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Modeling of acetylene detonation in a shock tube by the large particle method with TVD correction

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Abstract. A one-dimensional TVD correction scheme is described, which can be successfully applied not only in 1D calculations, but also in 2D - 3D modeling [1-2]. The advantage of the proposed scheme is the lack of solving matrix equations. The implementation of the scheme in conjunction with the large particle method was tested on the problems of arbitrary discontinuity breakup and strong point explosion. The modeling of acetylene combustion in a shock tube and its transition to detonation was performed depending on the conditions set on the surface of the tube, and the parameters of the problem.

1. Introduction

The scheme of the large particle method [3] consists of several stages corresponding to the scheme of splitting into processes. We use the TVD scheme as the most last stage of this method to correct the solution obtained after the execution of the previous stages. Hence the name of the method includes – «TVD correction». The large particle method modified in this way allows to increase the accuracy of the approximation to the second order, as well as to get rid of the need for the use of artificial viscosity.

Verification of the joint operation of the large particle scheme and the TVD correction was performed on the problem of decay of an arbitrary discontinuity and the problem of a strong point explosion. Although these test problems are one-dimensional in nature, they were simulated using a two-dimensional axisymmetric formulation, which allowed validating the applicability of one-dimensional TVD scheme in 2D modeling.

Numerical simulation in a shock tube was performed for stoichiometric mixture of enriched air and acetylene represented by four elements: air – $2.5\text{O}_2 + 5.2\text{N}_2$; acetylene – C_2H_2 ; nitrogen – N_2 ; combustion products – $\text{H}_2\text{O} + 2\text{CO}_2$. The proposed physical-chemical model uses tabular descriptions of the equilibrium thermodynamic state for each component of the gas mixture separately, but they do not have to be in a state of chemical equilibrium with respect to each other and can participate in mutual chemical conversion.

2. Mathematical model

The numerical method is based on the solution of a system of Euler equations written in the form of the mass, momentum, and energy conservation laws. The two-dimensional Euler equations can be represented as a system of conservation laws recorded in cylindrical coordinates (z, r) as follows:



$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial z} + \frac{\partial \mathbf{G}(\mathbf{U})}{\partial r} = \mathbf{S}(\mathbf{U}) \quad (1)$$

where \mathbf{U} is the column vector of the conserved quantities, \mathbf{F} and \mathbf{G} are the column vectors of flows along the coordinates z and r , respectively, and \mathbf{S} is the source vector. The number of components in the vectors is determined by the number of equations in system (1); this number, in turn, depends on the used physical model. When describing the processes of chemical conversion in combustible mixtures, the equations of conservation of the corresponding chemical components have to be added. Then the number of equations in (1) must be equal to $N + 4$, where N is the number of components of the mixture. The vector quantities from the system (1) can be written as:

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho Y \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \\ \rho uY \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \\ \rho vY \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ p \\ -r\nabla \mathbf{q} \\ r\rho W \end{bmatrix} \quad (2)$$

where ρ is the density of the substance; u and v are the components of the velocity vector, respectively, in z and r coordinates; E is the total specific energy; p is the pressure; $Y \equiv \{Y_1, \dots, Y_N\}$ – the mass fraction vector of the chemical components; $W(T, \rho, Y) \equiv \{W_1, \dots, W_N\}$ – the vector of the chemical reaction rate; \mathbf{q} – thermal conductivity flow. To close the system of equations (1)–(2), one should specify the equation of state or the system of equations by which the pressure in the form $p = p(T, \rho, Y)$ and its derivatives can be calculated:

$$\chi = \left(\frac{\partial p}{\partial \rho} \right)_{\rho, Y}, \quad k = \left(\frac{\partial p}{\partial \rho \varepsilon} \right)_{\rho, Y}, \quad \eta_i = \left(\frac{\partial p}{\partial Y_i} \right)_{\rho, \rho \varepsilon}, \quad \text{where } \varepsilon = E - \frac{u^2 + v^2}{2} \quad (3)$$

The pressure derivatives determined in (3) are needed for calculating the TVD dissipation, in particular, of the local speed of sound:

$$c^2 = \chi + k(\varepsilon + p / \rho) \quad (4)$$

The temperature used to calculate the partial pressure and the energy of the mixture components is determined based on the energy conservation equation for the mixture in a given calculation cell:

$$\varepsilon = \sum_i^N Y_i \varepsilon_i(T, Y_i \rho) \quad (5)$$

The numerical simulation used the functions $\varepsilon_i = \varepsilon_i(T, \rho)$ and $p_i = p_i(T, \rho)$ obtained in the form of tables, calculated with a given grid upon the parameters of temperature and density. A uniform temperature scale ranging from 200 K up to 6000 K with increments of 50 K and a density scale ranging from 10^{-8} up to $10^{2.5}$ kg/m³ with a uniform logarithmic step of 0.25 were used. For a realistic description of the thermodynamic properties of the substance, equilibrium tables calculated by NASA CEA for specific components of the burning mixture considered in the simulation were used.

The combustion rate of acetylene in the air, determined in accordance with the Arrhenius law:

$$W(T, \rho, Y_1, Y_2) = \bar{Y}_{O_2} B(T) \exp(-E_a / T) Y_1 Y_2 \rho \quad (6)$$

Were Y_1 – mass fraction of the enriched air; Y_2 – mass fraction of acetylene; \bar{Y}_{O_2} – fixed fraction of oxygen in the air (variable Y_1); $B(T) = 2.3 \cdot 10^{11} \text{ m}^3 \text{ mol/kg}^2 \text{ s}$; E_a – activation energy expressed in units of temperature is a fitting parameter.

3. TVD correction

Initially, the scheme of Total Variation Diminishing (TVD) was developed for the conservation equations for the one-dimensional plane case [4]. However, as shown in [5], it can be successfully

applied in both cylindrical and spherical geometry for one-dimensional gas dynamics problems. In the future, the TVD scheme has been widely used for the numerical solution of two-dimensional and three-dimensional gas dynamics problems [1-2]. Herewith, the same one-dimensional version of the scheme, applied alternately to different coordinate directions, was used. The possibility of using the TVD method in conjunction with the large particle method was described in [6] too.

Nonphysical oscillations are suppressed by adding the TVD correction after completion all of the large particle method stages. That is, after the values ρ_{ij}^{n+1} , u_{ij}^{n+1} , v_{ij}^{n+1} , E_{ij}^{n+1} , and Y_{ij}^{n+1} have been obtained on the $(n+1)$ -th time layer, they are supplemented with the correction that plays the part of numerical dissipation. Corrections to each of the mentioned quantities have the form of the divergence of correcting fluxes calculated on the basis of the TVD scheme. Note that in solving of two-dimensional equations of hydrodynamics use is made of one-dimensional TVD schemes applied alternately along the respective coordinate lines. Since all of the operations for calculating these fluxes are performed on gas-dynamical quantities determined for the moment t^{n+1} , the index showing their relation to the time layer can be omitted in their designation. The change of gas-dynamic quantities included in the column vector \mathbf{U}_{ij} from the definition (2) due to the considered dissipation can be presented in the following form:

$$\Delta \mathbf{U}_{ij} = \frac{\Delta t}{V_{ij}} \left[(\sigma \mathbf{f})_{i-1/2,j} - (\sigma \mathbf{f})_{i+1/2,j} + (\sigma \mathbf{f})_{i,j-1/2} - (\sigma \mathbf{f})_{i,j+1/2} \right] \quad (7)$$

Here $\mathbf{f}_{i+1/2,j}$ and $\mathbf{f}_{i,j+1/2}$ are the vector columns of correcting fluxes calculated from the formulas of the TVD scheme that yield a correction to the fluxes $\mathbf{F}_{i+1/2,j}$ and $\mathbf{G}_{i,j+1/2}$ of the components in the vector column \mathbf{U}_{ij} , respectively. Since the value of flux \mathbf{f} is determined by a one-dimensional TVD scheme for an arbitrary fixed coordinate direction on the computational grid, we need to consider in detail only one direction, for example, cells with variable index $i(z)$ at a fixed value of index $j(r)$. Then, the fluxes $\mathbf{f}_{i+1/2}$ (omit the index j) are commonly calculated by expanding the variations $\delta \mathbf{U}_{i+1/2} = \mathbf{U}_{i+1} - \mathbf{U}_i$ at the edge of the cells by eigenvectors of Jacobi matrix $(\partial \mathbf{F} / \partial \mathbf{U})_{i+1/2}$ and applying the scalar TVD scheme for each component of the series. The matrix $(\partial \mathbf{G} / \partial \mathbf{U})_{j+1/2}$ is used for another direction. This approach is a version of the solution of the linearized Riemann problem [7].

However, with respect to the gas dynamics conservation equations, this decomposition problem can be solved in a different way, without the use of Jacobi matrices treatment. The way proposed in this work consists in the application of known expressions for Riemann invariants:

$$\delta J_+ = \delta u + \frac{\delta p}{\rho c}, \quad \delta J_- = \delta u - \frac{\delta p}{\rho c}, \quad (8)$$

respectively, for the characteristics with the eigenvalues equal to $u \pm c$, where c is the local velocity of sound. Variations of the quantities from (8) are the total differentials only for the isentropic flow. In the case of an arbitrary flow, the entropy variation differs from zero $\delta s \neq 0$ and propagates along the characteristic with the eigenvalue equaled to u , i.e., it moves with the mass of the matter. Thus, any perturbation of gas-dynamic quantities can be decomposed to independent parts of the mentioned three types that propagate along the corresponding characteristics.

We determine the variations of the quantities necessary for the described decomposition:

$$\begin{aligned} \delta u_{i+1/2} &= u_{i+1} - u_i, & \delta v_{i+1/2} &= v_{i+1} - v_i, & \delta \rho_{i+1/2} &= \rho_{i+1} - \rho_i, & \delta \varepsilon_{i+1/2} &= \varepsilon_{i+1} - \varepsilon_i, \\ \delta e_{i+1/2}^k &= e_{i+1}^k - e_i^k, & \delta p_{i+1/2} &= p_{i+1} - p_i, & \delta s_{i+1/2} &= \delta \varepsilon_{i+1/2} - \frac{p_{i+1/2}}{\rho_{i+1/2}^2} \delta \rho_{i+1/2}. \end{aligned} \quad (9)$$

Next, we omit the spatial indices for the values defined at the cell boundaries. Then the decomposition vector α and the vector of its corresponding eigenvalues a will have the form:

$$\alpha \Delta z = \left[\frac{1}{c} \left(\delta u - \frac{\delta p}{\rho c} \right); \frac{1}{c} \left(\delta u + \frac{\delta p}{\rho c} \right); \frac{\delta v}{c}; \frac{\delta s}{c^2}; \delta Y \right] \quad (10)$$

$$a = [u - c; u + c; u; u; u] \quad (11)$$

For each characteristic solution $\alpha_{i+1/2}^l$, where $l=1,2,\dots,N+4$, corrective flows $\Phi_{i+1/2}^l$ are calculated using formulas for the scalar counter-flow TVD scheme [4]:

$$\Phi_{i+1/2}^l = \frac{\Delta z_{i+1/2}}{2} \left[\frac{1}{2} \psi(a_{i+1/2}^l)(g_{i+1}^l + g_i^l) - \psi(a_{i+1/2}^l + \gamma_{i+1/2}^l) \alpha_{i+1/2}^l \right] \quad (12)$$

where

$$\psi(x) = \begin{cases} |x|, & |x|/c \geq \delta \\ (x^2 + \delta^2)/2\delta, & |x|/c < \delta \end{cases} \quad (13)$$

$$\gamma_{i+1/2}^l = \frac{1}{2} \psi(a_{i+1/2}^l) \begin{cases} (g_{i+1}^l - g_i^l)/\alpha_{i+1/2}^l, & \alpha_{i+1/2}^l \neq 0 \\ 0, & \alpha_{i+1/2}^l = 0 \end{cases} \quad (14)$$

$$g_i^l = \min \text{mod}(\alpha_{i-1/2}^l, \alpha_{i+1/2}^l) \quad (15)$$

The $\min \text{mod}(x,y)$ function is the smallest argument in absolute value if all arguments have the same sign, or zero if the arguments have different signs.

Then, substituting the vector Φ into the expression (10) instead of the vector α , we can find the changes of flows for the values included in (10) in the form of variations. It should be borne in mind that Φ has the dimension of speed. Therefore, to avoid confusion, replace the symbol δ with the symbol Δ , and obtain a system of equations:

$$\Phi = \left[\frac{1}{c} \left(\Delta u - \frac{\Delta p}{\rho c} \right); \frac{1}{c} \left(\Delta u + \frac{\Delta p}{\rho c} \right); \frac{\Delta v}{c}; \frac{\Delta s}{c^2}; \Delta Y \right] \quad (16)$$

By solving this system of equations with respect to $\Delta u, \Delta p, \Delta v, \Delta s$ and ΔY one can find the correcting flows \mathbf{f} for the corresponding flows from the vector $\mathbf{F}(\mathbf{U})$ with the help of formulas:

$$\begin{aligned} \text{mass flow} - f_1 &= \Delta \rho; \\ \text{longitudinal pulse flux} - f_2 &= u \Delta \rho + \rho \Delta u; \\ \text{cross pulse flux} - f_3 &= \rho \Delta v + v \Delta \rho; \\ \text{flux of the total energy} - f_4 &= (E + p/\rho) \Delta \rho + \rho \Delta s + \rho u \Delta u + \rho v \Delta v; \\ \text{flux of the mass fraction} - f_{4+k} &= \Delta Y_k; \end{aligned} \quad (17)$$

where $\Delta p = -\rho c^2(\Phi_1 - \Phi_2)/2 - \sum_k \eta_k \Phi_{4+k}$; $\Delta u = c(\Phi_1 + \Phi_2)/2$; $\Delta v = \Phi_3 c$; $\Delta s = \Phi_4 c^2$;

$\Delta \rho = (\Delta p - k \rho \Delta s)/c^2$; $\Delta Y_k = \Phi_{4+k}$. These expressions are derived explicitly from system (16).

4. Simulation results

Calculations were made for a long pipe with a diameter of about 0.04 m and a length of 1 m to 6 m, sealed on one side. Initially, the pipe was filled with the rest stoichiometric acetylene-air mixture enriched with oxygen at a temperature of about 300 K, with a reduced density of 0.18 kg/m³ and a pressure of 0.142 Pa. Initiation of combustion was carried out by modeling Joule heat release from the electric spark of the spark plug. The energy of the spark plug stood out in a gas mixture with a constant power of 0.04 J per 1.5ms in a small volume at the axis adjacent to the closed end of the pipe.

Numerical simulation was performed by the modified large particle method with TVD correction in 2D axisymmetric coordinate system. The symmetric spatial difference scheme of the 2nd order without artificial viscosity was used. A homogeneous calculation grid with a cell size in both directions (axial and radial) equal to $9.77 \cdot 10^{-4}$ m was applied.

Simulation results for some variants were considered: variants differed in settings the conditions on the side walls – the slip or adhesion model, and differed in the value of activation energy (6) – low (53 kcal) or high (63.7 kcal).

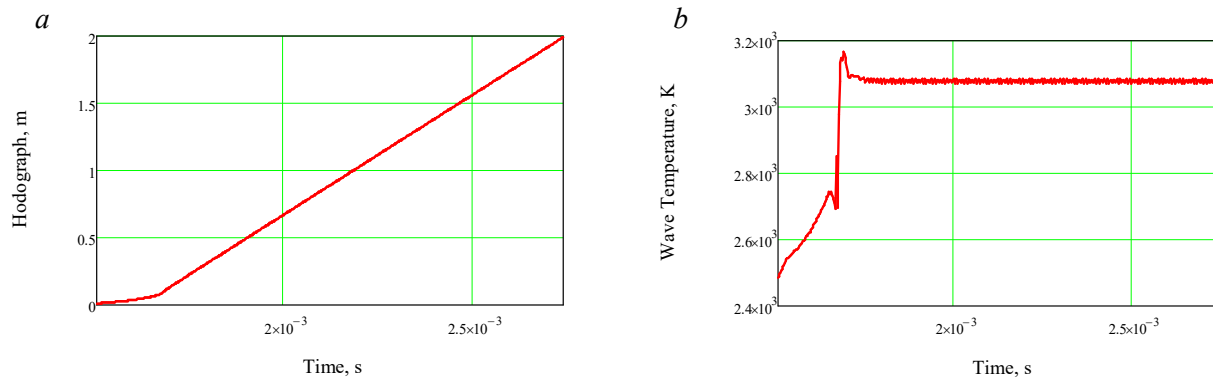


Figure 1. Combustion front dynamics at the axis for the adhesion and low activation energy:
a – front location; *b* – front temperature.

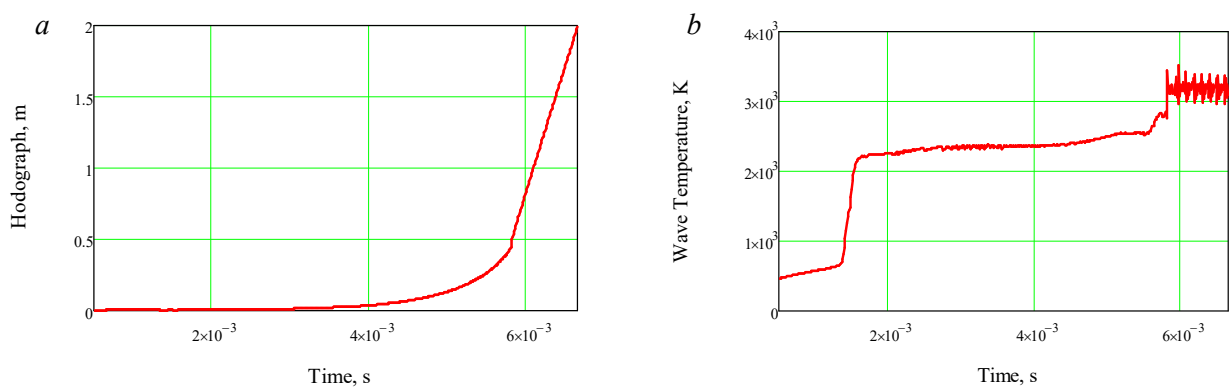


Figure 2. Combustion front dynamics at the axis for the adhesion and high activation energy:
a – front location; *b* – front temperature.

In the variant with the slip and low activation energy, the slow combustion of the mixture almost immediately after ignition passes into the detonation mode with a stable flat combustion front. Such an option, but with high activation energy gives a stable plane combustion wave, never passing into detonation. In the case of an adhesion and a low activation energy pattern of propagation of the combustion slightly different from the similar option with the slip. However, the detonation front is less stable here, judging by the small temperature oscillation on the wave front in axis (figure 1). In the high-energy version of the activation detonation occurs much later and the temperature oscillation at the wave front have a much higher amplitude (figure 2). This suggests that the surface of the detonation wave front is not flat and stationary. That can be seen in figure 3 where color maps of pressure distribution are represented for some moments in the range of the oscillation period. Here is shown a fragment of the pipe located in the vicinity of the detonation front at three (a, b, c) sequential time points divided with time interval equaled to 0.01ms. The detonation wave moves from up to down in the figure.

Conclusion

The use of TVD correction in conjunction with the large particle method improves the accuracy and stability of the latter. TVD correction extends capabilities of large particle method relatively to legitimately including second-order processes such as thermal conductivity and molecular viscosity in

the model. The simulation results showed the importance of taking into account the friction on the pipe walls. However, without taking into account viscous stresses, the effect of these boundary conditions disappears when the mesh cells decrease.

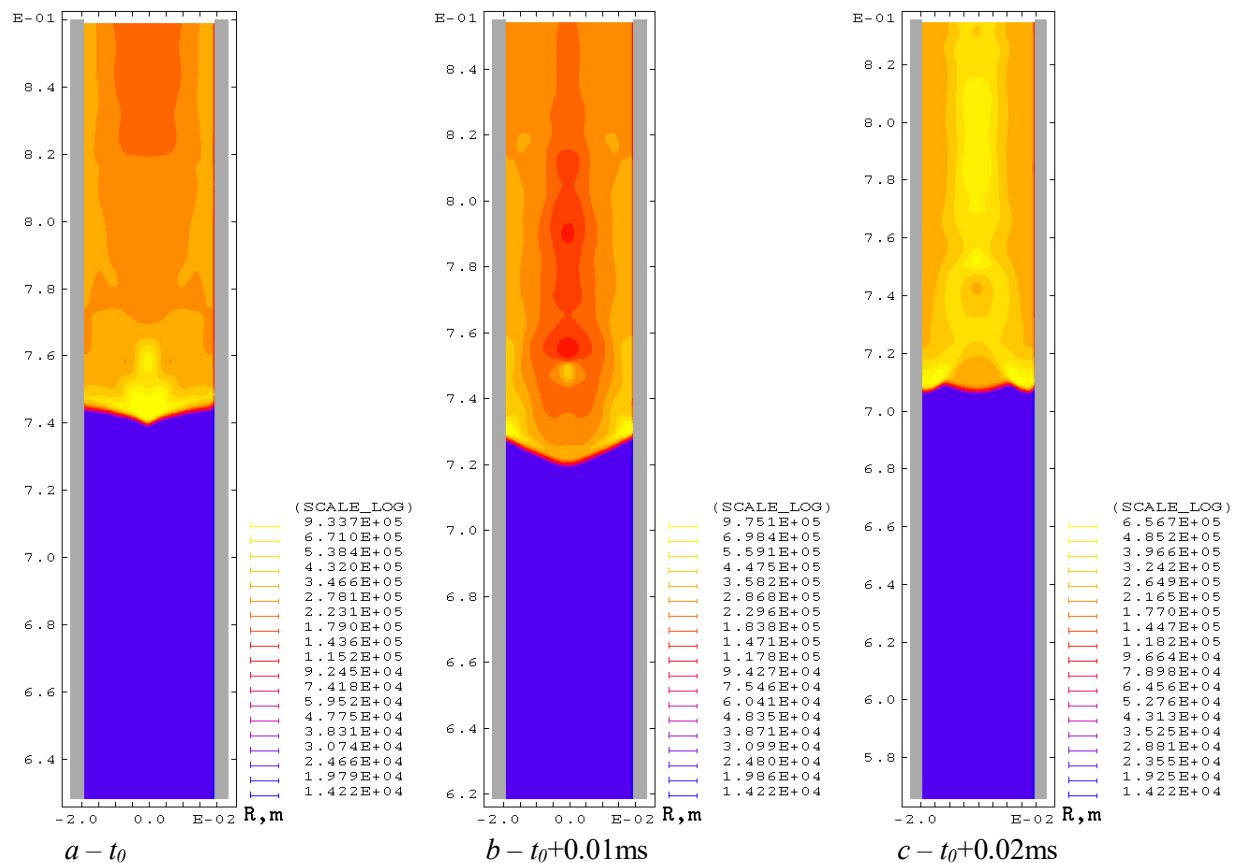


Figure 3. Color maps of pressure distribution at three sequential time points.

References

- [1] Moon J, Yee H C 1987 Numerical simulation by TVD schemes of complex shock reflections from airfoils at high angle of attack *AIAA Paper* **350** 1-17
- [2] Yee H C 1986 Linearized form of implicit TVD schemes for multidimensional Euler and Navier-Stokes equations *Int. J. Comp. Math. Appl.* **12A** 413-32
- [3] Belotserkovsky O M, Davydov Y M 1982 *Coarse particle (large particle) method in hydrodynamics* (Moscow, Nauka) p 392
- [4] Harten A 1983 High Resolution Schemes for Hyperbolic Conservation Laws *Journal of Computational Physics* **49** 357-93
- [5] Kozlov I M, Romanov G S, Suvorov A E 1993 Application of TVD-schemes for simulation of gas-dynamic flows with spherical or cylindrical symmetry *Journal of Engineering Physics and Thermophysics* **65** 296–301
- [6] Davydov Y M, Davydova I M 2003 Modern difference schemes of increased accuracy with decreasing the total variation on the solution for the actual problems of machine building a // *Mathematical modeling of systems and processes* **11** 4-18
- [7] Roe P L 1981 Approximate Riemann solvers, parameter vectors, and difference schemes *J. Comp. Phys.* **43** 357-72