

Technical Comments

Comments on "Elliptic Elements in Terms of Small Increments of Position and Velocity Components" and Generalization of the Solutions for an Arbitrary Initial Point

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THE valuable solutions of de Vries¹ to the "rendezvous" equations for a reference elliptic orbit of small eccentricity unfortunately contain a few algebraic errors. The following terms should be changed to read

$$e_0 (\frac{3}{2}B - 2B \cos v_0 - 6C v_0 \cos v_0)$$

instead of

$$e_0 (+2B \cos v_0 - 6 v_0 \sin v_0)$$

in the y equation, and

$$e_0 (-\frac{1}{3}E \cos v_0 - \frac{1}{6}E \cos 2v_0)$$

instead of

$$e_0 (-\frac{1}{6}E \cos v_0 - \frac{1}{3}E \cos 2v_0)$$

in the z equation.

deVries' solutions are restricted to an initial point located at perifocus of the reference elliptic orbit. The following solutions for x , y , and z are generalized to an arbitrary initial point. The symbols e and v correspond to e_0 and v_0 in Ref. 1 and $v(0)$ is the true anomaly of the initial point ($t = 0$) on the reference elliptic orbit.

Solutions to the small eccentricity, elliptic "rendezvous" equations of relative motion for an arbitrary initial point follow:

$$x = 2C + A \cos v + B \sin v + e \left\{ -\frac{3}{2}A + \frac{1}{2}A \cos 2v + \frac{1}{2}B \sin 2v - 3C v \sin v + \frac{1}{2}A [1 + \cos 2v(0)] \cos[v - v(0)] + 2A \sin v(0) \sin v - B \cos v(0) \sin v + \frac{1}{2}B [1 - \cos 2v(0)] \sin[v - v(0)] - \frac{3}{2}C \cos v + \frac{3}{2}C \cos[v - 2v(0)] 3C v(0) \sin v \right\}$$

$$y = D - 3C v - 2A \sin v + 2B \cos v + e \left\{ 3A [v - v(0)] - \frac{1}{2}A \sin 2v + \frac{1}{2}B \cos 2v + 9C \sin v - 6C v \cos v - A [1 + \cos 2v(0)] \sin[v - v(0)] + 4A \sin v(0) \cos v - 2B \cos v(0) \cos v + B [1 - \cos 2v(0)] \cos[v - v(0)] - 3C \sin[v - 2v(0)] + 6C v(0) \cos v - \frac{3}{2}A \sin 2v(0) + \frac{3}{2}B \cos 2v(0) - 12C \sin v(0) \right\}$$

$$z = E \cos v + F \sin v + e \left\{ \frac{E}{2} - \frac{E}{6} \cos 2v - \frac{F}{6} \sin 2v - \frac{E}{3} \cos 2v(0) \cos[v - v(0)] - \frac{2}{3}E \sin v(0) \sin v + \frac{F}{3} \cos v(0) \times \sin v - \frac{F}{6} [1 - \cos 2v(0)] \sin[v - v(0)] \right\}$$

where

$$A = -[3x(0) + 2y'(0)] \cos v(0) - x'(0) \sin v(0)$$

$$B = -[3x(0) + 2y'(0)] \sin v(0) + x'(0) \cos v(0)$$

$$C = 2x(0) + y'(0)$$

$$D = y(0) - 2x'(0) + 3v(0) [2x(0) + y'(0)]$$

$$E = z(0) \cos v(0) - z'(0) \sin v(0)$$

$$F = z(0) \sin v(0) + z'(0) \cos v(0)$$

Reference

¹ deVries, J. Pieter, "Elliptic elements in terms of small increments of position and velocity components," AIAA J. 1, 2626-2629 (1963).

A Computation of One-Dimensional Combustion of Methane

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SEVERAL problems involving the analysis of chemical kinetics have been considered recently. Particularly interesting are the problems in combustion. Several models have been examined by different authors,¹⁻³ and it is easy to foresee that more and more complex and sophisticated chemical phenomena will attract the researcher's interest in the future.

In gasdynamics, one assumes some basic information from chemistry, viz., the number of chemical species to be considered, the number and nature of the reactions, and the numerical values of forward and backward reaction rates. The problem is that of determining the chemical composition (i.e., the mass fraction of each specie) as a function of time, by integrating the differential equations that express the rate of production of each specie.

As pointed out in Ref. 4, the integration techniques for nonlinear, ordinary differential equations, based on Runge-Kutta or similar methods, are, in this case, handicapped by a stability criterion. The more complex the chemical phenomenon, the longer becomes the time needed on a computing machine to perform the numerical analysis.

The technique presented by Moretti seemed to circumvent that difficulty and provide an increase in the allowable step-size of several orders of magnitude.

Such a technique was based upon a manipulation of the nonlinear differential equations which reduces them to the linear form

$$y_i' = dy_i/dt = \sum a_{ij} y_j + b_i \quad (1)$$

where y_i is the concentration in moles per cubic centimeter of the i th species, t is time, and a_{ij} and b_i are constant during a time interval from t_n to t_{n+1} . The numerical solution of these equations requires the evaluation of the complex eigenvalues and eigenvectors of an n th order real matrix.

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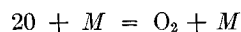
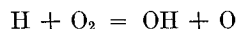
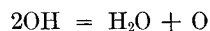
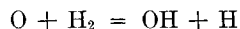
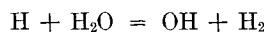
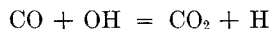
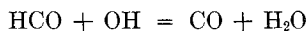
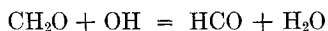
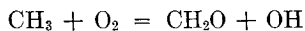
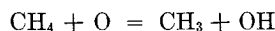
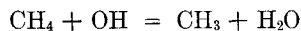
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The research outlined on this paper has a twofold purpose: 1) applying the technique of Ref. 4 to more complicated chemical problems, and 2) improving the numerical analysis of such a technique to make it practical in those problems. The combustion of methane in air has been analyzed.

The chemical model used is that of Ref. 2. The species considered are H, O, CO, CO₂, H₂, O₂, H₂O, OH, CHO, CH₂O, CH₃, CH₄, and N₂, the latter being considered an inert diluent. These species are identified with the subscripts 1, 2, 3, ..., 13, respectively. The following reactions are considered to occur:



where M is a catalyst. Each reaction has associated with it a forward and backward reaction rate denoted by f_j and b_j , respectively, for the j th reaction.

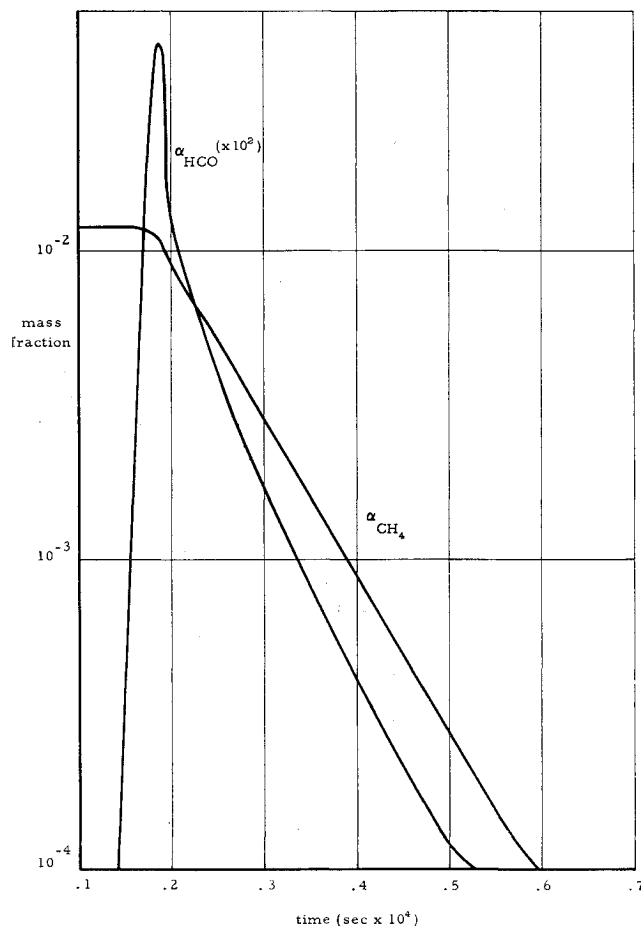


Fig. 1 Mass fractions vs time.

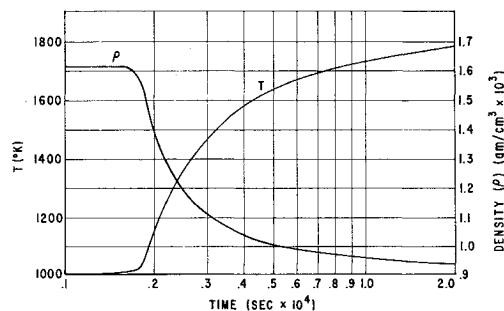


Fig. 2 Temperature and density vs time.

Governing Equations

The equations governing the system under consideration are:

Equation of State

$$P = \frac{P}{RT \sum (\alpha_i / w_i)} \quad (2)$$

Enthalpy Equation

$$h = \sum \alpha_i h_i \quad (3)$$

Time Rate of Change of Concentration Species i

$$y_i' = \dot{y}_i + (\rho' / \rho) y_i \quad (4)$$

where a prime means substantial differentiation with respect to time, and

$$\dot{y}_i = \frac{\rho}{w_i} \frac{d\alpha_i}{dt} = \sum_{j=1}^{13} [f_j \pi y_i^{\nu_{e'}} - b_j \pi y_i^{\nu_{e''}}] \quad (5)$$

In the foregoing equation, P is pressure, ρ density, T temperature, α mass fraction, W molecular weight, h static enthalpy (sensible + chemical), y concentration, t time, and $\nu_{e'}$ and $\nu_{e''}$ are stoichiometric coefficients for the reactants and the reaction products, respectively. The subscript i refers to the i th species, the subscript j to the j th chemical equation. We have the identity

$$\sum_{i=1}^{13} \alpha_i = 1 \quad (6)$$

Physically, the \dot{y}_i term represents the time rate of change of y_i as a result of chemical reactions.

The remaining formulation of the equations is similar to that of Ref. 4. The only difference is that in the present problem three of the concentrations, y_{10} , y_{11} , and y_{13} , are expressed in terms of the remaining nine and of the parameter γ , the ratio of the densities at the end and at the beginning of each step. The main step in the computation consists of solving a system of nine linear, ordinary nonhomogeneous differential equations:

$$y_i' = \sum_{j=1}^9 a_{ij} y_j + b_i \quad (7)$$

The solution of the set of Eqs. (7) is

$$y_i = \sum_{j=1}^9 \lambda_{ij} e^{r_j t} + c_i$$

where the eigenvalues r_j are the roots of the characteristic equation obtained from

$$|a_{ij} - r_j \delta_{ij}| = 0$$

and λ_{ij} are the eigenfunctions corresponding to the eigenvalues r_j , δ_{ij} is the Kronecker delta, and the c_i are determined from the known conditions at $t = 0$. In general, the r_j may be complex which increases the difficulty of obtaining the

exact solution of the Eqs. (7) to the point where it renders that method impractical for a system of this size. A different method has been developed by the senior author, as follows.

An approximate solution to Eq. (7) was assumed to be a truncated power series of the form

$$y_i = \sum_{k=0}^2 d_{ik} t^k$$

Substituting this assumed form of the solution into Eq. (7), we find that the residue is

$$R_i(t) = \sum_{k=0}^2 d_{ik} k t^{k-1} - \sum_{k=0}^2 \sum_{j=1}^9 a_{ij} d_{jk} t^k - b_i$$

or

$$R_i(t) = \sum_{k=1}^2 \left\{ d_{jk} k t^{k-1} - \sum_{j=1}^9 a_{ij} d_{jk} t^k \right\} - \sum_{j=1}^9 a_{ij} d_{j0} - b_i$$

Requiring that

$$\int_0^{\Delta t/2} R_i(t) dt = 0$$

$$\int_{\Delta t/2}^{\Delta t} R_i(t) dt = 0$$

yields the two additional conditions required for the evaluation of the d_k for each equation:

$$\begin{aligned} & \sum_{k=1}^2 \sum_{j=1}^9 \left\{ d_{jk} k t^{k-1} - \frac{a_{ij} d_{jk} t^{k+1}}{k+1} \right\} \Big|_0^{\Delta t/2} - \\ & \sum_{j=1}^9 a_{ij} d_{j0} t \Big|_0^{\Delta t/2} - b_i t \Big|_0^{\Delta t/2} = 0 \\ & \sum_{k=1}^2 \sum_{j=1}^9 \left\{ d_{jk} k t^{k-1} - \frac{a_{ij} d_{jk} t^{k+1}}{k+1} \right\} \Big|_{\Delta t/2}^{\Delta t} - \\ & \sum_{j=1}^9 a_{ij} d_{j0} t \Big|_{\Delta t/2}^{\Delta t} - b_i t \Big|_{\Delta t/2}^{\Delta t} = 0 \\ & \sum_{k=1}^2 \sum_{j=1}^9 \left\{ d_{jk} \left(\frac{\Delta t}{2} \right)^k - \frac{a_{ij} d_{jk}}{k+1} \left(\frac{\Delta t}{2} \right)^{k+1} \right\} - \\ & \sum_{j=1}^9 a_{ij} d_{j0} \left(\frac{\Delta t}{2} \right) - b_i \frac{\Delta t}{2} = 0 \\ & \sum_{k=1}^2 \sum_{j=1}^9 \left\{ d_{jk} \Delta t^k \left(\frac{2^k - 1}{2^k} \right) - \frac{a_{ij} d_{jk}}{k+1} \Delta t^{k+1} \left(\frac{2^{k+1} - 1}{2^{k+1}} \right) \right\} - \\ & \sum_{j=1}^9 a_{ij} d_{j0} \frac{\Delta t}{2} - b_i \frac{\Delta t}{2} = 0 \end{aligned}$$

There results a set of eighteen linear algebraic equations for the eighteen unknown d_k . The algebraic equations are then solved by triangularizing the coefficient matrix. The d_k being known, an explicit solution is given for each species over the time interval considered.

Numerical Results

A check of this method was made by solving the equations for the H-O system, and very good agreement with Ref. 4 was obtained. Further, a check between this method and the classic Runge-Kutta method for the methane combustion also indicated very close agreement.

The most important feature of this method is that it is not limited by any stability criteria, as is the case for the Runge-Kutta. Both this method and the method of Ref. 4 are at least one to two orders of magnitude faster than the Runge-Kutta in the computational time, and in certain cases are even several orders of magnitude faster. Their intrinsic stability allows larger step sizes to be taken in applications of the one-dimensional chemical computational to two-dimensional fluid flow problem with finite-rate chemistry.

In conclusion, it has been shown that the technique of Ref. 4 is applicable to the methane-air system. Representative mass fraction distributions (Fig. 1) and temperature density variations vs time (Fig. 2) have compared very well with Ref. 2. In fact, in many cases, the results have agreed to four significant figures. A direct extension of the Moretti method for a methane-air combustion problem would have been prohibitive, if not impossible, because of the difficulty involved with extracting the complex eigenvalues and eigenvectors of the larger matrix. That approach would also have been time consuming computationally which is the main disadvantage of the Runge-Kutta method. The method of this paper, while maintaining the accuracy of the Runge-Kutta method, has reduced the computational time by roughly an order of magnitude.

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