.6)$$

WENO schemes are a class of non-linear methods which have the capability to achieve arbitrarily high-order formal accuracy in smooth regions while maintaining stable, non-oscillatory and sharp discontinuity transitions. These schemes are a version of Essentially Non-Oscillatory (ENO) schemes which were first proposed by Harten et al. [86] in 1987. Liu et al. [87] proposed a weighted version of the ENO scheme, in which case, each of the candidate stencils is assigned a weight which determines the contribution of the stencil to the final approximation of the flux value. The weights are assigned in a way that an optimal value is reached in the stencils of smooth regions and a near zero value is reached in the stencils with discontinuities. These non-linear weights ω_j can be computed as

$$\omega_j = \frac{\bar{\omega}_j}{\sum_j \bar{\omega}_j}, \quad \text{where} \quad \bar{\omega}_j = \frac{\gamma_j}{\sum_j (\epsilon + \beta_j)^2}. \quad (3.7)$$

where γ_j represents linear weights, ϵ is a very small value which has been set to be 10^{-10} , and β_j is the smoothness indicator. In the present work, the third-, fifth- and seventh-order WENO schemes based on conserved variables are implemented. The third-order WENO scheme has been implemented as proposed by Titarev et al. [88] which requires four grid points and two small stencils yielding the reconstructed flux value as

$$\phi_{i+1/2}^L = \omega_0 \left(\frac{1}{2} \phi_{i-1} + \frac{1}{2} \phi_i \right) + \omega_1 \left(\frac{3}{2} \phi_i + \frac{1}{2} \phi_{i+1} \right), \quad (3.8)$$

where the non-linear weights ω_j and $\bar{\omega}_j$, and the numerical values of the linear weights γ_j and the smoothness indicators β_j ($j = 0, 1$) in Eq. (3.7) can be given as

$$\gamma_0 = \frac{1}{3}, \quad \gamma_1 = \frac{2}{3}, \quad \beta_0 = (\phi_{i-1} - \phi_{i-2})^2, \quad \text{and} \quad \beta_1 = (\phi_i - \phi_{i-1})^2. \quad (3.9)$$

The fifth-order WENO scheme has been implemented as proposed by Titarev et al. [88] which requires six grid points and three small stencils yielding the reconstructed flux value as

$$\phi_{i+1/2}^L = \omega_0 \left(\frac{1}{3} \phi_{i-1} + \frac{5}{6} \phi_i - \frac{1}{6} \phi_{i+1} \right) + \omega_1 \left(-\frac{1}{6} \phi_{i-2} + \frac{5}{6} \phi_{i-2} + \frac{1}{3} \phi_{i-1} \right) + \omega_2 \left(\frac{1}{3} \phi_{i-3} - \frac{7}{6} \phi_{i-2} + \frac{11}{6} \phi_{i-1} \right), \quad (3.10)$$

where the non-linear weights ω_j and $\bar{\omega}_j$, and the linear weights γ_j and the smoothness indicators β_j ($j = 0, 1, 2$) in Eq. (3.7) can be found in Appendix F. The seventh-order WENO scheme has been implemented as proposed by Balsara et al. [89] which requires eight grid points and four small stencils leading to the reconstructed intercell flux values as

$$\begin{aligned} \phi_{i+1/2}^L = & \omega_0 \left(-\frac{1}{4} \phi_{i-3} + \frac{13}{12} \phi_{i-2} - \frac{23}{12} \phi_{i-1} + \frac{25}{12} \phi_i \right) + \omega_1 \left(\frac{1}{12} \phi_{i-2} - \frac{5}{12} \phi_{i-1} + \frac{13}{12} \phi_i + \frac{1}{4} \phi_{i+1} \right) \\ & + \omega_2 \left(-\frac{1}{12} \phi_{i-1} + \frac{7}{12} \phi_i + \frac{7}{12} \phi_{i+1} - \frac{1}{12} \phi_{i+2} \right) + \omega_3 \left(\frac{1}{4} \phi_i + \frac{13}{12} \phi_{i+1} - \frac{5}{12} \phi_{i+2} + \frac{1}{12} \phi_{i+3} \right), \end{aligned} \quad (3.11)$$

where the non-linear weights ω_j and $\bar{\omega}_j$, and the corresponding numerical values of the linear weights γ_j and the smoothness indicators β_j ($j = 0, \dots, 3$) in Eq. (3.7) are provided in Appendix G.

3.1.2. The HLLC Riemann solver using the interpolated intercell flux values and the inviscid flux differentiation

In this work, the local Riemann problem is solved based on the predicted intercell flux values with the use of the directionally split approximate HLLC Riemann solver which is the modification of the HLL approximate Riemann solver, where the missing contact and shear waves are restored [61]. The HLLC Riemann solver approximates the

solution of the local Riemann problem taking into account three-wave patterns which separate the space and time domain, and the HLLC inviscid flux term in the spatial direction x can be given [61] by

$$\mathbf{F}^{\text{HLLC}} = \begin{cases} \mathbf{F}_L, & \text{if } 0 \leq S_L, \\ \mathbf{F}_L + S_L(\mathbf{U}_{*L} - \mathbf{U}_L), & \text{if } S_L \leq 0 \leq S_*, \\ \mathbf{F}_R + S_R(\mathbf{U}_{*R} - \mathbf{U}_R), & \text{if } S_* \leq 0 \leq S_R, \\ \mathbf{F}_R, & \text{if } 0 \geq S_R, \end{cases} \quad (3.12)$$

where $\mathbf{U}_L$ and $\mathbf{U}_R$ are the vectors of conservative variables, and $\mathbf{F}_L$ and $\mathbf{F}_R$ are the vectors of inviscid fluxes on the left 'L' and right 'R' sides of the cell-interface, respectively. The values of these vectors are obtained using the interpolation (reconstruction) schemes discussed above. Furthermore, $\mathbf{U}_{*k}$ ($k = L, R$) are the vectors of conservative variables taken in the contact wave region, which leads to the solution of the local Riemann problem as

$$\mathbf{U}_{*k} = \rho_k \left(\frac{S_k - u_k}{S_k - S_*} \right) \begin{bmatrix} 1 \\ S_* \\ v_k \\ w_k \\ \frac{E_k}{\rho_k} + (S_* - u_k) \left(S_* + \frac{p_k}{\rho_k(S_k - u_k)} \right) \\ Y_1 \\ \vdots \\ Y_s \end{bmatrix}, \quad (3.13)$$

where S_L and S_R are the wave speeds on the left 'L' and right 'R' sides of the cell-interface which can be given by

$$S_L = \min(u_L - a_L, u_R - a_R), \quad \text{and} \quad S_R = \max(u_L + a_L, u_R + a_R), \quad (3.14)$$

where a_k ($k = L, R$) is the speed of sound, and the wave speed S_* can be computed [79] as

$$S_* = \frac{p_R - p_L + \rho_L u_L (S_L - u_L) - \rho_R u_R (S_R - u_R)}{\rho_L (S_L - u_L) - \rho_R (S_R - u_R)}. \quad (3.15)$$

Relying on Eqs. (3.12)–(3.15), the mathematical formulation of the solution of the local Riemann problem is given in the spatial direction x which can also be used for the solution in other spatial directions y and z in a similar manner. It means that for the solution of the local Riemann problem in spatial direction y , S_* must be replaced by u_k , and v_k must be replaced by S_* , and u_k in the fifth element of the $\mathbf{U}_{*k}$ ($k = L, R$) vector must be replaced by v_k in Eq. (3.13). Similarly, for the solution of the local Riemann problem in spatial direction z , S_* must be replaced by u_k , and w_k must be replaced by S_* , and u_k in the fifth element of the $\mathbf{U}_{*k}$ ($k = L, R$) vector must be replaced by w_k in Eq. (3.13) when the algorithm of the HLLC approximate Riemann solver is implemented in the computer code. Furthermore, according to the mixed Godunov-type discretisation, the cell-centred values of the inviscid flux terms based on the solution of the local Riemann problem in spatial directions x , y and z can be computed as

$$\frac{\partial \mathbf{F}}{\partial x} \Big|_{i,j,k}^{\text{HLLC}} = \frac{\mathbf{F}_{i+\frac{1}{2},j,k}^{\text{HLLC}} - \mathbf{F}_{i-\frac{1}{2},j,k}^{\text{HLLC}}}{\Delta x}, \quad \frac{\partial \mathbf{G}}{\partial y} \Big|_{i,j,k}^{\text{HLLC}} = \frac{\mathbf{G}_{i,j+\frac{1}{2},k}^{\text{HLLC}} - \mathbf{G}_{i,j-\frac{1}{2},k}^{\text{HLLC}}}{\Delta y}, \quad \frac{\partial \mathbf{H}}{\partial z} \Big|_{i,j,k}^{\text{HLLC}} = \frac{\mathbf{H}_{i,j,k+\frac{1}{2}}^{\text{HLLC}} - \mathbf{H}_{i,j,k-\frac{1}{2}}^{\text{HLLC}}}{\Delta z}, \quad (3.16)$$

where $\mathbf{F}_{i-1/2,j,k}^{\text{HLLC}}$, $\mathbf{G}_{i,j-1/2,k}^{\text{HLLC}}$, $\mathbf{H}_{i,j,k-1/2}^{\text{HLLC}}$ are the left hand side intercell face flux values and $\mathbf{F}_{i+1/2,j,k}^{\text{HLLC}}$, $\mathbf{G}_{i,j+1/2,k}^{\text{HLLC}}$, $\mathbf{H}_{i,j,k+1/2}^{\text{HLLC}}$ are the right hand side intercell face flux values after using a high-order interpolation scheme and the information from the solution of the local Riemann problem with the HLLC approximate Riemann solver. One can see more details on different approximate Riemann solvers and the Godunov-type high-resolution flux differentiation in the context of FVM based discretisation techniques in the book of Trangenstein [90]. Furthermore, note that the spectral element method [91, 92], high-order Discontinuous Galerkin (DG) method [93] and high-order finite difference compact schemes [94] are used by other authors for solving compressible turbulent flow problems with DNS approach at low

Reynolds number flows. These schemes provide very high temporal and spatial accuracy, however, these schemes also require extremely powerful computational resources, therefore, their practical applicability are limited to low Reynolds number flows. In these methods, coupling of the MGD with chemical reactions is much more complex and the algorithms for such non-trivial coupling are still under development. Moreover, as highlighted by Ritos et al. [73], DNS techniques requires roughly four to five times more High-Performance Computing (HPC) resources in terms of the computational time compared to the Godunov-type very high-order, e.g. the use of a ninth-order WENO scheme, in the context of the Under-Resolved DNS or ILES technique. Therefore, to save computational time for the investigation of industrially relevant engineering applications when unsteady, viscous, compressible, chemically reacting MGD turbulent flows are concerned, the Under-Resolved DNS approach has been chosen in this work.

3.2. Modelling of viscous and diffusion terms

In the governing Eqs. (2.8)–(2.12), the viscous flux vector including additional diffusion terms in the total energy (2.11) and species transport (2.12) equations can be written as

$$\vec{V} = \frac{\partial \mathbf{F}_v}{\partial x} + \frac{\partial \mathbf{G}_v}{\partial y} + \frac{\partial \mathbf{H}_v}{\partial z}, \quad (3.17)$$

where the scalar forms of the viscous and diffusion terms $\vec{V}$ related to the continuity (2.8), momentum (2.9), total energy (2.11) and species transport (2.12) equations can be expressed by

$$V_{\text{continuity}} = 0, \quad (3.18)$$

$$V_{\text{momentum}}^x = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}, \quad (3.19)$$

$$V_{\text{momentum}}^y = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}, \quad (3.20)$$

$$V_{\text{momentum}}^z = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}, \quad (3.21)$$

$$\begin{aligned} V_{\text{energy}} = & u \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) + v \left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) + w \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) + \\ & + \tau_{xx} \frac{\partial u}{\partial x} + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{xz} \frac{\partial u}{\partial z} + \tau_{yx} \frac{\partial v}{\partial x} + \tau_{yy} \frac{\partial v}{\partial y} + \tau_{yz} \frac{\partial v}{\partial z} + \tau_{zx} \frac{\partial w}{\partial x} + \tau_{zy} \frac{\partial w}{\partial y} + \tau_{zz} \frac{\partial w}{\partial z} + \\ & + \frac{\partial}{\partial x} \left(\kappa \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\kappa \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\kappa \frac{\partial T}{\partial z} \right) + \sum_{s=1}^{N_s} (V_{\text{species}})_s h_s, \end{aligned} \quad (3.22)$$

where the additional diffusion term $\sum_{s=1}^{N_s} (V_{\text{species}})_s h_s$ is equal to $-\nabla \cdot (\sum_{s=1}^{N_s} \vec{J}_s h_s)$ in the total energy transport Eq. (2.11) (see its mathematical derivation in Appendix I), which can be computed as

$$(V_{\text{species}})_{s \neq e} = -\nabla \cdot \vec{J}_s = \rho D \left[\frac{\partial}{\partial x} \left(\frac{\partial Y_s}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial Y_s}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial Y_s}{\partial z} \right) \right], \quad (3.23)$$

$$(V_{\text{species}})_e = -\nabla \cdot \vec{J}_e = -\nabla \cdot \left[-\frac{1}{q_e} \sum_{s \neq e} q_s \vec{J}_s \right] = \frac{1}{q_e} \sum_{s \neq e} q_s \nabla \cdot \vec{J}_s = \frac{1}{q_e} \sum_{s \neq e} q_s (-V_{\text{species}})_{s \neq e}. \quad (3.24)$$

Note that Eqs. (3.23) and (3.24) are required to compute the diffusion terms in the species transport Eq. (2.12). Furthermore, when $s = e = N_s$ in the species diffusion term $\sum_{s=1}^{N_s} (V_{\text{species}})_s h_s$ in Eq. (3.22), the divergence of the mass diffusion flux of electrons has to be computed based on Eq. (3.24), otherwise, Eq. (3.23) has to be used to predict the divergence of the mass diffusion for each individual species. The spatial derivatives appearing in the

viscous and diffusion terms in Eqs. (3.19)–(3.24) are obtained from the Taylor series expansion and their order of accuracy depends on the order of the truncation error. To provide high accuracy of the numerical solution, second-, fourth- and sixth-order finite difference central schemes have been implemented in the algorithm, see Appendix H.

3.3. Numerical solution of the Poisson equation for the induced electric field

The Poisson equation (2.62) for the induced electric field has been solved by using the method of Successive Over-Relaxation (SOR), which is an iterative solver and a variant of the Gauss–Seidel method for solving a linear system of equations. To achieve highly accurate numerical solution, second-, fourth- and sixth-order accurate central finite difference discretisation schemes, based on Eqs. (3.26), (3.27) and (3.28), have been implemented for solving the Poisson Eq. (2.62) in the computer code, respectively. The relaxation factor $\lambda = 0.7$ of the SOR method, and the right hand side of the second-order elliptical Poisson Eq. (2.62) can be computed as

$$\mathbf{RHS} = u \left(\frac{\partial B_y}{\partial z} - \frac{\partial B_z}{\partial y} \right) + v \left(\frac{\partial B_z}{\partial x} - \frac{\partial B_x}{\partial z} \right) + w \left(\frac{\partial B_x}{\partial y} - \frac{\partial B_y}{\partial x} \right) + B_x \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) + B_y \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) + B_z \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right). \quad (3.25)$$

For solving the Poisson Eq. (2.62), the second-order accurate central finite difference formulation is as follows:

$$\varphi_{i,j,k}^{(n+1)} = (1 - \lambda)\varphi_{i,j,k}^{(n)} + \frac{\lambda}{\beta} \left[\frac{\varphi_{i+1,j,k}^{(n)} + \varphi_{i-1,j,k}^{(n+1)}}{(\Delta x)^2} + \frac{\varphi_{i,j+1,k}^{(n)} + \varphi_{i,j-1,k}^{(n+1)}}{(\Delta y)^2} + \frac{\varphi_{i,j,k+1}^{(n)} + \varphi_{i,j,k-1}^{(n+1)}}{(\Delta z)^2} - \mathbf{RHS}_{i,j,k}^{(n)} \right], \quad (3.26)$$

where, $\beta = 2 \left[\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right]$.

The fourth-order accurate central finite difference formulation using the SOR method can be written as

$$\begin{aligned} \varphi_{i,j,k}^{(n+1)} = (1 - \lambda)\varphi_{i,j,k}^{(n)} + \frac{\lambda}{\beta} & \left[\frac{-\varphi_{i+2,j,k}^{(n)} + 16\varphi_{i+1,j,k}^{(n)} + 16\varphi_{i-1,j,k}^{(n+1)} - \varphi_{i-2,j,k}^{(n+1)}}{(\Delta x)^2} + \right. \\ & + \frac{-\varphi_{i,j+2,k}^{(n)} + 16\varphi_{i,j+1,k}^{(n)} + 16\varphi_{i,j-1,k}^{(n+1)} - \varphi_{i,j-2,k}^{(n+1)}}{(\Delta y)^2} + \frac{-\varphi_{i,j,k+2}^{(n)} + 16\varphi_{i,j,k+1}^{(n)} + 16\varphi_{i,j,k-1}^{(n+1)} - \varphi_{i,j,k-2}^{(n+1)}}{(\Delta z)^2} \\ & \left. - 12 \mathbf{RHS}_{i,j,k}^{(n)} \right], \quad (3.27) \end{aligned}$$

where, $\beta = 30 \left[\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right]$.

The sixth-order central finite difference formulation using the SOR method can be given by

$$\begin{aligned} \varphi_{i,j,k}^{(n+1)} = (1 - \lambda)\varphi_{i,j,k}^{(n)} + \frac{\lambda}{\beta} & \left[\frac{2\varphi_{i+3,j,k}^{(n)} - 27\varphi_{i+2,j,k}^{(n)} + 270\varphi_{i+1,j,k}^{(n)} + 270\varphi_{i-1,j,k}^{(n+1)} - 27\varphi_{i-2,j,k}^{(n+1)} + 2\varphi_{i-3,j,k}^{(n+1)}}{(\Delta x)^2} + \right. \\ & + \frac{2\varphi_{i,j+3,k}^{(n)} - 27\varphi_{i,j+2,k}^{(n)} + 270\varphi_{i,j+1,k}^{(n)} + 270\varphi_{i,j-1,k}^{(n+1)} - 27\varphi_{i,j-2,k}^{(n+1)} + 2\varphi_{i,j-3,k}^{(n+1)}}{(\Delta y)^2} \\ & \left. + \frac{2\varphi_{i,j,k+3}^{(n)} - 27\varphi_{i,j,k+2}^{(n)} + 270\varphi_{i,j,k+1}^{(n)} + 270\varphi_{i,j,k-1}^{(n+1)} - 27\varphi_{i,j,k-2}^{(n+1)} + 2\varphi_{i,j,k-3}^{(n+1)}}{(\Delta z)^2} - 180 \mathbf{RHS}_{i,j,k}^{(n)} \right], \quad (3.28) \end{aligned}$$

where, $\beta = 490 \left[\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right]$.

Note that superscript (n) in Eqs. (3.26), (3.27) and (3.28) denotes the iteration step ($n = 1, \dots, n_{max}$) for the numerical solution of the Poisson (2.62) for the induced electric potential.

3.4. Time integration schemes using the Runge–Kutta method

The temporal solution is advanced using Runge–Kutta (RK) Total Variation Diminishing (TVD) schemes. Three explicit RK schemes have been implemented in the code. The governing Eqs. (2.15) can be re-arranged as

$$\frac{\partial \mathbf{U}}{\partial t} = -\frac{\partial \mathbf{F}}{\partial x} - \frac{\partial \mathbf{G}}{\partial y} - \frac{\partial \mathbf{H}}{\partial z} + \frac{\partial \mathbf{F}_v}{\partial x} + \frac{\partial \mathbf{G}_v}{\partial y} + \frac{\partial \mathbf{H}_v}{\partial z} + \mathbf{S} = \mathbf{R}(\mathbf{U}), \quad (3.29)$$

where $\mathbf{R}(\mathbf{U})$ stands for the numerical values of the right hand side which can be computed at different time levels (m). The first-order Runge–Kutta scheme is equivalent to the backward Euler scheme and can be written as

$$\mathbf{U}_{i,j,k}^{(m+1)} = \mathbf{U}_{i,j,k}^{(m)} + \Delta t \cdot \mathbf{R}[\mathbf{U}_{i,j,k}^{(m)}]. \quad (3.30)$$

The second-order Runge–Kutta TVD scheme can be formulated [79] as

Step 1:

$$\mathbf{U}_{i,j,k}^{(1)} = \mathbf{U}_{i,j,k}^{(m)} + \Delta t \cdot \mathbf{R}[\mathbf{U}_{i,j,k}^{(m)}], \quad (3.31)$$

Step 2:

$$\mathbf{U}_{i,j,k}^{(m+1)} = \frac{1}{2}\mathbf{U}_{i,j,k}^{(m)} + \frac{1}{2}\mathbf{U}_{i,j,k}^{(1)} + \frac{1}{2}\Delta t \cdot \mathbf{R}[\mathbf{U}_{i,j,k}^{(1)}]. \quad (3.32)$$

The third-order Runge–Kutta TVD time integration scheme can be expressed [88] by

Step 1:

$$\mathbf{U}_{i,j,k}^{(1)} = \mathbf{U}_{i,j,k}^{(m)} + \Delta t \cdot \mathbf{R}[\mathbf{U}_{i,j,k}^{(m)}], \quad (3.33)$$

Step 2:

$$\mathbf{U}_{i,j,k}^{(2)} = \frac{3}{4}\mathbf{U}_{i,j,k}^{(m)} + \frac{1}{4}\mathbf{U}_{i,j,k}^{(1)} + \frac{1}{4}\Delta t \cdot \mathbf{R}[\mathbf{U}_{i,j,k}^{(1)}], \quad (3.34)$$

Step 3:

$$\mathbf{U}_{i,j,k}^{(m+1)} = \frac{1}{3}\mathbf{U}_{i,j,k}^{(m)} + \frac{2}{3}\mathbf{U}_{i,j,k}^{(2)} + \frac{2}{3}\Delta t \cdot \mathbf{R}[\mathbf{U}_{i,j,k}^{(2)}]. \quad (3.35)$$

The time step is chosen according to Courant–Friedrich–Lewy (CFL) number. In the present work, the directionally split finite volume method is used, therefore, the CFL number must be less than equal to one ($\text{CFL} \leq 1$). The time step computation has been carried out as proposed by Toro [79], thus

$$\Delta t = \text{CFL} \cdot \min \left(\frac{\Delta x}{S_i^{\max}}, \frac{\Delta y}{S_j^{\max}}, \frac{\Delta z}{S_k^{\max}} \right), \quad (3.36)$$

where $S_i^{\max}$, $S_j^{\max}$, $S_k^{\max}$ with the use of the value of the local speed of sound $a_{i,j,k}^{(m)}$ at each time level (m) as

$$S_i^{\max} = \max [|u_{i,j,k}^{\max}| + a_{i,j,k}^{(m)}], \quad S_j^{\max} = \max [|v_{i,j,k}^{\max}| + a_{i,j,k}^{(m)}], \quad S_k^{\max} = \max [|w_{i,j,k}^{\max}| + a_{i,j,k}^{(m)}]. \quad (3.37)$$

3.5. Boundary condition specifications

High-resolution interpolation schemes and high-order finite difference central schemes for computing inviscid and viscous flux terms requires additional cells known as ghost cells near to the boundaries. The numerical implementation of the physically correct boundary conditions is crucial, because improper boundary conditions could generate non-physical wave propagations from the boundaries which affects the solution of the Riemann problem. Four different types of boundary conditions have been implemented in conjunction with the conservative variables in the computer code. Note that in the following mathematical description of the specification of boundary condition equations, the notation of negative indices stand for the ghost cells. To impose Dirichlet boundary conditions, the numerical value

of the unknown variable has to be specified, which are extrapolated using a linear extrapolation given as follows:

$$\Phi_{BC} \begin{cases} \rho_{-i} = 2(\rho_{BC}) - \rho_i, \\ u_{-i} = 2(u_{BC}) - u_i, \\ v_{-i} = 2(v_{BC}) - v_i, \\ w_{-i} = 2(w_{BC}) - w_i, \\ E_{-i} = 2 \left[\frac{p_{BC}}{\gamma - 1} + \frac{1}{2} \rho_{BC} (u_{BC}^2 + v_{BC}^2 + w_{BC}^2) \right] - E_i, \\ (\rho_s)_{-i} = 2(\rho_s)_{BC} - (\rho_s)_i. \end{cases} \quad (3.38)$$

Adiabatic no-slip boundary condition requires zero velocity at the wall and it means that heat transfer does not occur at the boundary. The resulting conditions are similar to reflective conditions which can be given [79] as

$$\Phi_{BC} = \left[\rho_{-i} = \rho_i, \quad u_{-i} = -u_i, \quad v_{-i} = -v_i, \quad w_{-i} = -w_i, \quad E_{-i} = E_i, \quad (\rho_s)_{-i} = (\rho_s)_i \right]. \quad (3.39)$$

The free-flow boundary conditions are similar to transmissive conditions which can be expressed [79] by

$$\Phi_{BC} = \left[\rho_{-i} = \rho_i, \quad u_{-i} = u_i, \quad v_{-i} = v_i, \quad w_{-i} = w_i, \quad E_{-i} = E_i, \quad (\rho_s)_{-i} = (\rho_s)_i \right]. \quad (3.40)$$

In the case of the symmetrical boundary condition, the normal derivative of the velocity component is equal to zero. The conditions given below assumes that x-wall is defined as a symmetric plane, thus

$$\Phi_{BC} = \left[\rho_{-i} = \rho_i, \quad u_{-i} = -u_i, \quad v_{-i} = v_i, \quad w_{-i} = w_i, \quad E_{-i} = E_i, \quad (\rho_s)_{-i} = (\rho_s)_i \right]. \quad (3.41)$$

3.6. Description of the computer code structure

For nearly hypersonic, unsteady, viscous, compressible, reacting magnetogasdynamics flows, the governing equations (2.8)–(2.12) along with the Dunn and Kang chemical kinetic model with 11 species and 26 chemical reactions, a multi-component Harten–Lax–van Leer Contact (HLLC) local Riemann solver, the Wilke model for temperature dependent transport properties coupled with the numerical solution of the Poisson equation for the electromagnetic effects have been implemented in an in-house code. The flow chart of the computer code structure is shown in Fig. 1 which represents a simplified form of the algorithm. The in-house code reads an input file which defines the problem setup such as geometrical dimensions of the test case, numerical schemes, initial and boundary conditions. Depending on the numerical setup file, memory is allocated to the variables and a structured mesh is generated. To place an object in the computational domain, the grid cells corresponding to the location of the object are flagged as 1, and the rest of the cells are flagged as 0. The computation of the inviscid and viscous fluxes is switched off for the cells marked as 1, and the computation is carried out for the cells marked as 0. The inclusion of the object placement flags is carried out during the structured mesh generation process. Similar to the boundary conditions, the ghost cells are also required for the reconstruction near to objects. However, in this case, the ghost cells are overlapping. To overcome the problem of overlapping, the algorithm checks if the reconstruction requires a flagged cell and assigns an appropriate value. Once this is done, the initial conditions are imposed on the domain, primitive and transport variables are computed, then the boundary conditions are imposed. After this initial process, the Runge–Kutta time integration loop starts in which case different flux values are computed over the domain. The looping over the domain is carried out in a particular order as highlighted in the flowchart (see Fig. 1). At the beginning of the loop, represented by red colour in Fig. 1, the flag conditions are checked and the high-order reconstruction is performed on the conservative variables. After the reconstruction, the inviscid-, viscous- and diffusion fluxes along with the source terms are computed, then the simulation is advanced in time. The Poisson equation for the induced electric field is solved with the computation of source terms. The residuals are computed in each time step and when the final physical time is reached, output and restart files are written in formats compatible with the TecPlot® [95] and the MATLAB® [96] software packages.

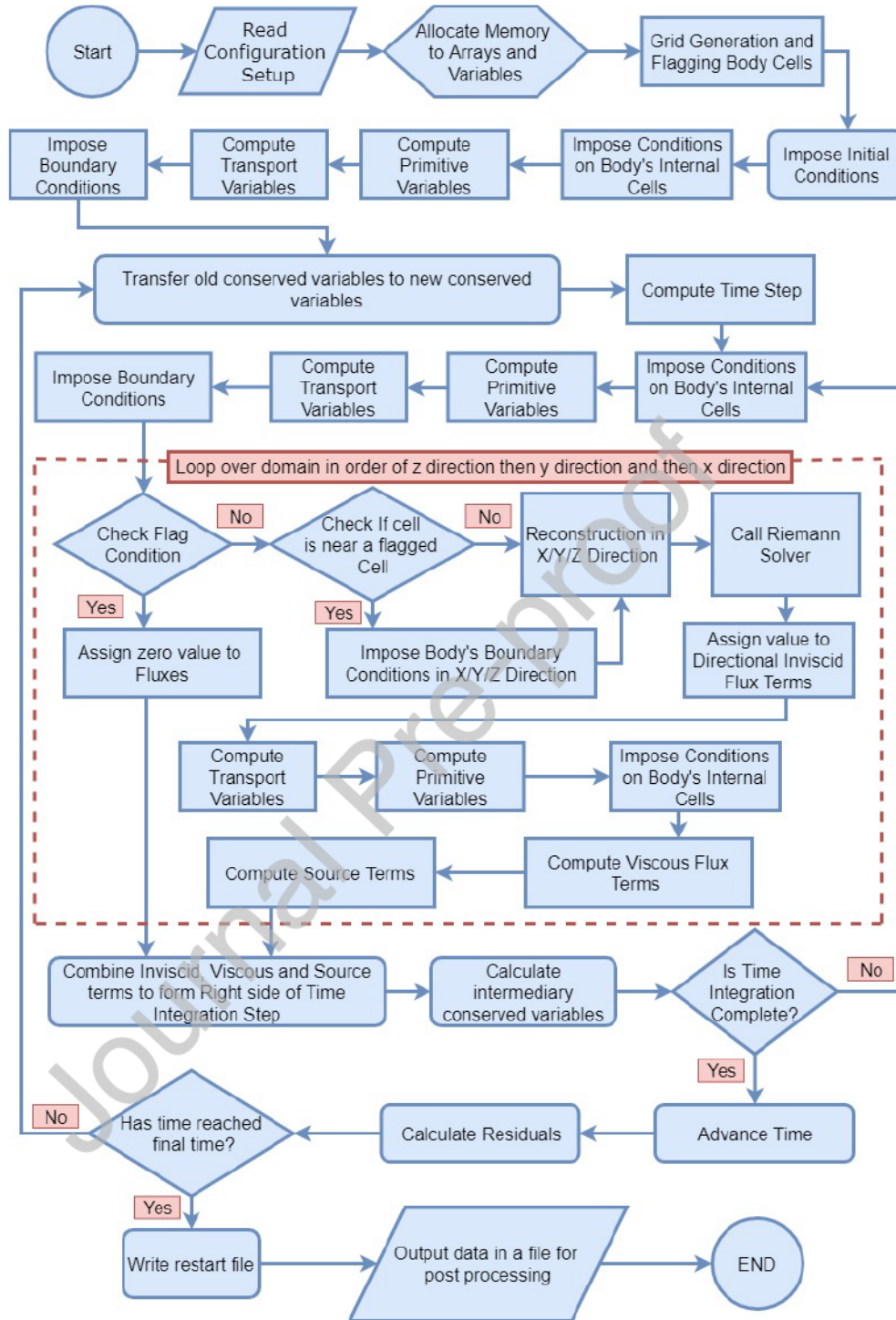


Figure 1: Flowchart of the implemented computer code structure and process

4. Results and Discussions

4.1. Validation and verification of the MGD model

Hartmann flow is a benchmark test problem for the validation of magnetic source terms. In Hartmann flow, a fluid which can be affected by magnetic field such as paramagnetic fluid or ferrofluid flows between two parallel flat plates under the influence of a pressure gradient in the presence of a constant magnetic field normal to the plates. In such conditions, an analytical solution for the outlet velocity profile exists which is given by

$$u(y) = \frac{1}{\sigma B_o^2} \left(\frac{dp}{dx} \right) \left[1 - \frac{\cosh\left(Ha \frac{y}{y_o}\right)}{\cosh(Ha)} \right], \quad -y_o \leq y \leq y_o, \quad (4.1)$$

where $u(y)$ is the x -velocity component at any y -coordinate, σ is the electrical conductivity of the fluid, B_o is the magnitude of the applied magnetic field, dp/dx is the pressure gradient, y_o is the characteristic length, and Ha is the dimensionless Hartmann number which is defined as

$$Ha = y_o B_o \sqrt{\frac{\sigma}{\mu}}, \quad (4.2)$$

where μ is the dynamic viscosity of fluid. The velocity distribution (4.1) can be further simplified by normalising the x -velocity component with the x -velocity component at the middle of the velocity profile. This results can be expressed in a dimensionless form which is used for validation purposes in the present work as follows:

$$\frac{u(y)}{u(0)} = \frac{\cosh(Ha) - \cosh\left(Ha \frac{y}{y_o}\right)}{\cosh(Ha) - 1}. \quad (4.3)$$

The present validation test case consists of a three-dimensional duct of the length of 0.5 m having a square cross-sectional area of 0.1 m² which is placed along the x -axis. At the inlet, Dirichlet boundary conditions are defined with $\rho = 1.225$ kg/m³, $u = 10$ m/s, $v = 0$ m/s, $w = 0$ m/s, and $p = 102325$ Pa leading to $Re = 67730$. At the outlet, Robin boundary conditions are defined with $p = 101325$ Pa and the normal derivative of velocity and density vanish. The fluid is composed of single species which has the electrical conductivity of 800 S/m and dynamic viscosity of 1.81×10^{-5} kg/(m s). A third-order WENO scheme has been employed for the discretisation of the inviscid flux terms along with a second-order central approximation for the viscous terms. The Poisson equation (2.62) is discretised with a second-order central finite difference formulation (3.26). The CFL number is 0.3 for the simulation time of 0.1 s using a third-order RK-TVD time integration scheme on the computational mesh of $300 \times 30 \times 30$ cells.

The comparison of numerical results with the analytical solution at different Hartmann numbers is shown in Fig. 2. The results indicate that there is no dispersion error and phase error in the results, however, the results do show some slight dissipation error near the wall. At Hartmann numbers of 20, 30, 40, 50, 75 and 100, the L_1 norms of the error are 1.60%, 1.71%, 1.52%, 1.31%, 0.98% and 0.72% which are shown in Figs. 2(a)–2(f), respectively. This slight dissipation error usually appears when approximate Riemann solvers are employed, however, it can be seen from results in Figs. 2(a)–2(f) that this error is decreasing when the Hartmann number is increasing. It means that when the strength of the magnetic field is increasing, the Maxwell stresses dominate the inertial and viscous stresses in the fluid flow. Since all of these errors are in between 0.72% and 1.71%, it can be concluded that a good agreement is achieved between the numerical results and the analytical solution. Therefore, these computational results indicate that the MGD model is implemented correctly and highlighting the robustness of the code.

The dissipation errors for different meshes at Hartmann number of 20 are shown in Fig. 3. For Mesh 1 ($160 \times 16 \times 16$), Mesh 2 ($200 \times 20 \times 20$), Mesh 3 ($240 \times 24 \times 24$), Mesh 4 ($300 \times 30 \times 30$) and Mesh 5 ($360 \times 36 \times 36$), the L_1 norms of the error are 5.07%, 3.27%, 2.81%, 1.60% and 0.67%, respectively. It means that the dissipation error is decreasing by refining the mesh at the expense of the increased computational time.

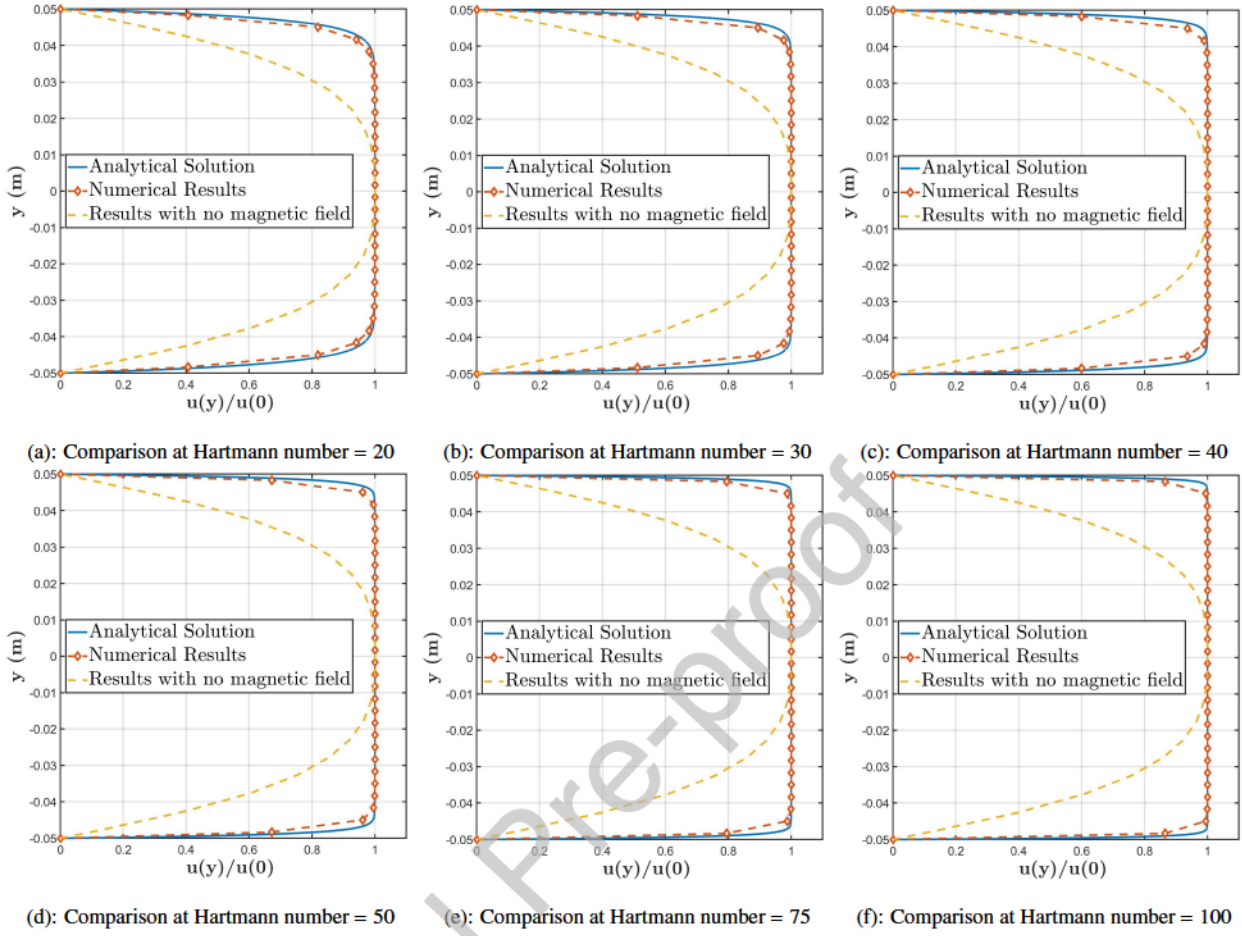


Figure 2: Validation and verification of the MGD model using the Hartmann flow problem at different Hartmann numbers

For a rigorous validation, the Hartmann flow cases are simulated with the magnetic field at different oblique orientations aligned in the YZ -plane. The analytical solution for these cases is provided by Altı [97] as

$$\frac{u(y)}{u(0)} = \frac{\cosh(Ha \cdot \cos \theta) - \cosh\left[(Ha \cdot \cos \theta) \cdot \frac{y}{y_0}\right]}{\cosh(Ha \cdot \cos \theta) - 1}, \quad (4.4)$$

where θ is the angle of orientation in the YZ -plane. The comparison of numerical results with analytical solution at Hartmann number of 30 with the magnetic field in the YZ -plane at angles of 15° and 30° orientations, the L_1 norms of the error are 1.55% and 1.04% which are shown in Figs. 5 and 6, respectively. At Hartmann number of 40 with the magnetic field in the YZ -plane at the angle of 15° , the L_1 norm of the error is 1.41% (see Fig. 7). At Hartmann number of 50 with the magnetic field in the YZ -plane at the angle of 30° , the L_1 norm of the error is 0.95% (see Fig. 8). Since all of these errors are in between 0.95% and 1.55%, it can be concluded again that a good agreement is achieved between the computational results and the analytical solution. Therefore, these numerical results indicate again that the MGD model is implemented correctly in the computer code.

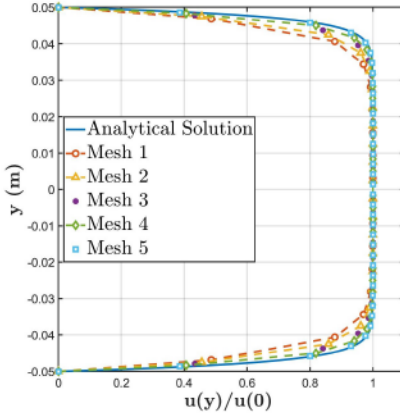


Figure 3: Comparison of the dissipation error for different meshes

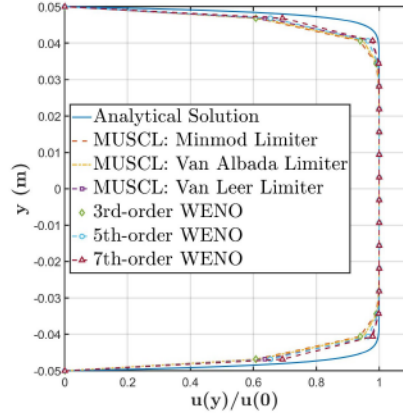


Figure 4: Comparison of the accuracy of different reconstruction schemes

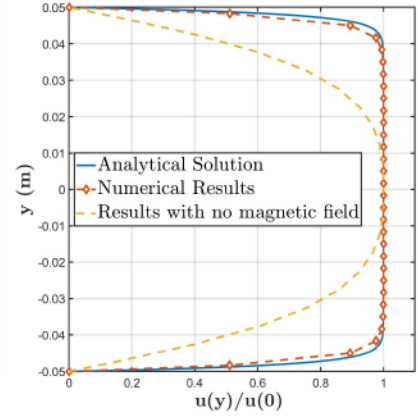


Figure 5: Comparison of results at Hartmann number of 30 with magnetic field at 15°

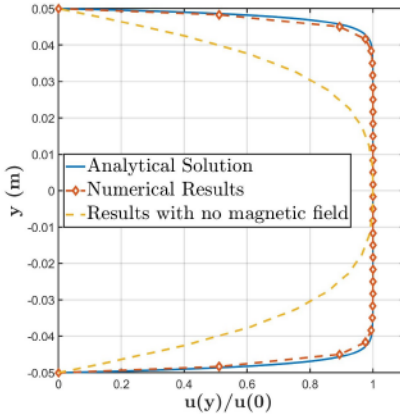


Figure 6: Comparison of results at Hartmann number of 30 with magnetic field at 30°

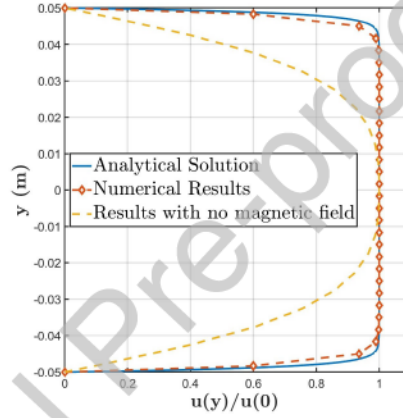


Figure 7: Comparison of results at Hartmann number of 40 with magnetic field at 15°

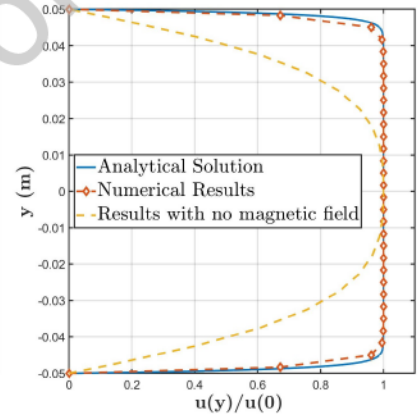


Figure 8: Comparison of results at Hartmann number of 50 with magnetic field at 30°

4.2. Error analysis for the implemented numerical schemes

The numerical results of different interpolation/reconstruction schemes for the Hartmann flow case at Hartmann number of 30 on the computational mesh of $200 \times 20 \times 20$ cells are shown in Fig. 4. The time integration scheme for comparison purposes is a third-order RK-TVD scheme with the CFL number of 0.3. To achieve highly accurate numerical solution, MUSCL and third-order WENO schemes are employed with a second-order central finite difference approximation for the Poisson equation (3.26) and the viscous terms. The fifth-order WENO scheme is used with a fourth-order central finite difference discretisation for the Poisson equation (3.27) and the viscous terms. Furthermore, the seventh-order WENO scheme is employed with a sixth-order discretisation for the Poisson equation (3.28). All the implemented reconstruction schemes showed again a good agreement between the numerical results and the analytical solution (see Fig. 4) which indicates that the implementation of the MGD model is correct. For the MUSCL scheme with the use of Minmod, Van-Leer and Van-Albada limiters, the L_1 norms of the error are 3.94%, 2.95% and 3.63% with the computational time of 8397 s, 8397 s and 8339 s, respectively. For the third-, fifth- and seventh-order WENO schemes, the L_1 norms of the error are 3.91%, 2.92% and 2.21% with computational time of 9139 s, 10685 s and 20414 s, respectively. As expected, on increasing the order of the WENO scheme, the L_1 norms of error are reducing and the computational time is increasing. One can see from Fig. 4 that the use of the seventh-order WENO scheme provided the most accurate result. Thus, it can be concluded that the dissipation error is reducing by increasing the size of the stencil. Among all the implemented reconstruction schemes for the inviscid flux terms, the MUSCL scheme with the use of the Minmod limiter led to the highest value in the L_1 norm. It is relevant to note for this

case that the MUSCL scheme with the Van–Leer limiter has approximately the same error as the fifth-order WENO scheme. The convergence of different time integration schemes is shown in Fig. 9. The third-order RK-TVD scheme consumes more computational time followed by the second-order RK scheme, and then first-order time integration scheme. Since, the flow physics involved in the Hartmann flow is relatively simple, the results for all three different time integration schemes exhibit identical numerical behaviour. It also conveys that all the results provided in this study have achieved the residuals below 10^{-6} which represents high accuracy in terms of scientific computing.

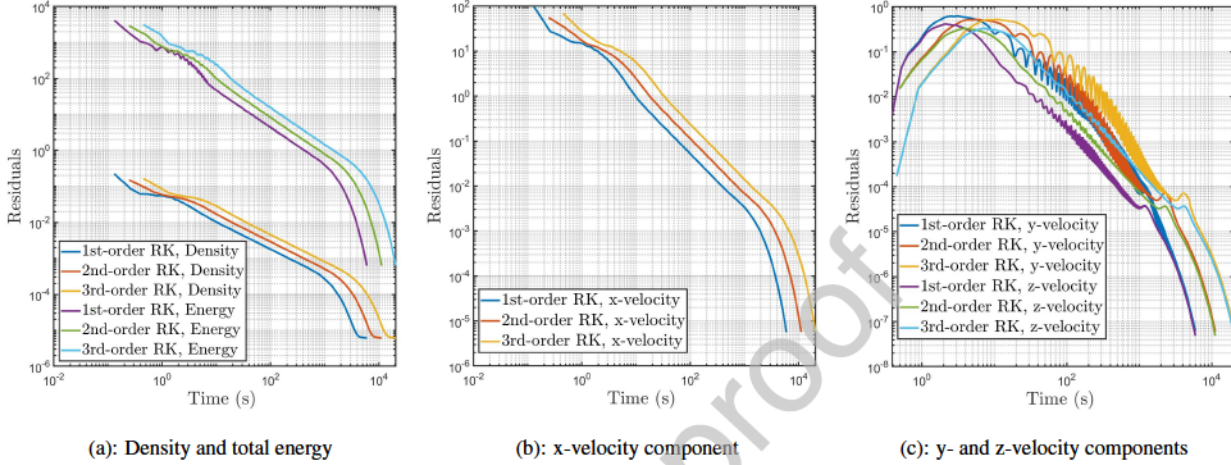


Figure 9: Residual history of primitive variables

4.3. Verification of the chemical reaction model

The verification of the implementation of chemical reactions is carried out by comparing the forward reaction rates at different temperatures with the experimental shock tube results. Due to the difference in the experimental setup of different authors as well as different chemical reaction models, the model is verified by the trend analysis in which case the observed reaction rates may not exactly match the experimental results, however, they should follow a similar trend with the values being in the ballpark region. As suggested by Park [40], for the verification of forward reaction rates of dissociation and exchange reactions, T_p and T_{tr} are used as controlling temperatures, respectively. In the case of the Dunn and Kang model [38], Figs. 10 and 11 show the reaction rate of the nitrogen dissociation when the third chemical species (M) is N_2 , O_2 , NO and N , O , respectively. Similarly, the nitrogen dissociation plots of the Park model [40] are shown in Figs. 16 and 17, respectively. The implemented reaction rates are approximately showing the same trends as presented by Bryon et al. [98] and Appleton et al. [99]. In addition to that, the numerical results agree with the experimental ones in the ballpark region. For the Dunn and Kang model [38], when the third body is N_2 , O_2 , NO and O , the reaction rates have higher values than the experimental ones, while in the case of the third body N , the reaction rate is lower than the experimental values. In the case of the Dunn and Kang model [38], Figs. 12 and 13 show the reaction rate of oxygen dissociation when the third chemical species (M) is N_2 , O_2 , NO , and N , O , respectively. Similarly, the oxygen dissociation plots of the Park model [40] are shown in Figs. 18 and 19, respectively. The reaction rates are approximately showing the same trends as given by Bortner et al. [100], Mathews et al. [101] and Johnston et al. [102]. For both chemical models, when the third body is O , the reaction rates have almost the same values as the experimental ones. For the Dunn and Kang model [38], in the case of the third body N_2 and NO , the implemented reaction rate agrees with the experimental ones in the ballpark region, while, in the case of the third body O_2 , the reaction rates have approximately the same values as the experimental ones. However, the value of the reaction rate for the third body N is much lower than the experimental value, because the Dunn and Kang model [38] is a one-temperature model where a couple of reaction rates are intentionally reduced to accommodate the limitations of one-temperature chemical reaction models. Since, the Park model [40] is a two-temperature model, therefore, none of the reaction rates is deliberately suppressed. For the similar reasons, the dissociation of nitrogen N_2 (see Figs. 10 and 16) and oxygen O_2 (see Figs. 13 and 19), the numerical results show slightly closer agreement with the experimental

data in the case of the Park model [40] compared to the Dunn and Kang model [38]. Note that the Dunn and Kang model [38] consists of 26 chemical reactions and has four more chemical reactions for ionisation compared to the two-temperature model of Park [40] which consists of 21 chemical reactions. The chemical reactions for modelling the ionisation process could be relevant to predict the fluid flow field in the radio blackout region. Finally, the reaction rates of the implemented exchange reactions are shown for the Dunn and Kang model [38] and the Park model [40] in Figs. 14–15 and Figs. 20–21, respectively. Similar trends can be observed as given by Bortner et al. [100] and Baulch et al. [103] compared to the corresponding experimental data. The verification of these six chemical reactions provides sufficient evidence that all the chemical reactions are simulated correctly. Furthermore, the implementation of both chemical reaction models discussed above is stable in the computer code.

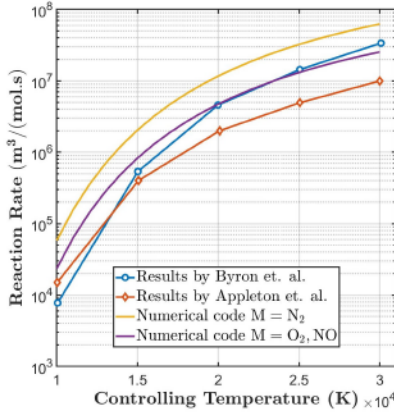
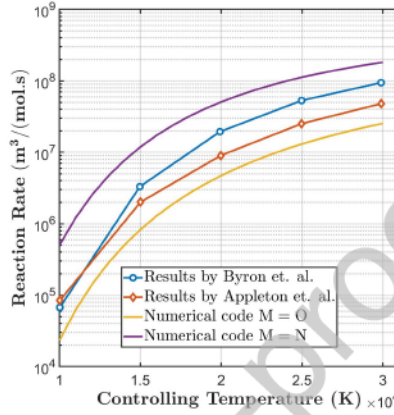
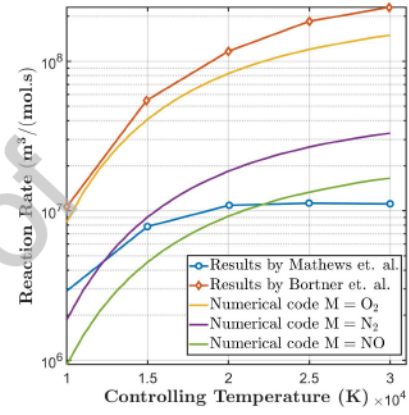


Figure 10: Verification of Nitrogen dissociation using the Dunn and Kang model [38], $N_2 + M \rightleftharpoons 2N + M$, where $M = N_2, O_2, NO$

Figure 11: Verification of Nitrogen dissociation using the Dunn and Kang model [38], $N_2 + M \rightleftharpoons 2N + M$, where $M = O, N$

Figure 12: Verification of Oxygen dissociation using the Dunn and Kang model [38], $O_2 + M \rightleftharpoons 2O + M$, where $M = N_2, O_2, NO$

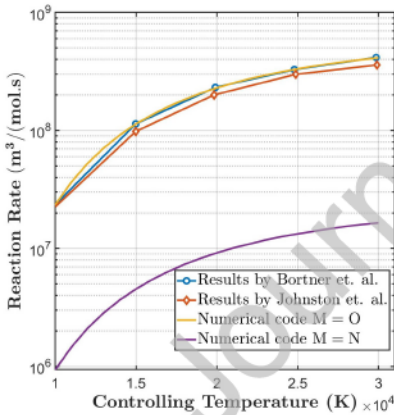
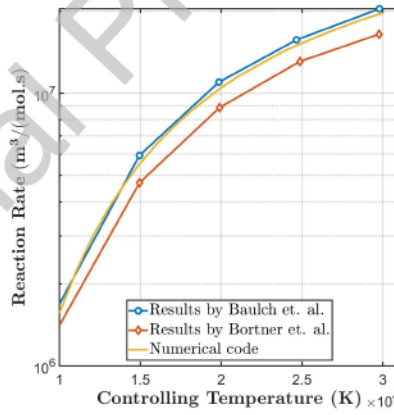
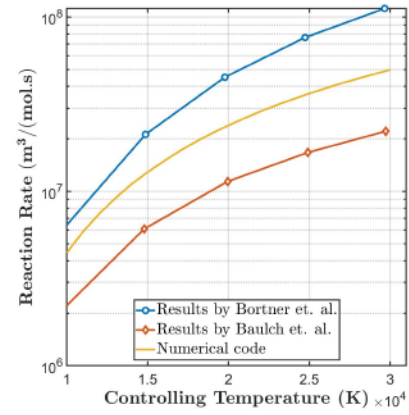


Figure 13: Verification of Oxygen dissociation using the Dunn and Kang model [38], $O_2 + M \rightleftharpoons 2O + M$, where $M = N, O$

Figure 14: Verification of exchange reaction involving Nitrogen using the Dunn and Kang model [38], $N_2 + O \rightleftharpoons NO + N$

Figure 15: Verification of exchange reaction involving Nitric oxide using the Dunn and Kang model [38], $NO + O \rightleftharpoons O_2 + N$

It is important to highlight that according to Park (2010) [62], the two-temperature model can be used successfully for investigating high-speed flows in shock tubes, however, it is not capable of predicting the physically correct shock standoff distance at intermediate hypersonic speeds when the Mach number is in between 10 and 15. As discussed in Section 2, Park [62] pointed out that two-temperature models are valid for most practical engineering applications, except for a) Martian and Titan entries, b) radio blackout, and c) rarefied rocket plume flows. Furthermore, according to Gnoffo et al. (1989) [41], the two-temperature model may be invalid for modelling viscous flows in the near wall region of the boundary layer, because the physical boundary conditions in terms of the vibrational-electronic and translational energies are inconsistent with the one-temperature approximation. Longo et al. (2007) [63] and Wang et al. (2017) [64] carried out a comparative study among the one-temperature models of Dunn and Kang (1973) [38] and

Gupta et al. (1990) [39] in comparison with the two-temperature model of Park et al. (1991) [42]. According to the work of Longo et al. [63], the one-temperature model of Dunn and Kang [38] predicted the shock standoff distance of the bow shock slightly more accurately in comparison with the two-temperature model of Park et al. [42] against measured data for a hypersonic flow at Mach number of 8.0. The knowledge on the physical behaviour of complex hypersonic shock structures around different blunt bodies is industrially relevant to predict the atmospheric re-entry trajectories of de-orbiting CubeSats, space debris or fragments of launch vehicles.

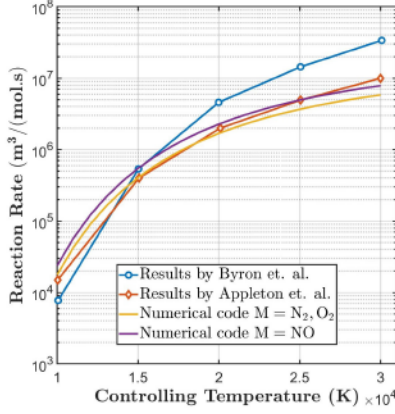
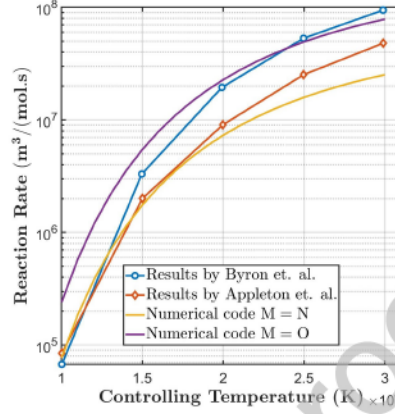
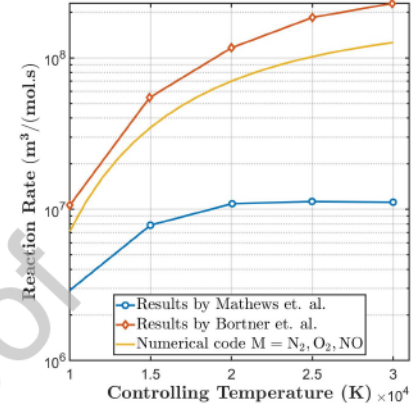


Figure 16: Verification of Nitrogen dissociation using the Park (1987) model [40], $N_2 + M \rightleftharpoons 2N + M$, where $M = N_2, O_2, NO$ Figure 17: Verification of Nitrogen dissociation using the Park (1987) model [40], $N_2 + M \rightleftharpoons 2N + M$, where $M = O, N$ Figure 18: Verification of Oxygen dissociation using the Park (1987) model [40], $O_2 + M \rightleftharpoons 2O + M$, where $M = N_2, O_2, NO$

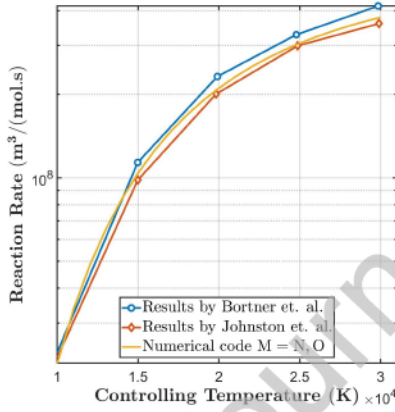
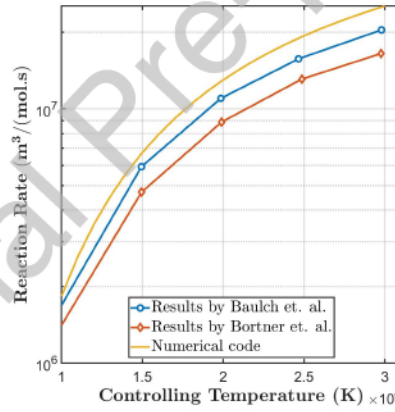
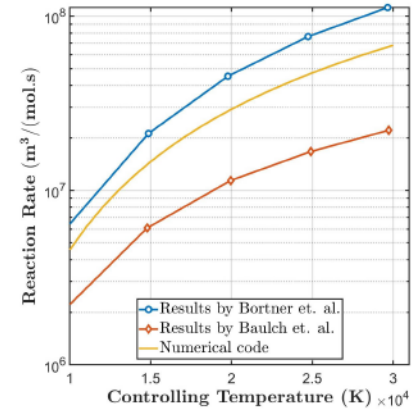


Figure 19: Verification of Oxygen dissociation using the Park (1987) model [40], $O_2 + M \rightleftharpoons 2O + M$, where $M = N, O$ Figure 20: Verification of exchange reaction involving Nitrogen using the Park (1987) model [40], $N_2 + O \rightleftharpoons NO + N$ Figure 21: Verification of exchange reaction involving Nitric oxide using the Park (1987) model [40], $NO + O \rightleftharpoons O_2 + N$

In the next section, we focus on the physical investigation of a compressible, viscous, nearly hypersonic chemically reacting magnetogasdynamic turbulent flow around different cube arrangements at Mach number of 3.0 at an altitude of 15 km. The vehicle travelling between the altitude of 15 to 65 km suffers from the radio blackout due to the high rate of ionisation. For the realistic modelling of these complex flows, the viscous effect in the boundary layer has to be taken into account and the accurate prediction of the shock standoff distance is indispensable for the understanding of the resolved shock structure formation in the wake region. A limited number of studies is available for understanding these viscous nearly hypersonic magnetogasdynamic turbulent flows around a sharp cornered blunt bodies. According to Gnoffo et al. [41] and Park [62], a) the two-temperature model is assumed to be invalid for modelling compressible, viscous, chemically reacting hypersonic turbulent flows in the boundary layer near to the solid wall due to the inconsistency of the boundary conditions; and b) the two-temperature model is invalid for the physically correct prediction of hypersonic fluid flows in the radio blackout region. Therefore, and to reduce the computational cost, the one-temperature chemical reaction model of Dunn and Kang [38] has been employed subsequently.

4.4. Shock structures around a cube

To investigate the formation of shock structures around a bluff object, a cube with a characteristic length (c) of 0.1 m placed in a three-dimensional rectangular domain. The rectangular domain extends one characteristic length in front of the cube in the spatial direction x , four characteristic lengths behind the cube in the direction x and three characteristic lengths from the sides in directions y and z . On the walls of the cube, no-slip boundary conditions are imposed. The inlet is defined with Dirichlet boundary conditions corresponding to two different free stream conditions. ‘SET-A’ conditions correspond to those conditions which are located at 15 km altitude above the sea level, where the air is a mixture of 78% nitrogen and 22% oxygen with the density of 0.19487 kg/m³ at the atmospheric pressure of 12110 Pa. ‘SET-B’ conditions correspond to those upstream conditions which exist in a vacuum type wind tunnel (see Table 1). The remaining five faces of the rectangular domain are defined with Neumann-type boundary conditions corresponding to free-flow boundary conditions. To reduce the computational time, an initial value problem in relation with the shock is given in the midway between the inlet and the cube surface. For the reconstruction of conservative variables, the third-order WENO scheme is used for the intercell flux interpolation of the inviscid terms, a second-order central approximation is employed for the viscous terms, the CFL number was 0.3, and the time integration has been carried out with a third-order RK-TVD scheme using a mesh consists of 4 293 214 cells. For validation purposes, the density immediately upstream and downstream of the shock are taken on the line passing through the centre of the cube which is compared to the analytical result which can be given by

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)M_1^2}{(\gamma - 1)M_1^2 + 2}, \quad (4.5)$$

where ρ_1 and ρ_2 are the density of air upstream and downstream of normal part of the bow shock wave, respectively.

Mach number	Density (kg/m ³)	Pressure (Pa)
1.25	1.7889	156470
1.50	1.3945	110400
1.75	1.0693	76125
2.00	0.8122	51799
2.25	0.6145	35051
2.50	0.4649	23271
2.75	0.3528	16121
3.00	0.2691	11034

Table 1: Freestream conditions SET-B

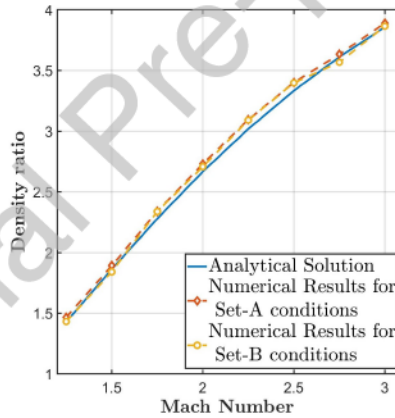


Figure 22: Comparison of density ratios at different supersonic Mach numbers and conditions

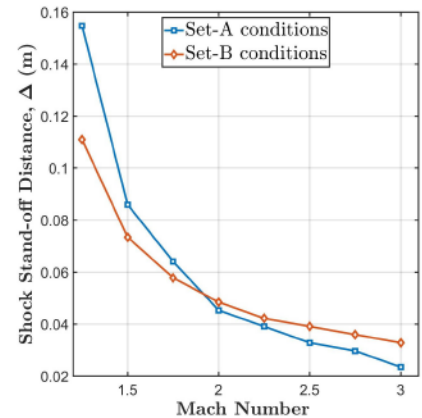


Figure 23: Comparison of shock standoff distances for different conditions

As highlighted by Anderson [104], the results from the two-dimensional theory is applicable for three-dimensional shocks for a point immediately behind a shock surface. The comparison of the numerical results of the density ratio with the analytical solution obtained at different Mach numbers is shown in Fig. 22. For ‘SET-A’ conditions, at Mach numbers of 1.25, 1.50, 1.75, 2.0, 2.25, 2.50, 2.75 and 3.0, the relative errors are 2.62%, 1.55%, 2.60%, 2.37%, 2.53%, 2.03%, 0.61% and 0.85%, respectively. For ‘SET-B’ conditions, at Mach numbers of 1.25, 1.50, 1.75, 2.0, 2.25, 2.50, 2.75 and 3.0, the relative errors are 0.16%, 1.13%, 2.57%, 1.51%, 2.40%, 1.94%, 1.22% and 0.22%, respectively. It means that for ‘SET-A’ and ‘SET-B’ conditions, the average relative errors are 1.895% and 1.393%, respectively. Note that at these Mach numbers, the temperature was not high enough to cause the chemical dissociation of air.

The shock standoff distance obtained for different upstream Mach numbers (M) at different conditions which is shown in Fig. 23. The blue line corresponds to the SET-A conditions follows the trend line of $\Delta = (0.2099) M^{-2.029}$, and the red line corresponds to the SET-B conditions follows the trend line of $\Delta = (0.1311) M^{-1.326}$. These trends shows that the shock standoff distance decreases with the increment of the Mach number. The difference in shock

standoff distance of the two set of conditions can be explained in terms of stagnation enthalpy of the flow. Therefore, in *SET-B* flow conditions, the stagnation enthalpy for the entire Mach number range is 402 kJ/kg. On the other hand, in *SET-A* flow conditions, the stagnation enthalpy is increasing when the Mach number is increasing and ranges between 285.64 kJ/kg for Mach numbers 1.25 to 609.43 kJ/kg, and at Mach number of 3.0. Since, it is a well-established knowledge that the stagnation temperature remains constant across a shock wave, and the ratio of the static temperature across a shock wave is a only a function of the Mach number. Therefore, at a particular Mach number, the flow condition with higher stagnation enthalpy will have a higher downstream static temperature resulting in higher values of coefficient of viscosity and thermal conductivity, therefore, causing higher viscous dissipation leading to a shorter standoff distance. It means that at a particular Mach number, the flow condition with higher stagnation enthalpy is having shorter shock standoff distance.

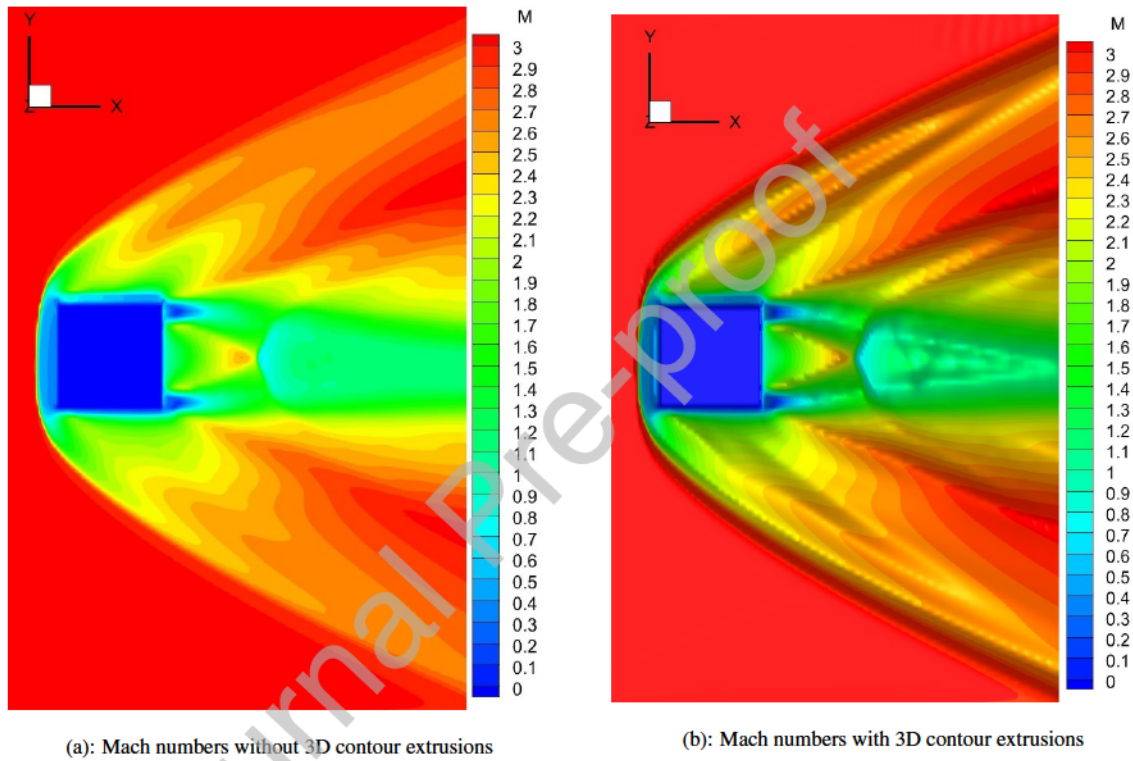


Figure 24: Mach number contours on central XY-plane at Mach number of 3.0 with '*SET-A*' conditions

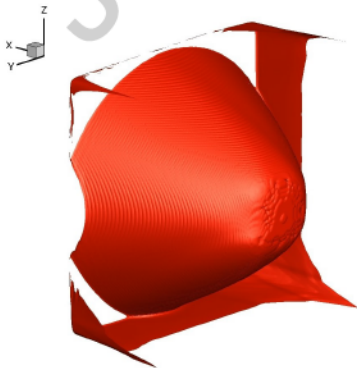


Figure 25: Bow shock iso-surface at $Ma = 3.0$ with '*SET-A*' conditions

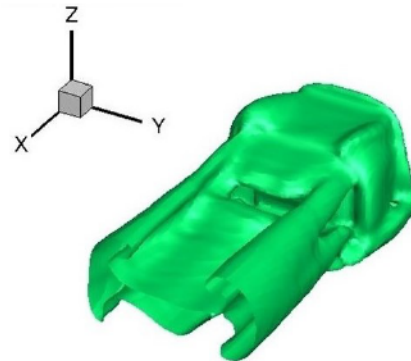


Figure 26: Iso-surface of the sonic envelope

The Mach number contours at Mach number of 3.0 freestream conditions on the XY -plane passing through the centre of the cube which is shown in Fig. 24(a). As can be seen in Fig. 24(b), the Mach number contours with the three-dimensional effects produced by using the TecPlot® [95] post-processing software package. In this case, the two-dimensional plot is converted into a three-dimensional plot by utilising the values of the local Mach number for the third axes to visualise the three-dimensional effects by generating elevation and depth, respectively. It is observed that all characteristic waves are being captured by the solver, which highlights again the robustness of the algorithm. The solver is capable of capturing the normal part as well as the curved part of the bow shock and also capturing the vortices being shed from the corners of the cube. The structure of the bow shock wave is similar to the Schlieren images obtained by the experimental work of Seltner et al. [53] and Rees et al. [54]. Moreover, the results show in Fig. 22 that the density ratio immediately behind the normal part of the shock wave is in close agreement with the analytical results, highlighting that the magnitude of the shocks obtained from the numerical investigation are correctly captured. Furthermore, the comparison of the shock standoff distance with the analytical work of Askari [55] and Olivier [56] shows that the obtained shock wave appears on the correct scale. It means that the solver is capable of resolving the subsequent shock structures originating from different shocks and contact waves interactions. These observed shock structures appear in the works of Golubev et al. [50] and Gerasimov et al. [51], however, these are much more detailed and resolved in the present study than in any previously reported results.

The flow immediately downstream of the normal part of the bow shock is subsonic at roughly Mach number of 0.43485. Ahead of the edges, the shock is still separated and highly curved, because of which a small separation bubble exists between the edge of the cube and the curved part of the shock. The curved part of the bow shock is acting as a combination of multiple oblique shocks of varying strength with the strength of each oblique shock decreasing with the increment of the distance from the wall. The separation bubble is accompanied by a small expansion fan. The flow downstream of the curved part of shock is supersonic, which after a certain downstream length is turning into itself, resulting in a reattachment shock. This reattachment shock is the combination of weak oblique shocks of varying strength, which is eventually coalescing with the main bow shock at around downstream position of 2.5 times the characteristic length behind the cube. The reattachment shock is developing, because the presence of separation bubble creates a thin envelop of subsonic flow surrounding the cube. At the end of the cube, near the edges, there is a circulation in subsonic flow in the form of counter rotating vortex pairs, because of which the supersonic flow above this sonic envelope is turning away from itself, creating an expansion fan and further accelerating the flow. In the wake of the body, the accelerated flow from the top expansion fan meets with the accelerated flow from the bottom expansion fan, which creates a Mach disk bounded by two weak oblique shocks. Further downstream in the wake these weak oblique shocks are coalescing with the previously generated expansion wave which creates subsequent reflected shocks. Furthermore, a very weak shock-train structure is observed in the downstream of the Mach disk. This shock-train is diminishing in size linearly and consists of weak expansion waves followed by even weaker reflected oblique shocks. The described flow physics is occurring in a three-dimensional space which is resulting in iso-surfaces which are shown in Figs. 25 and 26. The initial strong bow shock shown in Fig. 25 and the sonic envelope shown in Fig. 26 encloses the subsonic flow. Similar, however weaker, shock structures are observed for lower Mach numbers and identical shock structure patterns are observed for *SET-B* conditions.

Bailey et al. [105] provided experimental results for the shock structures around the sphere and Sinclair et al. [106] performed the computations on sphere at Mach number of 3.0. On comparing the two results, it is inferred that the shock structures in the case of the sphere are less complex compared to the cube. The primary difference can be seen in the curvature of the curved part of the bow shock, where the curvature is much sharper in the case of the cube. Moreover, in the case of the sphere, no separation bubble exists which results in less complex sonic envelope. Since there is no separation bubble in this case, the reattachment shock generated downstream due to boundary layer is absent. The curvature of the sphere is allowing the flow to expand due to the supersonic flow is not turning into itself which is resulting in much simpler shock structures.

4.5. Comparison of different reconstruction schemes

The comparison of results obtained from using different interpolation/reconstruction schemes are shown in Figs. 27 and 28. These results are obtained for the cube which is placed in the supersonic flow of Mach number of 2.0. The Mach number, density and temperatures at a line passing through $z = 0.1$ m are shown in Figs. 27(a) to 27(c) which location corresponds to the line parallel to the edge of the cube at one characteristic length away from the surface. It can be concluded that there is no significant difference in the shock standoff distance, in the shape of the bow shock

and in the overall shock structure. However, as can be seen in the temperature plots, some minor differences are observed near the end of the cube and in the wake. The temperature profiles when the fifth-order WENO scheme is employed with a fourth-order viscous scheme are overshooting the temperature profiles compared to the case when the seventh-order WENO scheme with a sixth-order viscous scheme was used. However, the temperature profiles of the third-order WENO scheme with a second-order viscous approximation are undershot in this case. The Mach number, density and temperatures at a line passing through $y = 0.05$ m are shown in Figs. 28(a) to 28(c) which location corresponds to the line parallel to the line passing through centre of the surface. All of these three plots further reinforce the conclusions discussed above. It can also be concluded that the differences in the numerical results are diminishing as the distance from the surface is increasing.

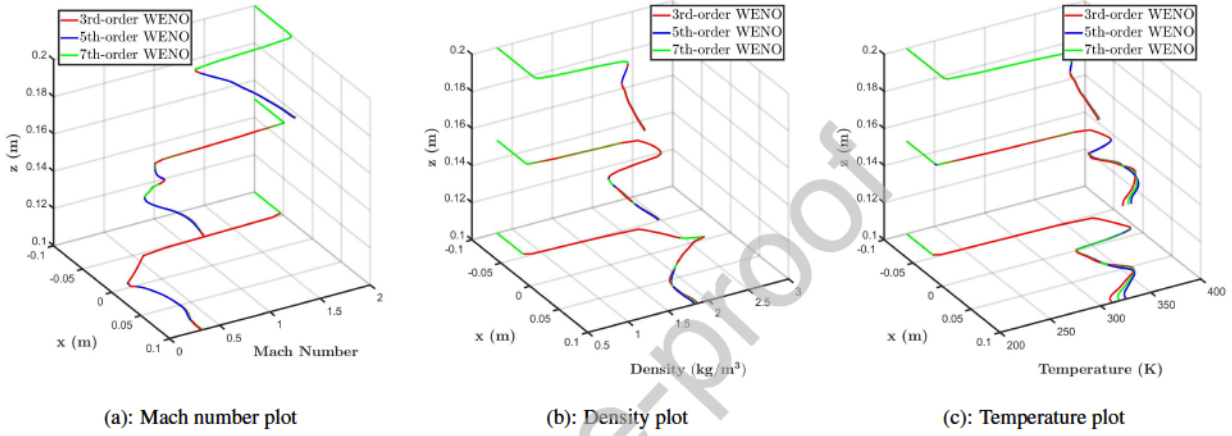


Figure 27: Comparison of (a) Mach number, (b) density and (c) temperature for different reconstruction schemes at a line passing through $z = 0.1$ m

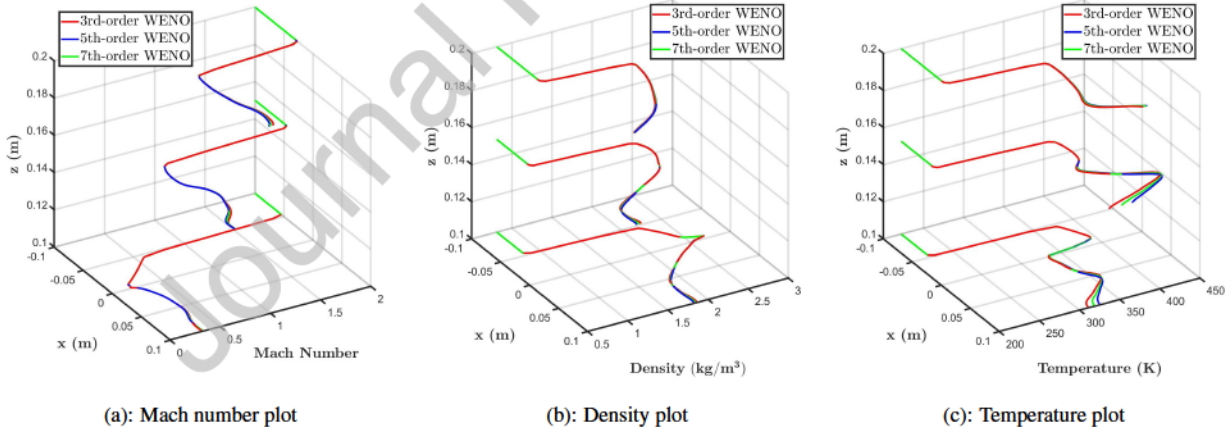


Figure 28: Comparison of (a) Mach number, (b) density and (c) temperature for different reconstruction schemes at a line passing through $y = 0.05$ m

4.6. Shock structures for bow shock interactions

The Mach contours on the YZ -plane depicting the interaction of Mach number of 3.0 bow shocks for side-by-side arrangement of the bodies are shown in Fig. 29. The first slice in Fig. 30 is passing through the middle of the two cubes, the second slice is coincident to the end surface of these two cubes, and the third slice represents the flow field at downstream location of the half of the characteristic length. The interaction of the two bow shocks in this arrangement does not change the shock standoff distance. At the half of the characteristic length from the front surface of the cubes, the two bow shocks are about to intersect each other. The coalescence of these two shocks generates a Mach disk

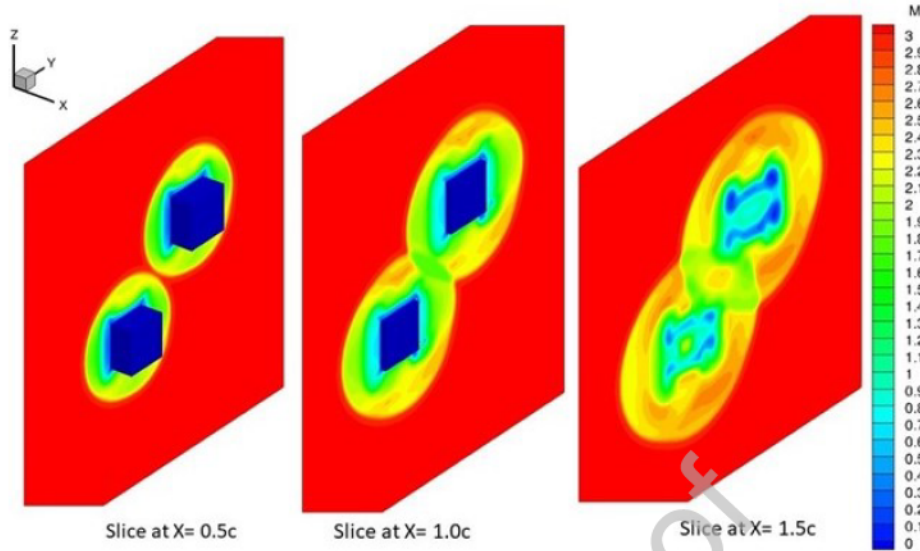


Figure 29: Mach contours on the YZ-plane depicting the interaction of Mach number of 3.0 bow shocks for side-by-side arrangement

bounded by the two reflected oblique shocks. As can be seen at slice- $X = 1.0c$ in Fig. 29, the Mach disk is in the shape of an ellipse with a sharp vertex. This shock arrangement is expanding downstream. As these oblique shocks are moving away from each other, they eventually generate an expansion fan between them, which is again accelerating the flow to Mach number of around 3.0. The oblique shock originating from the Mach disk is intersecting with the expansion fan originating from the end of the body which is resulting in the formation of two weak oblique shocks. These shock structures are gradually starting to diminish in a shock-train pattern further downstream. On comparing the case of upstream Mach number of 2.0 with Mach number of 3.0, it can be observed that in the case of upstream Mach number of 2.0, the shock interaction is weaker and the shock structures are relatively simpler, because at the point of the intersection, only a Mach disk is generated with no oblique shock reflections. Therefore, it does not result any formation of the subsequent expansion fan and shock structures.

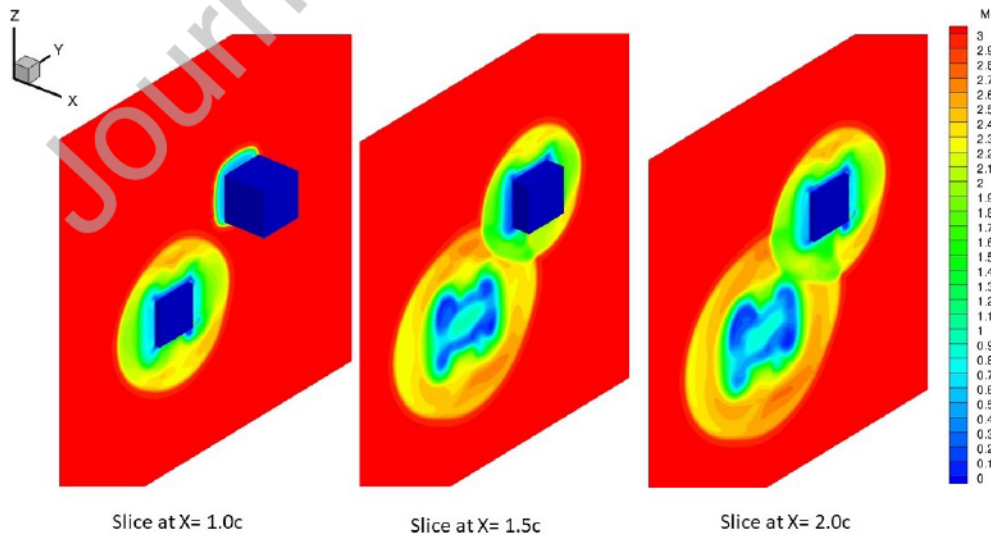


Figure 30: Mach contours on the YZ-plane depicting the interaction of Mach number of 3.0 bow shocks for staggered arrangement

The Mach contours on different YZ -plane depicting the interaction of Mach number of 3.0 bow shocks for staggered arrangement of the bodies are shown in Fig. 30. The first slice in Fig. 30 is coincident to the end surface of the first cube, the second slice is passing through the middle of the second cube, and the third slice is coincident to the end surface of the second cube. Similar to the previous case, the coalescence of the two shocks generates a Mach disk bounded by the two reflected oblique shocks, however, in this case, the oblique shock has different strengths. The oblique shock on the side of the first cube is stronger than the oblique shock on the side of the second cube. Due to this difference in the strength of the oblique shocks, the expansion fan is not symmetric and is deflected towards the wake of the first cube. In this case, the generated expansion fan is weaker than the one generated in the previous case. It means that the expansion fan is capable of accelerating the flow to Mach number of around 2.75. The oblique shock generated towards the first cube is intersecting with the oblique shocks generated in the wake of the first cube. These interactions reflect into the weaker oblique shocks with more weaker expansion fan. These shock structures gradually start to diminish further downstream in a shock-train pattern. Similar to the previous case, the shock interaction for the upstream Mach number of 2.0 is weak with relatively simpler flow physics. However, compared to the previous case, a Mach disk is generated with one reflected oblique shock at the point of intersection, which is deflected towards the first cube. This oblique shock is capable of generating an extremely weak expansion fan between itself and the surface of the second cube. This expansion fan accelerates the flow at Mach number from around 1.3 to 1.5.

4.7. Remarks on numerical artefacts

It is important to mention that CFD codes are susceptible to numerical artefacts. In certain cases, they tend to show severe instabilities called as the carbuncle phenomenon [107–109] that originates in the numerical capturing of shocks. In the code used in the present study, no such phenomenon is observed. The solver does not exhibit any dispersion and phase shift error [109, 110]. The dissipation error due to the HLLC approximate Riemann solver component is present, however, it can be reduced by refining the mesh or by using a higher-order interpolation/reconstruction scheme. As can be observed in every high fidelity compressible solver, the numerical artefacts due to the smearing of shocks have been observed in this code as well, however, the effect of the smearing is extremely mild and is not affecting the modelled fluid flow physics. However, for coarser meshes, these numerical artefacts could have an impact on capturing the physically correct fluid flow by distorting the symmetry of the bow shock. Therefore, a proper grid convergence (mesh sensitivity) study is required before performing any simulations using this methodology. Different CFD solvers use different mesh refinement techniques [111–113] for removing these numerical artefacts. However, employing such techniques will further increase the computational time for modelling these complex physical problems.

5. Summary and Conclusions

This work proposed a fully-coupled numerical approach for solving unsteady, viscous, compressible, chemically reacting turbulent MGD problems in the supersonic and nearly hypersonic fluid flow regimes relevant to aerospace applications. The Dunn and Kang [38] one-temperature chemical kinetic model was incorporated into the context of an under-resolved DNS approach taking into account 11 species and 26 chemical reactions. The appropriate choice of the one-temperature chemical reaction model of Dunn and Kang [38] was discussed in comparison with the two-temperature model of Park [40]. The reaction rate controlling temperature suggested by Park [40] has also been implemented and taken into account for the verification of the chemical model which was discussed in Section 4.3. The electromagnetic effect in the source terms of the momentum and energy equations was computed by solving a Poisson equation (2.62) in conjunction with the chemical reactions, because the current density is coupled with the product of charged species. The temperature dependence of the transport properties were taken into account with the use of the Wilke model [49]. For supersonic and hypersonic flows, a third-, fifth- and seventh-order WENO were employed with a second-, fourth- and sixth-order central viscous flux discretisation schemes, respectively. The local Riemann problem was solved by using a multi-component HLLC approximate Riemann solver. Note that the combination of these modelling approaches led to a novel combination of mathematical modelling approaches for solving compressible chemically reacting turbulent MGD problems in the context of the under-resolved DNS approach.

The magnetic source terms were validated using the classical benchmark problem of the Hartmann flow. The thermodynamic and transport model for multi-species flow and the cuboid object placement using the flag technique were validated by performing numerical simulations in the supersonic fluid flow regime. The implemented chemical

reaction model was verified by comparing implemented reaction rates against various experimental shock tube results. For the shock tube test problem, the numerical results show slightly closer agreement with the experimental data in the case of the Park (1987) model [40] compared to the Dunn and Kang model [38]. However, note that the Dunn and Kang model [38] consists of 26 chemical reactions and has four more chemical reactions for ionisation in comparison with the two-temperature model of Park [40] which consists of 21 chemical reactions. The chemical reactions for modelling the ionisation process could be relevant to predict the fluid flow field in the radio blackout region. The verification of these chemical reaction models provided sufficient evidence that all the chemical reactions were simulated correctly. The implementation of these chemical reaction models was stable in the computer code. A comparative study among different high-order numerical schemes was carried out using the Hartmann flow test problem at low Mach number. In each validation and verification study, a good agreement is achieved between the numerical results and analytical solutions. The accuracy, stability and robustness of the implemented computer code was highlighted in this work. The solver did not exhibit any dispersion or phase shift error. The dissipation error due to the HLLC approximate Riemann solver component was present, however, it can be reduced by refining the density of the computational mesh. Due to the smearing of the shock, numerical artefacts are extremely minor, therefore, the code was found to be free from the carbuncle phenomenon. It was also found that the solver adequately captured the physical behaviour of the fluid flow field for different Mach number range. Note that the implementation of the in-house code used in this study is applicable to investigate physical problems in rectangular domains. The further extension of the code to treat curvilinear domains and complex geometries is the subject of future work.

The numerical investigation on the sharp-cornered bluff body, i.e., a cuboid object in this case, showed the generation of the strong bow shock. For this problem, the gas flow was dense, therefore the continuum approach was employed, otherwise, particle-based methods should be used for rarefied gas flows. It is relevant to emphasise again that according to Gnoffo et al. [41] and Park [62], a) the two-temperature model is assumed to be invalid for modelling compressible, viscous, chemically reacting hypersonic turbulent flows in the viscous boundary layer due to the inconsistency of the physical boundary conditions; and b) the two-temperature model is invalid for the physically correct prediction of hypersonic fluid flows in the radio blackout region. Therefore, in addition to that, in order to reduce the computational cost, the one-temperature chemical reaction model of Dunn and Kang [38] was employed for the investigation of each physical problem in conjunction with cuboid objects in this work. The curved part of the bow shock acted as a combination of multiple oblique shocks of varying strength which resulted in a highly non-linear flow. In comparison with blunt bodies, the bow shock was accompanied by the separation bubble and reattachment oblique shocks near the edges of the front face of the cube and expansion fans near the edges of the back end of the cube. It was concluded from the shock standoff distance study at various upstream Mach numbers for a different set of conditions that the shock standoff distance decreased with increasing upstream Mach number. At a particular Mach number with different fluid flow conditions, the shock standoff distance was found to be shorter for a flow with higher stagnation enthalpy. A detailed explanation of the shock standoff distance and interaction between the sonic envelop and the multiple oblique shocks over the cube was given in this paper.

For the multi-component turbulent airflow over the cube at Mach numbers of 2.0 and 3.0, a particular attention was devoted to the interaction of bow shocks for side-by-side and staggered arrangements. The interaction of bow shocks generated by the two bodies resulted in a generation of a Mach disk accompanied by two oblique shocks and a downstream expansion fan. The shock structures arising due to these interactions are weaker in the case of staggered formation than in a side-by-side formation. Therefore, if one wants to minimise the drag of two flying bodies, these bodies should fly in a staggered formation. However, in the case of de-orbiting satellites or fragmenting launch vehicles, side-by-side arrangements should be considered to maximise drag to increase the chance of deterioration. The main finding of this work was that for supersonic flows over the cube, the shock structures were observed to be much more resolved compared to any previously reported work, especially in the wake region.

Appendix A. Derivation of the Equation of the Magnetic Induction Field

To derive an equation of the magnetic induction field $\vec{B}$, the electric field vector $\vec{E}$ can be obtained from Ohm's law (2.6) and the current density $\vec{j}$ can be derived from Ampere's law (2.5), and with the substitution of Eqs. (2.6)

and (2.5) in the Faraday's law (2.4), one can write the following derivation as

$$\begin{aligned}\nabla \times \vec{E} &= \nabla \times \left(\frac{\vec{J}}{\sigma} - \vec{u} \times \vec{B} \right) = \nabla \times \left(\frac{\epsilon_0 c^2}{\sigma} \nabla \times \vec{B} - \vec{u} \times \vec{B} \right) = \nabla \times \left[\frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right) - \vec{u} \times \vec{B} \right] = \\ &= -\nabla \times (\vec{u} \times \vec{B}) + \nabla \times \left[\frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right) \right] = \nabla \cdot (\vec{u} \otimes \vec{B} - \vec{B} \otimes \vec{u}) + \nabla \times \left[\frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right) \right] = -\frac{\partial \vec{B}}{\partial t}.\end{aligned}\quad (\text{A.1})$$

Therefore, the mathematical form of the equation of the magnetic induction field $\vec{B}$ can be given as

$$\frac{\partial \vec{B}}{\partial t} + \nabla \cdot (\vec{u} \otimes \vec{B} - \vec{B} \otimes \vec{u}) + \nabla \times \left[\frac{1}{\sigma} \left(\nabla \times \frac{\vec{B}}{\mu_e} \right) \right] = 0. \quad (\text{A.2})$$

Appendix B. Thermodynamic Properties and Electronic Energy Data of Species

Species	Molar Mass, M (kg/mol) · 10 ⁻³	Enthalpy of formation, h_f^0 (J/kg) · 10 ⁶	Characteristic Vibrational Temperature, θ_v (K)	Specific Heat at constant Volume, C_v J/(kg·K)	Pressure, C_p J/(kg·K)
N_2	28.000	0.0	3395	742.36	1039.3
O_2	32.000	0.0	2239	649.57	909.39
NO	30.000	3.0	2817	692.87	970.02
N_2^+	27.9994514	54.3	3395	742.38	1039.3
O_2^+	31.9994514	36.6	2239	649.58	909.41
NO^+	29.9994514	32.8	2817	692.88	970.04
N	14.000000	33.6	0	890.83	1484.7
O	16.000	15.4	0	779.48	1299.1
N^+	13.9994514	134.0	0	890.87	1484.8
O^+	15.9994514	97.7	0	779.51	1299.2
e^-	0.0005486	0	0	22734000	37889000

Table B.2: Thermodynamic properties of species

Level	Species O_2		Species O^+		Species O		Species N		Species N^+	
	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g
0	0.0	3	0.0	4	0.0	5	0.0	4	0.0	1
1	1.13916	2	3.858334	10	0.027707	3	2.766469	10	0.007007	3
2	1.89847	1	5.822349	6	0.032657	1	4.149309	6	0.018819	5
3	4.75597	1	-	-	2.283028	5	-	-	2.203657	5
4	4.99124	6	-	-	4.861993	1	-	-	4.703183	1
5	5.09227	3	-	-	-	-	-	-	6.731252	5
6	7.18986	3	-	-	-	-	-	-	13.271908	15

Table B.3: Electronic energy data of species O_2 , O^+ , O , N and N^+

Level	Species N_2		Species N_2^+		Species NO		Species O_2^+		Species NO^+	
	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g	θ_{el} (K) · 10 ⁴	g
0	-	-	0.0	2	0.0	4	0.0	4	0.0	1
1	0.0	1	1.318997	4	5.467346	8	4.735441	8	7.508968	3
2	7.223157	3	3.663323	2	6.317139	2	5.837399	4	8.525462	6
3	8.577863	6	3.668877	4	6.599451	4	5.841427	6	8.903572	6
4	8.605027	6	5.985305	8	6.599451	4	6.229896	4	9.746982	3
5	9.535119	3	6.618366	8	7.049998	4	6.733468	2	10.005530	1
6	9.805638	1	7.598992	4	7.491055	4	7.121937	4	10.280336	2
7	9.968268	2	7.625508	4	7.628875	2	7.654284	4	10.571386	2
8	10.489764	2	8.201019	4	8.676188	4	8.819692	4	-	-
9	11.164895	5	8.416835	4	8.714431	2	8.891630	4	-	-
10	12.258365	1	8.632651	8	8.886077	4	9.423977	8	-	-
11	12.488569	6	8.920406	8	8.981756	4	9.495916	4	-	-
12	12.824761	6	9.208161	4	8.988446	2	9.592026	2	-	-
13	13.380609	10	9.222549	4	9.042702	2	9.985099	2	-	-
14	14.042964	6	9.293768	2	9.064284	2	10.359181	4	-	-
15	15.049588	6	9.639794	2	9.111763	4	-	-	-	-
16	-	-	10.359181	4	-	-	-	-	-	-

Table B.4: Electronic energy data of species N_2 , N_2^+ , NO , O_2^+ and NO^+

Appendix C. Chemical Kinetic Model

- **Dissociative:**

Here, $M = N_2, O_2, NO, N$ and O .



- **Exchange:**



- **Dissociative Recombination:**



- **Charge Exchange:**



- **Electron Impact Ionisation:**



For computing the chemical reactions, the coefficients of the one-temperature chemical kinetic model of Dunn and Kang (1973) [38], and the two-temperature model of Park (1987) [40] are tabulated by Gnoffo et al. (1989) [41].

Appendix D. Viscosity Curve Fits

- Viscosity is obtained in g/(cm·s), and to convert it into SI unit, one should multiply it by factor of 0.1 [39].
- For temperatures less than 1000 K, the Sutherland viscosity law for air may be used for all species [39].
- The charged species viscosities are given here for the limiting the electron pressure p_m . For different electron pressures, these values should be corrected by the tile formula (2.50) given in the text [39].

Species	$A_{\mu,s}$	$B_{\mu,s}$	$C_{\mu,s}$
N_2	0.0203	0.4329	-11.8153
O_2	0.0484	-0.1455	-8.9231
NO	0.0452	-0.0609	-9.4596
N_2^+	0.0	2.5	-32.0827
O_2^+	0.0	2.5	-32.0148
NO^+	0.0	2.5	-32.0453
N	0.0120	0.5930	-12.3805
O	0.205	0.4257	-11.5803
N^+	0.0	2.5	-32.4285
O^+	0.0	2.5	-32.3606
e^-	0.0	2.5	-37.4475

Table D.5: Constants for viscosity curve fits [39]

Appendix E. Thermal Conductivity Curve Fits

- Thermal conductivity is obtained in cal/(cm·s·K), and to convert it into SI unit, one should multiply it by factor of 418.4 [39].
- For temperatures less than 1000 K, the Sutherland viscosity law for air may be used for all species [39].
- The charged species thermal conductivities are given for the limiting electron pressure p_m . For different electron pressures, these values should be corrected by the tile formula (2.50) given in the text [39].

Species	$A_{K_{f,s}}$	$B_{K_{f,s}}$	$C_{K_{f,s}}$	$D_{K_{f,s}}$	$E_{K_{f,s}}$
N_2	0.03607	-1.07503	11.95029	-57.90063	93.21782
O_2	0.07987	-2.58428	31.25959	-166.76267	321.69820
NO	0.02792	-0.87133	10.17967	-52.03466	88.67060
N_2^+	0.0	-0.03723	0.84192	-3.59040	-18.65620
O_2^+	-0.08373	2.75459	-33.74529	185.13274	-401.50753
NO^+	-0.06836	2.57829	-35.72737	219.09215	-519.00261
N	0.0	0.0	0.01619	0.55022	-12.92190
O	0.0	0.0	0.03310	0.22834	-11.58116
N^+	0.0	0.0	0.03088	2.06339	-31.51368
O^+	-0.04013	1.32468	-16.22091	89.96782	-208.57442
e^-	0.0	0.0	0.00032	2.49375	-27.89805

Table E.6: Constants for thermal conductivity curve fits [39]

Appendix F. Fifth-Order WENO Interpolation: Equations for Linear Weights and Smoothness Indicators

In Eq. (3.10), the linear weights and smoothness indicators are required for computing non-linear weights as

$$\gamma_0 = \frac{1}{10}, \quad \gamma_1 = \frac{6}{10}, \quad \gamma_2 = \frac{6}{10}, \quad (F.1)$$

$$\beta_0 = \frac{13}{12} (\phi_{i-1} - 2\phi_i + \phi_{i+1})^2 + \frac{1}{4} (3\phi_{i-1} - 4\phi_i + \phi_{i+1})^2, \quad (F.2)$$

$$\beta_1 = \frac{13}{12} (\phi_{i-2} - 2\phi_{i-1} + \phi_i)^2 + \frac{1}{4} (\phi_{i-2} - \phi_i)^2, \quad (F.3)$$

$$\beta_2 = \frac{13}{12} (\phi_{i-3} - 2\phi_{i-2} + \phi_{i-1})^2 + \frac{1}{4} (\phi_{i-3} - 4\phi_{i-2} + 3\phi_{i-1})^2. \quad (F.4)$$

Appendix G. Seventh-Order WENO Interpolation: Equations for Linear Weights and Smoothness Indicators

In Eq. (3.11), the linear weights and smoothness indicators are required for computing non-linear weights as

$$\gamma_0 = \frac{1}{35}, \quad \gamma_1 = \frac{12}{35}, \quad \gamma_2 = \frac{18}{35}, \quad \gamma_3 = \frac{4}{35}, \quad (G.1)$$

$$\beta_0 = \phi_{i-3} (547\phi_{i-3} - 3882\phi_{i-2} + 4642\phi_{i-1} - 1854\phi_i) + 2107\phi_i^2 + \phi_{i-2} (7043\phi_{i-2} - 17246\phi_{i-1} + 7042\phi_i) + \phi_{i-1} (11003\phi_{i-1} - 9402\phi_i), \quad (G.2)$$

$$\beta_1 = \phi_{i-2} (267\phi_{i-2} - 1642\phi_{i-1} + 1602\phi_i - 494\phi_{i+1}) + 547\phi_{i+1}^2 + \phi_{i-1} (2843\phi_{i-1} - 5966\phi_i + 1922\phi_{i+1}) + \phi_i (3443\phi_i - 2522\phi_{i+1}), \quad (G.3)$$

$$\beta_2 = \phi_{i-1} (547\phi_{i-1} - 2522\phi_i + 1922\phi_{i+1} - 494\phi_{i+2}) + 267\phi_{i+2}^2 + \phi_i (3443\phi_i - 5966\phi_{i+1} + 1602\phi_{i+2}) + \phi_{i+1} (2843\phi_{i+1} - 1642\phi_{i+2}), \quad (G.4)$$

$$\beta_3 = \phi_i (2107\phi_i - 9402\phi_{i+1} + 7042\phi_{i+2} - 1854\phi_{i+3}) + 547\phi_{i+3}^2 + \phi_{i+1} (11003\phi_{i+1} - 17246\phi_{i+2} + 4642\phi_{i+3}) + \phi_{i+2} (7043\phi_{i+2} - 3882\phi_{i+3}). \quad (G.5)$$

Appendix H. Finite Difference Schemes for Viscous Flux Discretisation

For the discretisation of the viscous flux terms with central finite difference approximations, ϕ represents the variable whose derivative is needed to be computed in Eqs. (3.18) to (3.24). These mathematical formulations are in spatial direction x and can also be used for other spatial directions in a similar manner.

Second-order formulation of Taylor series:

$$\left. \frac{\partial \phi}{\partial x} \right|_{i,j,k} = \frac{\phi_{i+1,j,k} - \phi_{i-1,j,k}}{2\Delta x} + O(\Delta x^2). \quad (\text{H.1})$$

Fourth-order formulation of Taylor series:

$$\left. \frac{\partial \phi}{\partial x} \right|_{i,j,k} = \frac{-\phi_{i+2,j,k} + 8\phi_{i+1,j,k} - 8\phi_{i-1,j,k} + \phi_{i-2,j,k}}{12\Delta x} + O(\Delta x^4). \quad (\text{H.2})$$

Sixth-order formulation of Taylor series:

$$\left. \frac{\partial \phi}{\partial x} \right|_{i,j,k} = \frac{\phi_{i+3,j,k} - 9\phi_{i+2,j,k} + 45\phi_{i+1,j,k} - 45\phi_{i-1,j,k} + 9\phi_{i-2,j,k} - \phi_{i-3,j,k}}{60\Delta x} + O(\Delta x^6). \quad (\text{H.3})$$

Appendix I. Diffusive term in energy equation

In the total energy Eq. (2.11), the term $-\nabla \cdot (\sum_s^{N_s} J_s h_s)$ can be simplified as

$$-\nabla \cdot \left(\sum_s^{N_s} J_s h_s \right) = -\nabla \cdot (J_{N_2} h_{N_2} + J_{O_2} h_{O_2} + \dots + J_e h_e) = -\nabla \cdot (J_{N_2} h_{N_2}) - \nabla \cdot (J_{O_2} h_{O_2}) - \dots - \nabla \cdot (J_e h_e), \quad (\text{I.1})$$

because h_s is the enthalpy of formation and it is a constant in terms of differentiation, thus

$$-\nabla \cdot \left(\sum_s^{N_s} J_s h_s \right) = -h_{N_2} \nabla J_{N_2} - h_{O_2} \nabla J_{O_2} - \dots - h_e \nabla J_e = h_{N_2} (-\nabla J_{N_2}) + h_{O_2} (-\nabla J_{O_2}) + \dots + h_e (-\nabla J_e), \quad (\text{I.2})$$

and as given by Eqs. (3.23) and (3.24), $-\nabla J_s = (V_{species})_s$, therefore, Eq. (I.2) becomes

$$-\nabla \cdot \left(\sum_s^{N_s} J_s h_s \right) = h_{N_2} (V_{species})_{N_2} + h_{O_2} (V_{species})_{O_2} + \dots + h_e (V_{species})_e = \sum_s^{N_s} (V_{species})_s h_s. \quad (\text{I.3})$$

Acknowledgements

The present research work was financially supported by the Centre for Computational Engineering Sciences at Cranfield University under project code EEB6001R. We would also like to acknowledge the IT support and the use of the High Performance Computing (HPC) facilities at Cranfield University, UK.

Conflict of Interest

None Declared. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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2022-03-09

Elsevier

<https://doi.org/10.1016/j.apm.2022.02.041>

Chaudhary H, Könözy L, Rana ZA. (2022) A novel combination of mathematical modelling approaches for simulating nearly hypersonic, viscous, reacting magnetogasdynamic flows, Applied Mathematical Modelling, Volume 107, July 2022, pp. 464-507