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Detonation Front Theories: Using High-Resolution DNS to Define Extended Asymptotic Scalings and Models

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When the detonation reaction-zone length, η_r, is short in comparison to the dimensions of the explosive piece being burnt, the detonation can be viewed as a propagating surface (or front) separating burnt from unburnt material. If the product of the shock curvature, κ, and η_r is small (i.e., the scaled shock curvature satisfies $|\kappa\eta_r| << 1$), then to leading order the speed of this surface, $D_n(\kappa)$ is a function only of κ. It is in this limit that the original version of the asymptotic detonation front theory, called detonation shock dynamics (DSD) [1], derives the propagation law, $D_n(\kappa)$. In this lecture, we compare $D_n(\kappa)$-theory with the results obtained with high-resolution direct numerical simulations (DNS), and then use the DNS results to guide the development of extended asymptotic front theories with enhanced predictive capabilities.

The asymptotics that supports the original DSD model is based on the three assumptions: (1) weak shock curvature, with $\kappa\eta_r = O(\varepsilon)$, (2) quasi-steady dynamics on the slow time $\tau = \varepsilon t D_{CJ}/\eta_r$ and (3) a near Chapman-Jouget (CJ) detonation, with $1 - D_n/D_{CJ} = O(\varepsilon)$, where D_{CJ} is the CJ detonation speed. When filtered through this asymptotics, the solutions to the 3D Euler equations yield the intrinsic front dynamics (depending only on front specific quantities), $D_n(\kappa)$. This dynamics corresponds to a reaction-zone structure that is steady and quasi-1D (a nozzle flow in the shock-normal direction). A parabolic PDE controls the front evolution. Comparison of the predictions of this theory with DNS reveal that the long-time dynamics for weakly curved waves is well represented. At shorter times and for more highly curved waves, local errors in the shock position (of a few reaction-zone lengths) are observed.

Recent modifications of the above asymptotics by Yao and Stewart [2] replace assumption (3) with $1-D_n/D_{CJ} = O(1)$, which allows a richer dynamics, with both τ and κ entering the leading order theory. Here we use high-resolution DNS to gauge the relative importance of terms in the 2D reactive Euler equations for detonation flows, such as the steady ratestick flow shown in Figure 1. The average magnitude, in the shock-normal direction, of the terms in this component of the momentum equation is shown in Figure 2. From these results, we reach the following conclusions: (1) the flow is nearly quasi-1D, (2) the curvature terms are the dominant correction, (3) time dependence grows in importance as the edge of the explosive is approached and (4) transverse flow is not significant. Thus, except near the edge, time dependence is a higher-order correction to the flow than is the curvature.

These results motivated us to carry the original DSD asymptotics to $O(\varepsilon^2)$, where time-dependence enters the theory. An expanded region of validity for our asymptotic expansions was obtained by developing an expansion for $\kappa(D_n, ...)$ rather than one for $D_n(\kappa, ...)$. When carried through $O(\varepsilon^2)$, the analysis yields the intrinsic propagation law

$$\kappa = a*(D_{CJ}-D_n)/D_n + b*\{(D_{CJ}-D_n)/D_n\}^2 + \delta^2*(c/D_n^2)*d(D_{CJ}-D_n)/d(\delta^2 t),$$

where the form of the expansion was selected to reflect the expected behavior of the solution as $D_n \to 0$. This propagation law yields a hyperbolic PDE for the front propagation law. A comparison of the $O(\varepsilon)$ and the extended $O(\varepsilon^2)$ theory with DNS (for the problem of Figure 1) is shown in Figure 3. The extended theory is in good agreement with the DNS.

For the detonating explosive stick problem shown in Figure 1, the quality of the comparison of the $D_n(\kappa)$ theory and the extended theory with the DNS is in large measure a function of the density of the inert adjacent to the explosive that acts as confinement. Both theories compare favorably with the DNS for high-density confinement. When the density of the confinement is reduced beyond that used in the example of Figure 3, even the extended theory compares less favorably with DNS near the explosive/inert boundary. The results shown in Figure 2 indicate a new asymptotics is required (with κ

and time derivatives entering at the same order). A layer problem for the explosive/inert boundary region is formulated using this asymptotics, with the resulting PDE being solved numerically.

All the results discussed above assumed a reaction rate that is state-independent. The problem was reformulated for a state-dependent rate depending on pressure to a power. Besides the behavior shown above, this model shows detonation extinction in regions where κ becomes to large.

[1] Bdzil, J. B., and Stewart, D. S., "Modeling two-dimensional detonation with detonation shock dynamics," *Physics of Fluids A*, 1, 1261-1267 (1989).

[2] Yao, Jin, and Stewart, D. S., "On the dynamics of multi-dimensional detonation," *Journal of Fluid Mechanics*, 309, 225-275 (1996).

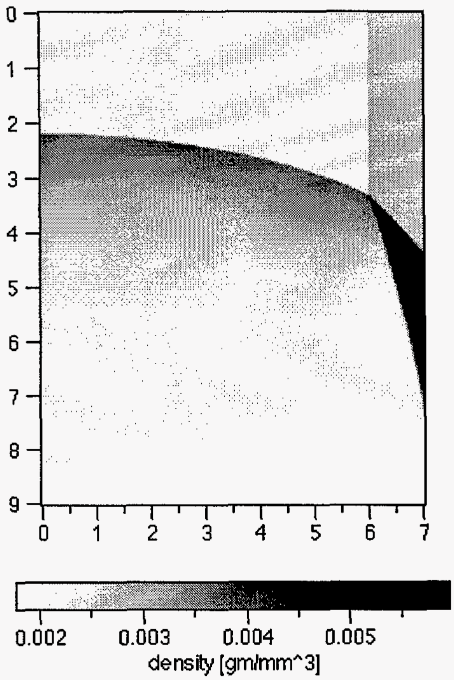
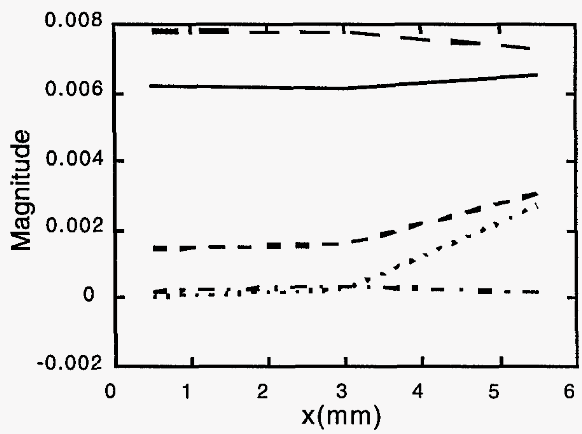


Figure 1



$$|\vec{\nabla}\alpha|\frac{\partial}{\partial\alpha}\left(\rho(u_\alpha - D_n)^2\right) + |\vec{\nabla}\alpha|\frac{\partial P}{\partial\alpha} + \rho(u_\alpha - D_n)u_\alpha\kappa + \frac{2\rho(u_\alpha - D_n)}{D_n}\frac{dD_n}{dt} + \rho\frac{du_\alpha}{dt} + (u_\alpha - D_n)\frac{d\rho}{dt} + \text{transverse} = 0$$

Figure 2

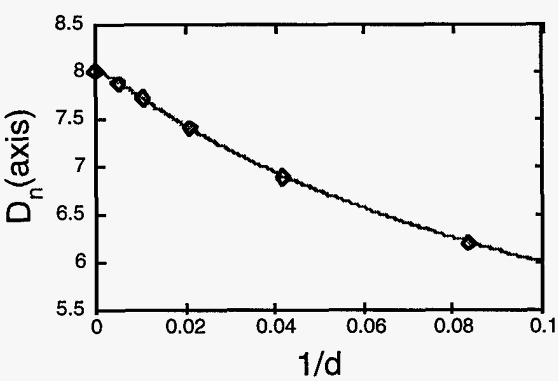


Figure 3a

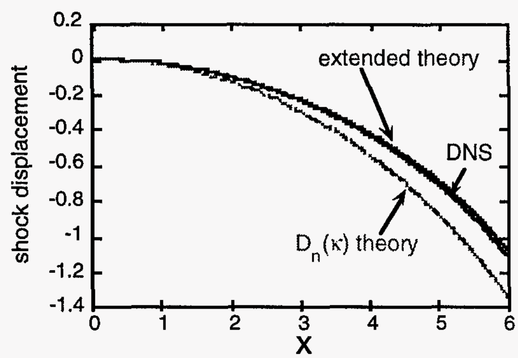


Figure 3b

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