Numerical Characteristics of Non-equilibrium Air Chemistry in Hypersonic Flow

Seong-Lyong Kim [1], Honam Ok [2], Seung- Ho. Ra [3], Insun Kim [4],

1. saintl@kari.re.kr 2. honam@kari.re.kr 3. ra@kari.re.kr 4. iskim@kari.re.kr
(Rocket System Integration Dept., Korea Aerospace Research Institute, Taejon City 305-333 Republic of Korea)
Corresponding author ***Seong-Lyong Kim***

Abstract

Hypersonic flow calculations need the analysis of the non-equilibrium air chemistry. Many researches reveal the physical aspects of air chemistry, but the numerical characteristics are still unknown. This paper treats the numerical characteristics of air chemistry compared with the hydrogen oxygen combustion, especially the time step sizes of the time integration method, the eigenvalue characteristics of the chemical Jacobian. For the study, a constant volume reaction and a hypersonic flow are considered. The constant volume reaction considers only species and energy equation, so the effects of flow can be neglected. Simple and fast calculation of the constant volume reaction makes it possible to view the characteristics of chemical reactions.

In the constant volume reaction, two reaction cases, air chemistry and hydrogen–oxygen combustion, are considered under the condition of 4,000K temperature, 10 atmosphere. Linear stability analysis of the constant volume reaction shows that the implicit scheme time step size is 10^3 times larger than that of explicit scheme in both reactions, which carries confidence to the use of the implicit schemes.

Figure 1 and 2 show that the negative real eigenvalue of the chemical Jacobian of the hydrogen combustion is 10^2 times larger than that of air chemistry. Therefore the time step size of the hydrogen combustion is 10^{-2} times smaller because the inverse of the negative eigenvalue is the characteristic time scale of the reaction. The difference of time step sizes agrees with the fact that the air chemistry is a slow reaction compared with the hydrogen oxygen.

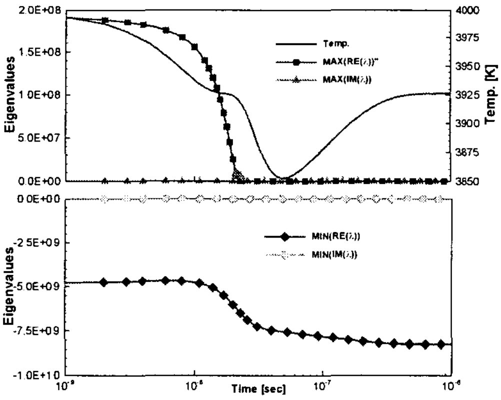

Fig. 1 Eigenvalue of Hydrogen-Oxygen Combustion

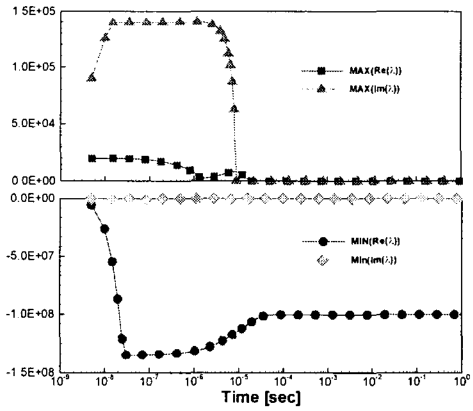

Fig. 2 Eigenvalue of Air chemistry

In the initial state of both reactions, the positive eigenvalue that is known to be a source of numerical instabilities appears, but the absolute value is different. The positive eigenvalue of the air chemistry is 10^{-5} times smaller than the negative eigenvalue, while the ratio of the hydrogen combustion is 10^{-1}. This implies that the stiffness of air chemistry calculation would be less sensitive than that of hydrogen combustion, and that the instability shown in hydrogen combustion rarely would appear in air chemistry.

This study applied the partially implicit time integration method to the constant volume reaction and hypersonic flow for stable and efficient calculations. The chemical Jacobian of the partially implicit scheme composes of lower triangular components of the full chemical Jacobian, which make it possible to save the computing time. Furthermore all the eigenvalue of the Jacobian are negative real, and thus the partially implicit scheme could reduce the stiffness due to positive eigenvalue. However its efficiency depends on the species ordering. In application of the partially implicit scheme, it shows the same results as the fully implicit one, the dependency of species ordering does not appear.

In hypersonic flow test, the LU-SGS scheme for the time integration, and AUSM-PW+ for the flux splitting, are adopted. Test case is an axisymmetric blunt body under the flow of Mach number of 16.34, wall temperature of 294.4K, free stream temperature 500K. CFL number is 0.4, and 17 reaction steps with 2 temperature model is used for the chemical reaction. The results show that the two schemes converge with the same rate, and the flow fields of the two scheme are the same as shown in Fig. 3.

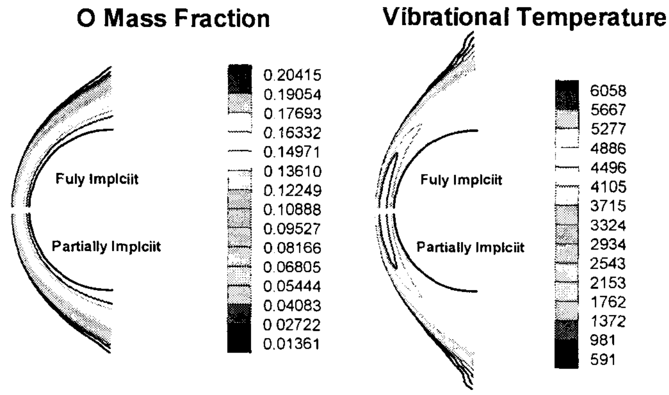

Fig. 3. Comparison of partially and fully implicit schemes

The computing time of the partially implicit scheme is 10% lower than that of the fully implicit scheme. The species ordering dependency also did not appear.

Keyword: *Hypersonic Flow, Partially Implicit Method, Non-equilibrium Air Chemistry*