Stability Analysis of a Fully Coupled Implicit Scheme for Inviscid Chemical Non-Equilibrium Flows

Yu Wang, Jinsheng Cai and Kun Qu*

National Key Laboratory of Science and Technology on Aerodynamic Design and Research, Northwestern Polytechnical University, Xi'an 710072, China

Received 21 April 2015; Accepted (in revised version) 13 October 2015

Abstract. Von Neumann stability theory is applied to analyze the stability of a fully coupled implicit (FCI) scheme based on the lower-upper symmetric Gauss-Seidel (LU-SGS) method for inviscid chemical non-equilibrium flows. The FCI scheme shows excellent stability except the case of the flows involving strong recombination reactions, and can weaken or even eliminate the instability resulting from the stiffness problem, which occurs in the subsonic high-temperature region of the hypersonic flow field. In addition, when the full Jacobian of chemical source term is diagonalized, the stability of the FCI scheme relies heavily on the flow conditions. Especially in the case of high temperature and subsonic state, the *CFL* number satisfying the stability is very small. Moreover, we also consider the effect of the space step, and demonstrate that the stability of the FCI scheme with the diagonalized Jacobian can be improved by reducing the space step. Therefore, we propose an improved method on the grid distribution according to the flow conditions. Numerical tests validate sufficiently the foregoing analyses. Based on the improved grid, the *CFL* number can be quickly ramped up to large values for convergence acceleration.

AMS subject classifications: 65M12, 65F10, 76K05

Key words: Stability, LU-SGS, non-equilibrium flows, Euler equations, flux Jacobian, grid refinement.

1 Introduction

The numerical computation of hypersonic flow fields has received increasing attention with the development of hypersonic vehicles. High-temperature effects [1] and multiple time scales make it difficult to compute hypersonic flow fields, especially nonequilibrium flows.

http://www.global-sci.org/aamm

©2016 Global Science Press

^{*}Corresponding author.

Email: wangyu@mail.nwpu.edu.cn (Y. Wang), kunqu@nwpu.edu.cn (K. Qu), caijsh@nwpu.edu.cn (J. S. Cai)

One of the difficulties encountered in solving non-equilibrium flows is the "stiffness problem" [2]. That is, the chemical source term in the species equations is sometimes excessively large compared to the convective terms. Non-equilibrium effect results in a large difference between the time scales of the chemical reaction and the fluid dynamics, making it very difficult to determine an appropriate time step or *CFL* number. Inappropriate treatment of the stiffness problem results in a non-physical solution or divergent numerical solutions.

There are currently two approaches to dealing with the stiffness problem. In the first approach, the gas dynamic equations (i.e., the Navier-Stokes (NS) or Euler equations) and the species equations are solved separately and iteratively. This approach is called the "loosely coupled method" [3–5]. In the second approach, which is called the "coupled implicit method" [6–9, 25], the two sets of equations are solved simultaneously in a coupled implicit form. The loosely coupled method can be easily implemented but is numerically less stable than the coupled implicit method and is not well-suited for solving real-time problems. The coupled implicit method offers faster convergence and provides a better description of non-equilibrium effects. However, the coupled implicit method results in a complex, large block matrix system. The solution of such a large linear system requires large amounts of computer memory, especially when there is a large number of chemical species.

As a result of continuous improvements in computer performance and computing techniques, many of the difficulties of the coupled implicit method have been gradually overcome. Bussing [6] used the coupled point implicit method to solve the Euler equations for chemical non-equilibrium problems. Eberhardt [7] and Candler [8] separately used a fully coupled implicit (FCI) method, which is based on the LU-SGS and GSLR schemes, to solve the NS equations for thermochemical non-equilibrium problems. Spiegel [9, 10] also employed FCI method to solve the NS equations for chemical non-equilibrium problems using an unstructured hybrid grid.

However, alomost all of the numerical computations of non-equilibrium flows based on the coupled implicit method are limited by the time step or *CFL* number. To prevent a non-physical solution or divergent numerical solutions, a very small *CFL* number has been adopted in many studies [6–8], resulting in very slow convergence rate and long computing time. Moreover, setting the *CFL* number is an empirical and experimental exercise. From a mathematical perspective, for non-homogeneous nonlinear differential equation sets, if some of the source terms are positive or the Jacobian matrix of the source terms has positive eigenvalues, the equation sets have "growing" solutions [11], and numerical methods are unstable [12,13]. For general chemical kinetics, strong chemical reactions in non-equilibrium flows lead to dominant non-linear effects. In fact, even the fully coupled method faces robustness difficulties because of these effects [14]. Thus, the stability and convergence of the coupled implicit scheme must be specifically investigated to determine the effect of the chemical source term on numerical computations, and to determine a reasonable time step. At present, there is very little related theoretical research on the stability and convergence of the coupled implicit scheme. Venkateswaran [14] has