# NONDIFFUSIVE THERMAL EXPLOSION IN A NARROW VESSEL

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A central problem in the theory of homogeneous reactive materials is a precise description of the manner in which an explosive event develops in a given sample for a prescribed set of initial and boundary conditions. While the evolution is a function of the physico-chemical properties of the material, it also depends crucially on the size of the container. In this paper we examine the ignition and subsequent explosion of a reactive material in a planar, one-dimensional configuration, wherein the material is confined to a narrow region, or slot, between two rigid parallel plates. Such a geometry is quite common in experimental setups. The material is assumed to be a polytropic fluid, undergoing an exothermic reaction governed by Arrhenius kinetics with activation temperature $1/\epsilon$ in suitably scaled units, where $\epsilon \ll 1$. The initial state is taken to be weakly nonuniform, with the temperature decreasing monotonically from one wall to the other by an order $\epsilon$ amount. The system is modelled by the reactive Euler equations.

Earlier studies have examined the course of events in a configuration for which the width of the region is large enough for the acoustic time across it to be comparable to a characteristic induction time at the initial state. For these wider regions, order $\epsilon$ departures from the initial state are governed by Clarke's equations [1], [2], representing a balance between acoustics and weak but *nonlinear* chemical heat addition. Differential chemical heating of neigboring parcels produces pressure waves that travel across the slot, thereby setting up significant pressure gradients. The induction period typically culminates in a localized thermal runaway, characterized by singularities in the pressure, temperature and velocity perturbations, while perturbation in density remains bounded. A nearly-constant-volume explosion occurs at the runaway location, heralding the birth of a supersonic reaction wave that emerges from the runaway site, decelerates as it proceeds into the colder material, and eventually transits into a ZND detonation. Almost the entire post-runaway event can be described by means of an asymptotic analysis in the limit of large activation energy. Even the small amount of numerical effort needed to complete the picture can be dispensed with by invoking the Newtonian limit of nearly-equal specific heats, $\gamma - 1 \ll 1$. Details can be found in [2] – [5].

Our present concern is with narrower regions for which $\alpha$, the ratio of acoustic to induction times, is considerably smaller than unity: $\alpha \ll 1$. It is immediately clear that the system must now evolve differently during the induction stage, as acoustic waves can traverse the region many times during the characteristic induction time, thereby ensuring that pressure evolution is spatially uniform, at least at leading order. It is of interest then to determine how this difference in early evolution affects the subsequent events; in particular, the structure of the runaway, the strength of the local explosion, and the resulting wave system. Once again the initial state is prescribed to be one with a small (order $\epsilon$)

temperature variation across the slot. The analysis is based on the distinguished limit

$$\alpha = O(\gamma - 1) = O(\sqrt{\epsilon}) \ll 1.$$

This limit allows one to construct an analytical solution upto the end of the local explosion. Post-explosion wave development requires an accurate and well-resolved numerical solution which we provide.

The very early stage of evolution, lasting only a fraction $\alpha$ of the initial induction time, and characterized by small, $O(\alpha\epsilon)$ departures from the initial state, is now governed by the *linearized* version of Clarke's equations, representing acoustics driven by linearized chemical heating. The pressure disturbance in this zone has a spatially uniform but temporally growing component, on which is superposed a weaker, periodic oscillation. The temperature perturbation also grows in time, while the velocity disturbance is bounded.

The linear growth takes the solution into the induction stage proper, where pressure and temperature disturbances grow to be of order $\epsilon$, while the velocity disturbance remains at order $\alpha\epsilon$. Here the governing equations are *almost* Clarke's, but the narrowness of the domain causes the acceleration term in the momentum equation to be multiplied by the factor $\alpha^2$. As a result pressure gradients are negligible to leading order. This stage requires a two-time analysis, because the leading-order perturbations, varying on the induction time scale $t$, are corrected by high-frequency periodic oscillations, varying on the fast time $t/\alpha$. This stage was analyzed in considerable detail in [6] under a different distinguished limit, $\alpha = O(\epsilon)$ and $\gamma - 1 = O(1)$, and for a more general set of initial conditions than those considered here, but without the inclusion of the high-frequency terms.

The induction stage becomes singular at $t = 1$, the *constant-pressure* induction time. This is in contrast to the induction singularity in a wider sample, which develops at a time that is part way between the constant-pressure and constant-volume induction times. The nature of the singularity is different as well. While the $O(\epsilon)$ temperature disturbance becomes logarithmicaly singular locally at the hot wall, the pressure disturbance develops a weaker logarithmic singularity, at order $\epsilon\alpha$, across the *entire* domain. Velocity disturbance becomes globally singular as well.

The induction singularities are resolved in a temporally thin layer, $1 - t = O(\alpha)$ and away from a thin corner region, $O(\alpha)$ in spatial extent, near the hot wall. Here Clarke's equations emerge, not unexpectedly, since spatial and temporal scales now enjoy coequal status. The solution in this layer must match that in the corner region, which has a locally self-similar structure. It is here that the small-disturbance solution breaks down and gives way to an explosion, characterized by a rapidly self-focussing kernel, in which temperature excursions and reactant depletion are of order unity. In stark contrast to conventional diffusionless explosions studied heretofore, the pressure disturbances, although larger than those in the induction stage, may grow here only to order $\alpha$, or to order unity, depending upon whether a parameter involving the initial temperature gradient is above or below a critical value. In either case, the reactant within the explosive kernel is fully depleted and the temperature there increases by an order-unity amount. In particular the constant-volume explosion, and the high-speed supersonic reaction wave resulting therefrom, are now absent.

The events following the local explosion at the hot wall are studied numerically, by adopting a high-resolution, adaptive approach. The computations reveal that detonation is now attained through a SWACER-like mechanism, whereby an initially weak shock is approached and then propelled by the flame behind it, rather than through the deceleration of a supersonic, weak detonation, as seen in regions of larger size.

## References

[1] J. F. Clarke, *Finite amplitude waves in combustible gases*, The Mathematics of Combustion, Frontiers in Applied mathematics, J. D. Buckmaster, ed., SIAM, Philadelphia (1985), pp. 183–245.

[2] T. L. Jackson, A. K. Kapila and D. S. Stewart, *Evolution of a reaction center in an explosive material*, SIAM J. Appl. Math., 49 (1989), pp. 432–458.

[3] A. K. Kapila and J. W. Dold, *A theoretical picture of shock-to-detonation transition in a homogeneous explosive*, 9th Symposium (International) on Detonation (1991), pp. 111–118.

[4] M. Short, *On the critical conditions for the initiation of detonation in a non-uniformly perturbed reactive fluid*, SIAM J. Appl. Math., 57 (1997), pp. 1242–1280.

[5] P. A. Blythe and D. G. Crighton, *Shock-generated ignition: the induction zone*, Proc. R. Soc. Lond., A426 (1989), pp. 189–209.

[6] D. R. Kassoy, N. Riley, J. Bebernes and A. Bressan, *The confined nondiffusive thermal explosion with spatially homogeneous pressure variation*, Combust. Sci. and Tech., 63 (1989), pp. 45–62.