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Letter to the Editors

Reply to the Letter of Ramshaw and Dukowicz*

Ramshaw and Dukowicz [1] claim that the article by Kansa [2] contains some misleading statements about APACHE [3], and about its suitability to combustion problems with large chemical heat release. These statements in [2] must be read contextually. Such statements were paraphrased from the APACHE [3] user's manual. As stated in [2], one must examine the application to determine which numerical scheme is most appropriate.

In several places, in the article by Kansa [2] it was stated that only low-speed subsonic flows would be considered. In Section VII, a situation in which large amounts of rapid chemical heat release such as ignition was given. A question is asked: Which numerical procedure, an ICE-like scheme which uses the method of successive substitution (MSS) iterative scheme or a stiff solver which uses a variant of the Newton–Raphson (NR) iterative scheme, is best suited for subsonic ignition-like conditions?

Because of the amount of matrix manipulation necessary in the stiff solved schemes, one naturally asks if a simplier scheme is perhaps more efficient. The time step used in the determining factor in estimating the radius of convergence of either the MSS or NR iterative schemes. Ramshaw and Dukowicz state that the APACHE code was designed primarily for transonic or supersonic combusting flows, whereas Kansa [2] restricted his stiff PDE solver to subsonic flows. The time step restrictions in Kansa [2] were placed primarily upon the Jacobian, Eq. (70) to enforce well conditioning, whereas in the APACHE code (cf. p. 39), the time step stability was taken to be the minimum of the convective, viscous momentum, species diffusion, thermal conduction, and radiative time step stability restrictions.

As Gustafsson [4] pointed out in his analysis of the shallow water equations, there exists a critical time step Δt_c above which the MSS scheme will diverge, but the NR scheme will converge. Below Δt_c, however, the MSS scheme is far more efficient in iterating to convergence than the NR scheme. The smaller the time step, the more advantageous is the MSS scheme compared to the NR scheme.

The comments that were in Sections II and VII of Kansa [2] regarding the APACHE scheme came from paraphrasing the following two paragraphs on page 34 of the APACHE [3] manual:

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Under unusual cirsumstances the iteration procedure may converge exceedingly slowly, or not at all. It is therefore desirable to establish an upper bound on ν, at which the iteration is arbitrarily terminated if it has not already converged. When this occurs a warning message is printed out, but the calculation is allowed to continue. This bound is currently taken to be 500.

Convergence difficulties may be experienced in low-speed reactive flow problems with large rates of chemical heat release. In such problems p^* differs greatly from p^{n+1} in the region of heat release. On the next cycle, then, these large pressure variations produce large variations in the explicit velocities u^T and v^T. The iteration must work inordinately hard to liquidate these large pressure and velocity variations. In such problems, it may be both more efficient and more accurate to simply run the calculation explicitly. Modifications to overcome this difficulty will be incorporated into later versions of APACHE.

Westbrook [5] found that problems arose when using the ICE method for treating the strongly exothermic chemical reaction in gasoline combustion simulations. He developed a generalized ICE method whereby the pressure corrections consists of not just mass changes, but also the internal energy and species corrections, thereby simultaneously coupling all equations within the iteration scheme. He pointed out that systematic errors occurred in the ICE model for problems with significant energy dissipation rates from exothermic chemical reactions. He concluded that the ICE method should only be used in those situations in which the fluid pressure variations are due principally to density variations. Note that in the stiff PDE treatment of Kansa [2] the generalized ICE treatment of Westbrook [5] has been incorporated within the NR iteration scheme.

Kansa [2] found that during an ignition phase in which very large amounts of heat were rapidly released, the NR scheme converged within three iterations, with frequent updating of the Jacobian each iterative cycle. Three iterations with frequent Jacobian updating, is not uncommon for stiff ordinary differential equations (ODE) packages in very severe circumstances. As long as the Jacobian is well conditioned, time steps several hundred times the CFL time step restriction may be taken. Convergence may occur with only one iteration, updating the Jacobian every three to five cycles.

In a fixed Eulerian grid scheme, ICE-like schemes might be preferable in transonic or supersonic combustion flows because the time step stability restrictions ensure also that the MSS time step restriction holds; this ensures a reasonably rapid convergence rate for the APACHE code. It was noted in Kansa [2] in several places that the fixed Eulerian grid stiff ODE solver should be used only for low subsonic combustion codes.

REFERENCES

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