16. **Darabiha N.** Transient behaviour of laminar counterflow hydrogen — air diffusion flames with complex chemistry. To appear in Combust. Sci. and Technol., 1991.
17. **Stahl G., Warnatz J.** Numerical investigation of time-dependent properties and extinction of strained methane — and propane — air flamelets // Combust. Flames.— 1991.— 85.— P. 285—299.
18. **Rolon J. C.** PhD thesis. Theoretical and experimental study of a counterflow diffusion flame. Ecole Centrale Paris, 1988.
19. **Djavdan E.** PhD thesis. Theoretical and experimental study of strained laminar premixed propane — air flames. Ecole Centrale Paris, 1990.
20. **Kee R. J., Miller J. A., Evans G. H. et al.** A computational model of the structure and extinction of strained, opposed flow, premixed methane — air flames // 22nd Symp. (Int.) on Combust., The Combust. Inst., 1988.— P. 1479—1494.
21. **Smooke M. D., Crump J., Seshadri K. et al.** Comparison between experimental measurements and numerical calculations of the structure of counterflow, diluted, methane — air premixed flames. Yale Univ. Report. ME—100—90.— 1990.
22. **Kee R. J., Miller J. A., Jefferson T. H.** CHEMKIN: A general-purpose, transportable, Fortran chemical kinetics code package. Sandia National Lab. Report, SAND80-8003.— 1980.
23. **Kee R. J., Warnatz J., Miller J. A.** A Fortran computer code package for the evaluation of gas-phase viscosities, conductivities, and diffusion coefficients. Sandia National Lab. Report, SAND83-8209.— 1983.
24. **Warming R. F., Beam R. M.** An extension of A-stability to alternating direction implicit methods. BIT — 1979.— 19.— P. 395—417.
25. **Darabiha N., Giovangigli V.** Vectorized computation of complex chemistry flames // Proc. of Int. Symp. on High Performance Computing/L. Delhaye and E. Gelenbe (Eds.).— Elsevier Sci. Publ. B. V. (North Holland), 1989.

УДК 621.452.226

R. F. Walter

RECENT ADVANCES IN COMPUTATIONAL ANALYSIS OF HYPERSONIC VEHICLES

W. J. Schafer Associates, Inc.
Albuquerque, New Mexico
USA

Abstract

The nonequilibrium gasdynamics processes of importance to hypersonic aerobraking vehicles are reviewed. Recent improvements in understanding these phenomena and in the detailed numerical modeling of these processes will be discussed. The paper concludes by describing the extent to which these models have been incorporated into multidimensional computational fluid dynamics (CFD) computer codes.

Physical Gasdynamics
Processes in the aerobraking environment

The chemistry and radiation processes which determine the heat transfer and aerodynamic force characteristics of aerobraking vehicles have been described in a series of excellent review papers [1—4]. Recently these considerations were extended to include the specific flight environments of manned missions to Mars, which employ aerobraking in both the Earth and the Martian atmospheres. Briefly, the one novel aspect of the AOTV flight environment when compared to those encountered by previous reentry systems such as Apollo; Soyuz, or the Space Shuttle Orbiter is the importance of nonequilibrium radiation in determining the heat transfer. This arises from the fact that the aerobraking vehicles will accomplish the required deceleration over a relatively long period of time (hundreds of seconds at high altitudes (70—100 km), whereas the Apollo spacecraft experienced peak heating and deceleration over a much shorter time (15 sec) at lower altitudes. This resulted in a situation whereby convective heat transfer dominated the thermal loads for Apollo. In contrast, the large phy-

sical size of proposed aerobraking vehicles produces a thicker shock layer and, therefore, greater radiative heat transfer rates to the body. At the same time, the large size and lower air density results in lower convective heat transfer to the aerobraking vehicles.

The effect of the new high altitude, long-duration flight regime on the dominant heat transfer mechainsms is of vital concern in the planning and design of aerobraking spacecraft. Since very little data from previous reentry vehicle programs is applicable to this new regime, a new design data base and design tools must be developed. This involves a joint theoretical/experimental endeavor. The theoretical aspect has two complementary parts: 1) development of three-dimensional flow solvers which accurately calculate the fluid dynamics and 2) development of realistic models of physical gasdynamic processes in the flow which strongly affect the heat transfer and pressure distributions. The physical gasdynamic processes include chemical reactions, vibrational excitation and dissociation, ionization, electronic excitation, and radiation. A much improved level of understanding of these phenomena has resulted from recent aerothermodynamics research programs. This paper reviews several areas of this work; later, we shall discuss the extent to which these results and new models have been folded into state-of-the-art computer codes.

Park and his collaborators have made especially significant contributions in the development of new physical models of non-equilibrium radiation. Their effort began with an attempt to understand why nonequilibrium radiation did not make a more noticeable contribution to the heat transfer coefficient observed on the Apollo spacecraft. This led to the formulation of theories for the collision-limiting and truncation mechanisms which together reduced the radiative heat transfer in the Apollo flight environment [2]. In the AOTV environment, however, the nonequilibrium radiative heat flux is expected to be between 10 and 100 w/cm^2, which is comparable to the convective heat transfer to such a vehicle. The magnitude of this heat load cannot be predicted by conventional equilibrium air codes, because the basic characteristics of the radiation are governed by the lack of thermal and chemical equilibrium among the excited gas species.

Since radiation heat transfer is expected to be very important for aerobraking vehicles, it is necessary to understand the essential elements for accurate calculations of these processes. There are two primary sources of radiation: atomic species and molecular species. The accurate calculation of their respective contributions requires a fairly precise knowledge of both the radiating species number densities and the radiative lifetimes of the excited states. There are two basic approaches to the latter problem: experimental measurements and computational chemistry, in which the required properties are calculated by solving Schrodinger's equation for the exsited state potential curves. This exciting new technique, which really became a practical alternative only with the advent of the Cray-2 supercomputer, has been used to determine a number of constants of importance to the aerobraking environment.

The other aspect of this problem — that of computing excited state number densities — usually involves the solution of a set of equations which describe the collisional and radiative transitions that add to and subtract from the energy levels of interest in each species. The most comprehensive approach to this problem involves the solution of the Master Equation of chemical physics. However, in practice this approach is too unwieldy, and simplified analytical approaches are desired. Such approaches were developed by Schwartz, Slawsky, and Herzfeld (SSH theory) in the 1950's and by Landau and Teller in the 1930's. Their well-known models are simple to use, but unfortunately they have been shown to be inaccurate at the high temperatures associated with the aerobraking flight environment. Lee conducted a systematic revision of this work in 1984—85 and produced some simple but significantly improved modifications to the

Landau — Teller theory [6—7]. Park has made further refinements to these models, and he has introduced the two-temperature model of vibrational and electronic excitation, which has been incorporated into his NEQAIR and STRAP/SPRAP codes [2]. NEQAIR is used to calculate the radiation heat transfer properties for a prescribed set of gas species at a given temperature, while STRAP and SPRAP perform a 1D integration along a streamline to calculate this radiation in a shock tube experiment or at a stagnation point.

An important question in the formulation of these models is the nature of the coupling between vibrational excitation and dissociation. The degree of dissociation has a strong effect on both the heat transfer to a vehicle and its aerodynamic force coefficients, and the amount of radiation from the gas is quite sensitive to its vibrational state. For these reasons, the chemistry model used in a computational aerothermodynamics code must accurately describe the effect of the vibrational state on the dissociation rate. In this research area, some exciting new results have recently been obtained; these promise to clarify some mysteries which have lingered since the 1950's. A number of models of this coupling process were developed in the 1959—63 time frame by workers at the AVCO and Calspan laboratories in the United States. However, none of these theories were able to predict the observed result that vibrational nonequilibrium significantly inhibits the dissociation rate. Park's two-temperature model is an attempt to predict the slower dissociation rates from a semi-empirical basis. The average temperature used in this model involves the product of the vibrational and translational temperatures, the first raised to an arbitrary power (less than one) and the second raised to one minus that power.

Recently attempts have been made to provide a sound theoretical basis for Park's semi-empirical model by solving a set of Master Equations numerically using transition rates calculated from SSH theory and also by using an approach based on Direct Simulation Monte-Carlo techniques. Using the former approach, Sharma, et al. predicted the existence of a bottleneck in the exchange rates among nitrogen molecules which results in a bimodal distribution of vibrational energy among the levels [8]. However, Olynick, et al. found no such behavior when they performed a DSMC analysis of the same problem [9]. More recently, Landrum and Candler repeated the analysis of Sharma, et al., using a nearly identical methodology, but allowing for vibrational-translational relaxation due to collisions with atoms and also for a variable inverse range parameter [10]. The latter quantity has an especially strong effect on vibrational exchange rates. The goal of this work is to develop a physically based model of the dissociation process which is simple enough to use for engineering purposes in CFD codes with thermochemical nonequilibrium.

An important capability which complements available experimental results is afforded by the impact of Cray 2-class supercomputers on computational chemistry, and the maturing of this discipline as a predictive tool for complex molecular configurations. This discipline involves the solution of Schrodinger's equation to calculate the chemical and radiative properties of atoms and molecules. Cooper, et al. have described the application of this discipline to species and problems of interest for aerobraking vehicles [1, 5]. Briefly, these applications include the calculation of radiative intensity factors, high-temperature gas transport properties, and rate constants for atomic and molecular excitation, ionization, and chemical reactions. This approach is especially valuable at high temperatures which cannot be achieved in laboratory test facilities and for radical and ionic species which are difficult to produce in quantities sufficient for measurements under these conditions. One payoff of this effort has been the computation of new energy partition functions for high temperature air; these have been incorporated in the NONEQ code of Whiting and Park [4]. A number of computational chemistry analyses driven by the

requirements of aerobraking mission applications are currently in progress or planned for the future. These include calculations of the rate constant for the exchange reaction $N + O_2 \rightarrow NO + O$, analyses of vibrational excitation and dissociation in N_2, and determination of improved values for rate constants for dissociation reactions involving CO and CO_2.

The latter are of special importance for aerobraking in the Martian atmosphere. In a recent review of chemical kinetic problems for future NASA missions, Park concluded that the present experimental data base for thermochemical rate parameters is inadequate for accurate modeling [4]. This situation offers additional opportunities for computational chemistry to provide needed rate data. In addition to the processes listed above, these reactions include dissociation of C_2 and N_2, three-body neutral exchange processes involving CN, the associative ionization process $C + O \rightarrow \rightarrow CO^+ + e^-$, the charge exchange reaction $CO^+ + C \rightarrow CO + C^+$, and all reactions involving NCO. Until these issues are resolved, there is an uncertainty associated with all Martian aerobraking calculations, which is difficult to quantify.

Navier — Stokes Equation Solvers

Several computer codes have been developed in the U. S. to solve the Navier — Stokes equations coupled with the equations of nonequilibrium gasdynamics. These include the LAURA and NEQ2D programs. First developed in 1984—85 by Gnoffo, the LAURA code appears to be the most mature of the Navier — Stokes solvers which incorporate the fluid physics important for aerobraking applications [11]. LAURA is an upwind-biased, point-implicit relaxation algorithm. It employs a finite-volume formulation to solve the Navier — Stokes equations in three dimensions for viscous hypersonic flows in thermal and chemical nonequilibrium. The point-implicit strategy involves the implicit treatment of variables at each cell center for the advanced iteration level. The latest available data from neighbor cells are used in the evaluation of the left-hand side of the equations. Hence, only a single level of storage is required. The inviscid components of flux across the cell boundaries are evaluated with Roe's averaging and Harten's entropy fix together with limiters derived from Yee's symmetric total variation diminishing (TVD) scheme. The point-implicit relaxation strategy enables the LAURA code to remain stable at large Courant numbers without the need to solve large block tridiagonal systems, while the special treatment of the flux vector components enhances the robustness of the solution in the presence of shock waves.

One of the principal modifications to the LAURA code from its original equilibrium air version was the addition of a model of nonequilibrium gasdynamics phenomena. The code currently includes continuity equations for 11 species: N_2, O_2, NO, N, O, N^+, O^+, N_2^+, O_2^+, NO^+, and e^-. A number of kinetics models for thermal, vibrational, and electronic nonequilibrium have been implemented in LAURA, including Park's 1987 two-temperature model, Park's 1991 update of this model, and the 1973 Dunn — Kang model of collisional plasma processes. The code also allows for variable wall catalycity. The basic LAURA code consists of approximately 15,000 lines of FORTRAN. When the LORAN radiation model is coupled to LAURA, the length increases to 22,000 lines. New thermodynamic and transport properties derived by Gupta and Yos were recently added to LAURA. These are considered good up to 30,000 K. In principle, LAURA can solve the Navier — Stokes equations for the flow field about any 3D blunt body. However, in practice some limitations associated with computer architecture add complications. For example, the largest allowed memory queue for the Cray YMP is 8 million words. Since a 3D Navier — Stokes solution could require at least 20 million words of storage, some jobs cannot be run without new approaches to memory management. Gnoffo is presently investigating a macro-tasking version of LAURA, in which one processor does the radiation calculations while another solves the fluid dynamics.

The coupled solution would be reached via asynchronous relaxation, which could also allow for networking.

The LAURA code has been used in an extensive series of validation studies which encompass a wide body of ground and flight test data [11]. The ground test data include wind tunnel tests of an aerobraking configuration, ballistic range data for a sphere at $M = 15.3$, and shock tunnel data for a cylinder in partially dissociated nitrogen at 5.59 km/sec. The flight data included both the FIRE II and RAM-C III experiments. Although the code results were generally in good agreement with test data, the one quantity with which LAURA experienced some difficulty was the electron density profile measured on RAM-C III. The Dunn — Kang chemical kinetic model appeared to give better qualitative agreement with the experiment than did the Park two-temperature model. However, both versions are considered to be in poor quantitative agreement with experiment. In fact, single-temperature shock-fitted viscous shock layer calculations are in better agreement for the electron density profile on RAM-C III. This suggests that the thermochemical nonequilibrium models require modification.

Candler's NEQ2D code was developed originally with MacCormack at Stanford University, and subsequently modified in collaboration with Park [12]. This code was developed to solve the Navier — Stokes equations in two dimensions using a physical model which contains most of the reacting chemical species important in the aerobraking regime. (The code includes constitutive relations for N_2, O_2, N, O, NO, NO^+, and e^-; fifteen differential equations are solved simultaneously.) Candler's method allowed for full coupling between the chemistry and fluid dynamics. The radiative power emitted by the gas between 0.2 and 1.5 μm is computed by coupling the converged results with Park's NEQAIR algorithm. This approach assumes that the amount of radiative emission is small compared to the total energy content of the gas, so that the radiative heat loss is not coupled to the flowfield calculation (the tangent-slab approximation). The fully coupled chemistry-fluid dynamics equation set is solved using the implicit Gauss — Seidel line relaxation technique proposed by MacCormack. This reduces the size of the full block matrix which must be stored and solved with the implicit method. The flux vectors are treated in an implicit manner and differenced using flux splitting; the chemical and thermal source vector is also treated implicitly. This implicit treatment allows the use of large time steps. The effects of adding the stiff chemical reaction equations were illustrated by an increase in convergence time of the Gauss — Seidel algorithm. For a perfect gas, convergence was achieved in 100 iterations. For a simplified chemistry model with five species this increased to 500—700 iterations, and 100 additional iterations were required with the seven-species model.

Validation of the NEQ2D code has consisted of comparisons with RAM-C II flight data and with DSMC calculations of AFE heat transfer characteristics. RAM-C II was selected as the most appropriate flight test example because of the absence of ablation products. Calculations were performed for several flight conditions with a 1050-point grid. The success of this code in predicting the measured electron density distribution is open to some question. Although Candler has stated in two publications that the agreement with experiment is «good», examination of the curves reveals that they exhibit greatly differing slope behaviors. Gnoffo attributes this to the use of a noncatalytic wall boundary condition for electron-ion recombination. This causes the computed peak in the electron density distribution to occur near the wall, whereas the experimental data indicate that this peak is near the shock. Candler concludes that these results suggest inadequacies in the models of translation-vibration and electron-vibration exchange processes. His modeling of an aerobraking configuration also raised questions about the nature of the boundary condition for wall catalycity. The NEQ2D code predicted a stagnation point convective heating

value which was 40 % lower than the value calculated by Moss, et al. with the G2 DSMC code. This discrepancy points to the need for a good understanding of the nature of this process for materials of interest for the thermal protection system. As we have noted, the NEQ2D code has not been extended to three dimensions, so it is probably unwise to compare its predictions directly to a 3D Navier — Stokes solver such as LAURA.

REFERENCES

1. **Peterson V. L. et al.** Supercomputer requirements for selected disciplines important to aerospace // Proc. IEEE.— 1989.— 77.— P. 1038.
2. **Park Chul.** Radiation Enhancement by nonequilibrium in earth's atmosphere // J. Spacecraft.— 1985.— 22, 27.
3. **Park Chul.** A review of reaction rates in high temperature air // AIAA-89-1740, 1989.
4. **Park Chul et al.** Chemical-kinetic problems of future NASA missions // AIAA-91-0464, 1991.
5. **Cooper D. M. et al.** Computational chemistry and aeroassisted orbital transfer vehicles // J. Spacecraft.— 1985.— 22.— P. 60.
6. **Lee Jong-Hun.** Basic governing equations for the flight regimes of aeroassisted orbital transfer vehicles // AIAA-84-1929, 1984.
7. **Lee Jong-Hun.** Electron-impact vibrational excitation rates in the flow field of aeroassisted orbital transfer vehicles // AIAA-85-1035, 1985.
8. **Sharma Surendra P., Huo Winifred M., Park Chul.** The rate parameters for coupled vibration-dissociation in a generalized SSH approximation // AIAA-88-2714, 1988.
9. **Olynick D., Moss J., Hassan H.** Monte Carlo simulation of vibrational relaxation in nitrogen // AIAA-90-1767, 1990.
10. **Landrum D., Candler G.** Vibration-dissociation coupling in nonequilibrium flows // AIAA-91-0466, 1991.
11. **Gnoffo P. A.** Code calibration program in support of the aeroassist. flight experiment // J. Spacecraft.— 1990.— 27.— P. 131.
12. **Candler G. V., MacCormack R. W.** Computation of weakly ionized hypersonic flows in thermochemical nonequilibrium // J. Thermophysics and Heat Transfer.— 1991.— 5.— P. 266.

УДК 452.225

П. К. Третьяков

ОПРЕДЕЛЕНИЕ ТЕПЛОПОДВОДА К ПОТОКУ В КАНАЛЕ С ПСЕВДОСКАЧКОМ

Подвод тепла за счет горения топлива в канале со сверхзвуковой скоростью потока приводит к его торможению. Возникающая газодинамическая структура характерна для псевдоскачка и существенно неоднородна по сечению канала. Наличие горения и малая длительность эксперимента не позволяют получить подробную информацию о параметрах течения. Наиболее доступные данные в этой ситуации — измерения статического давления на стенке канала, которые используются для определения полноты сгорания или количества тепла, подведенного к потоку.

Применение одномерной методики в ряде случаев может привести к получению нефизического результата, когда полнота сгорания превышает единицу. Предложенный метод основан на закономерностях изменения коэффициента неоднородности, который вводится из условия одномерного представления уравнений сохранения (импульса и неразрывности). Используется разница давлений для изотермического течения и с теплоподводом, трение и теплоотвод в стенку учитываются. Приведены примеры применения к известным в литературе экспериментам с горением водорода и керосина.

Торможение сверхзвукового потока с переходом к дозвуковому течению сопровождается возникновением сложной волновой структуры, получившей название псевдоскачка. Такая ситуация характерна для многих газодинамических устройств. Одно из первых исследований в этом направлении — работа [1]. Отметим, что при горении в канале со сверхзвуковой скоростью потока также возможна реализация структуры псевдоскачка.

Нетрудно показать, что при возникновении псевдоскачка в канале постоянного сечения для адиабатического случая одномерные уравнения сохранения выполняются только для сечений в начале и в конце псевдоскачка (см., например, [2]). В промежуточных сечениях, если в каче-