The reaction rate obtained by Strachan can be written down as:

$$
\begin{aligned}
R(T, \rho) &= \kappa(\rho)\exp(-(E_a + f\rho_a/\rho)\kappa T)(pico - s) \\
\kappa(\rho) &= \exp(a - b\rho_a/\rho) \\
\underline{a} &= 1.82561 \\
b &= 0.290392 \\
f &= 0.356 \\
E_a &= 21.472 \text{ (kcal/mol)} \qquad (1)
\end{aligned}
$$

where ρ_a is the initial density of the material.

If T_{CJ} is the Chapman-Jouguet temperature, the rate R may be written as:

$$
\begin{aligned}
R(T,\rho) &= \kappa \exp(-1/\in)\exp\left(\frac{T - T_{CJ}}{\in}\right) \\
&\quad \exp(-f\rho_a/\rho/\kappa T + E_a/\kappa T_{CJ}) \\
\in &= \frac{\kappa T_{CJ}}{E_a} \sim 0.13 \\
T - T_{CJ} &\sim \in \quad . \qquad (2)
\end{aligned}
$$

Thus ϵ provides one with a small dimensionless parameter with which to perform an asymptotic analysis of the reactive Euler equations. One can now use the methods developed in [1], where the reactive Euler equations are written in the shock-based frame of reference to obtain a formal solution to $\vartheta(\epsilon)$ as:

- Note that an extra assumption has been made in this model, viz., that the factor of $(1 - \lambda_r)$ which appears in the conventional form for the single-step Arrhenius rate has been replaced by $(1 - \lambda_r)^{1/2}$. Physically this allows the reaction to be complete within a reaction zone of finite width. This is a reasonable assumption as long as the major fraction of the energy is released within a short distance. We have experimented with retaining the linear factor of $(1 - \lambda_r)$ in our analysis, unsuccessfully.
- Furthermore, for the moment we utilized a polytropic equation of state to describe the explosive. We expect to replace it shortly with a realistic equation of state obtained directly from the MD simulations.

A nonlinear $D_n - \kappa$ relation was obtained from this formalism and used to compute the shape of a steady-state detonation front for the case of an unconfined cylinder of macroscopic dimension (Fig. 2), thereby completing the initial phase of the transportation of the reactive MD simulations to the continuum level.

[1] M. Short and J.B. Bdzil, "Propagation Laws for Steady Curved Detonations with Chain-Branching Mechanisms," *J. Fluid Mech.* **479**, 39-64 (2003).

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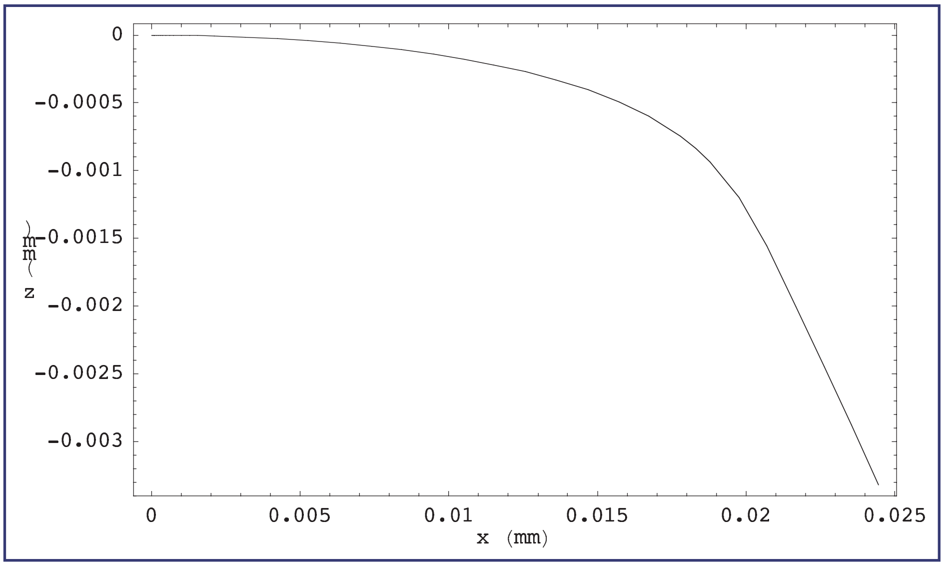

Figure 2—
Shape of the detonation front for an unconfined cylinder.

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