

# A SINGULAR-PERTURBATION ANALYSIS OF THE BURNING-RATE EIGENVALUE FOR A TWO-TEMPERATURE MODEL OF DEFLAGRATIONS IN CONFINED POROUS ENERGETIC MATERIALS

Stephen B. Margolis<sup>†</sup> and Melvin R. Baer<sup>‡</sup>

<sup>†</sup>Sandia National Laboratories  
Livermore, California 94551-0969 USA  
E-mail: margoli@sandia.gov

<sup>‡</sup>Sandia National Laboratories  
Albuquerque, New Mexico 87185-0834 USA  
E-mail: mrbaer@sandia.gov

## Extended Abstract

The combustion behavior of porous energetic materials is of increasing interest in predicting how such materials will perform after a period of long-term storage and/or exposure to abnormal thermal environments. Materials such as the nitramine propellants HMX and RDX, for example, find numerous applications in the fields of propulsion and pyrotechnics. Though manufactured and placed in a system while in a pristine state, partial decomposition can occur and significant void fractions can develop over time, either because of an inherent degree of metastability in the formulation or because of various accident scenarios that are associated with brief periods of elevated temperatures. During combustion, significant two-phase flow effects in such damaged materials play an important role, especially when the material is under confinement. Under these conditions, pressure-driven convective permeation of hot gases into the pores of the unburned solid occurs (*cf.* [1] and the literature review in [2]), leading to a superadiabatic preheating effect that accelerates the propagation speed and ultimately results in a convection-dominated mode of burning. During this transition from so-called conductive to convective burning, both conduction and convection play significant roles and must be considered in any model that describes this burning regime. In addition, as convective gas velocities increase in the two-phase regions, temperature-nonequilibrium effects associated with finite rates of heat transfer between the co-existing gaseous and condensed phases will also begin to influence the propagation speed. The purpose of this study is to analyze some of the influences associated with the latter.

A sketch of the physical problem is shown in Figure 1. In general, we consider a confined or partially confined geometry, in which case there is an overpressure-driven gas flow into the unburned porous material. It is assumed that melting of the solid occurs at a prescribed temperature and that subsequent to melting, a single-step exothermic reaction converts the liquid reactants to gaseous products, giving rise to a deflagration wave that propagates from right to left in the direction of the unburned propellant. The structure of the combustion wave consists of a solid/gas preheat region, the melting surface that marks the left boundary of a liquid/gas preheat region, and a relatively thin exothermic reaction zone in which chemical reaction occurs. Although it is not necessary to consider the details in the present work, there also exists, for weak permeabilities, a gas-permeation boundary layer within the solid/gas preheat region in which the gas pressure decreases rapidly from its value at the surface of the solid, to values close to the ambient deep within the porous material ([1]). In the present work, we focus on the calculation of the burning-rate eigenvalue corresponding to quasi-steady, planar propagation of the combustion wave. The effects of confinement are modeled by specifying the pressure difference, or overpressure, between the product gas in the burned region to the right of the

reaction zone and the gas deep within the unburned solid to the left of the material surface.

Various effects that are associated with two-phase flow in porous energetic-material deflagration, and that are relevant to the present work, have been analyzed in several recent theoretical studies (*cf.* [1], [3], [4]). In particular, the porous-material models considered thus far, which represent specific formulations of more general reactive two-phase-flow descriptions (*cf.* [5]), have generally considered the case of a porous solid with a reactive bubbling melt layer at the surface, a feature that is frequently observed during combustion of nitramine propellants. Though much of this analysis has been restricted to the single-temperature limit associated with infinite rates of interphase heat transfer, it was previously shown for the unconfined problem that the first effects of large but finite rates of interphase heat transfer are felt primarily in the liquid/gas reaction zone ([3]). In the present work, we consider the more general confined problem previously analyzed in the single-temperature limit [1], at the same time allowing for more significant two-temperature effects arising from increased resistance to interphase heat transfer. In particular, we generalize the earlier unconfined and/or single-temperature results by allowing for an overpressure in the gaseous phase external to the porous solid, and exploit the limit in which the gas-to-liquid thermal-conductivity ratio can be considered a small parameter. It is then shown that the leading-order effects on the burning rate associated with finite rates of interphase heat transfer again occur in the liquid/gas reaction region, but the asymptotic limit just described permits much more general results than those obtained previously. These are achieved through the application of nonstandard techniques in matched asymptotic expansions associated with the appearance of an infinite number of logarithmic terms in the asymptotic development.

Thus, in the parameter regime considered here, the problem reduces to a nontrivial eigenvalue calculation in the thin reaction region where final conversion of the liquid to gaseous products occurs. Although a closed-form solution to that problem is not generally available, it turns out that for realistically small gas-to-liquid thermal-conductivity ratios, solutions in the reaction zone take on a singular-perturbation character that can be exploited to derive an asymptotic expansion of the burning-rate eigenvalue. However, because there appear an infinite number of logarithmic terms in the subsequent asymptotic development that must be included in order to arrive at the desired level of approximation, the resulting problem requires a generalized, nonstandard approach to the usual formalism associated with the method of matched asymptotic expansions. The subsequent analysis [6] then ultimately provides a modified expression for the leading-order burning-rate eigenvalue in which the finite rate of interphase heat transfer appears explicitly.

Additional results that come out of this analysis include the degree of temperature nonequilibrium as a function of a reaction-progress variable, as shown in Figure 2, and the behavior of the normalized deflagration velocity as a function of various parameters, as shown in Figure 3. The physical effect of temperature nonequilibrium, which decreases the rate of heat transfer from the reacting liquid phase to the gas-phase products, and thus allows a greater amount of thermal energy to remain in the reacting phase, is to increase both the propagation speed and the sharpness of the transition to “convective” burning (relative to the single-temperature limit) as the overpressure increases. Indeed, for sufficiently small values of the scaled interphase heat-transfer rate, the temperature profile of the reactive liquid phase becomes non-monotonic (Figure 4), rising above the final burned temperature and thus supporting a faster reaction rate, before decreasing, in a thin equilibration sublayer, to approach the gas temperature as the reaction goes to completion. The end result arising from this thermal nonequilibrium is a factor in the expression for the normalized burning rate that reflects finite values of the scaled interphase heat-transfer coefficient and collapses to unity in the single-temperature limit.

## Acknowledgment

This work was supported by the United States Department of Energy under Contract DE-AC04-94AL85000.

## References

- [1] S. B. Margolis, *Influence of pressure-driven gas permeation on the quasi-steady burning of porous energetic materials*, Combustion Theory and Modelling, Vol. 2 (1998), pp. 95–113.
- [2] B. W. Asay, S. F. Son and J. B. Bdzil, *The role of gas permeation in convective burning*, International Journal of Multiphase Flow, Vol. 22 (1996), pp. 923–952.
- [3] S. B. Margolis and F. A. Williams, *Effects of two-phase flow on the deflagration of porous energetic materials*, Journal of Propulsion and Power, Vol. 11 (1995), pp. 759–768.
- [4] A. M. Telengator, S. B. Margolis and F. A. Williams, *Stability of quasi-steady deflagrations in confined porous energetic materials*, Combustion Science and Technology, 2001, to appear.
- [5] M. R. Baer and J. W. Nunziato, *A two-phase mixture theory for the deflagration-to-detonation transition (DDT) in reactive granular materials*, International Journal of Multiphase Flow, Vol. 12 (1986), pp. 861–889.
- [6] S. B. Margolis and M. R. Baer, *A singular-perturbation analysis of the burning-rate eigenvalue for a two-temperature model of deflagrations in confined porous energetic materials*, 2001, submitted for publication.

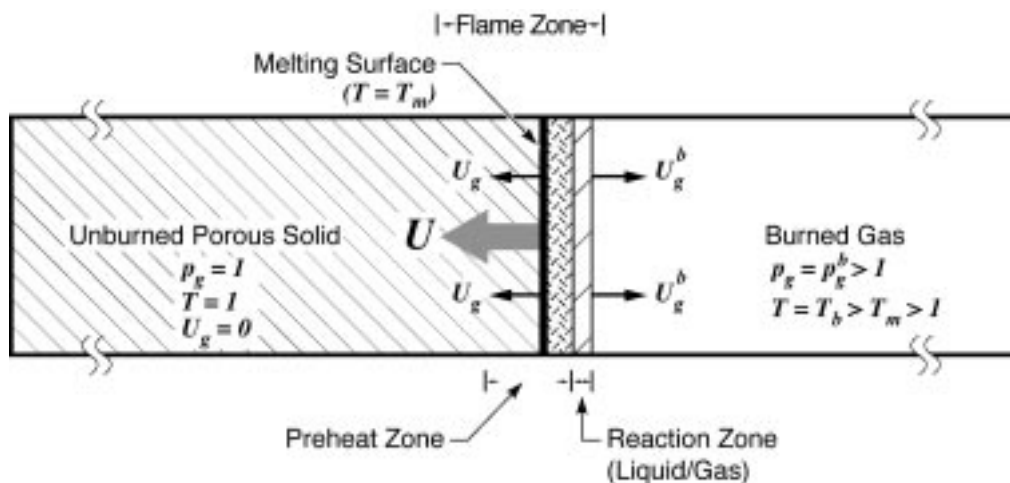


Figure 1. Physical sketch of the model. The two-phase-flow nature of the problem is enhanced by the effects of confinement, which leads to a pressure-driven permeation of the burned gas into the pores of the unburned solid.

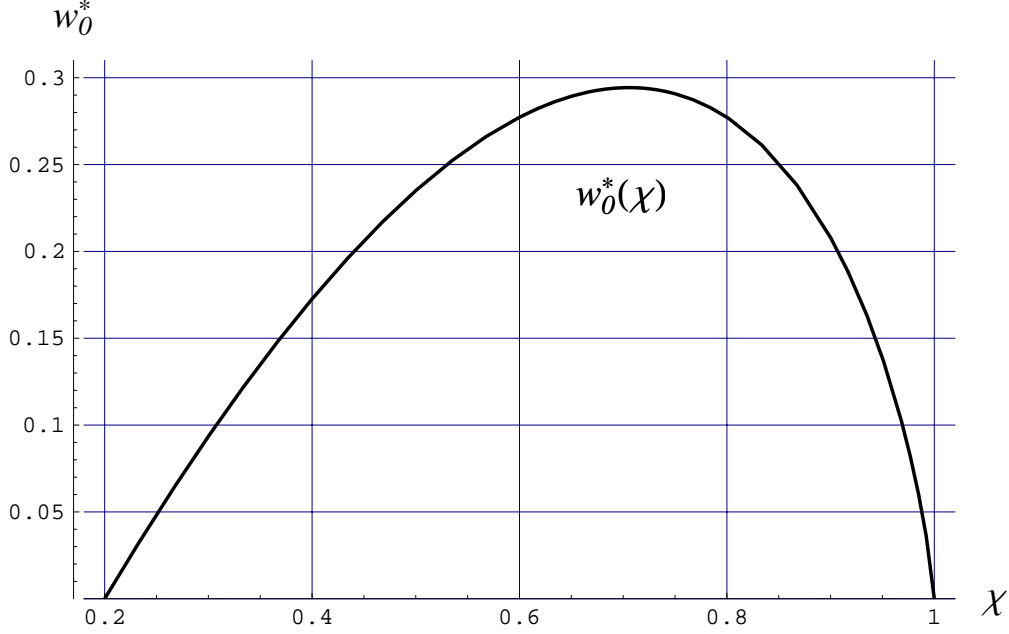


Figure 2. Profile of the normalized temperature-difference approximation  $w_0^*$  for porosity  $\alpha_s = 0.2$ . Temperature nonequilibrium between the reactive condensed and gas-product phases persists through most of the two-phase reaction region, with equilibrium achieved in a thin sublayer as the reaction approaches completion (*i.e.*, as the gas-phase volume fraction  $\chi \rightarrow 1$ ).

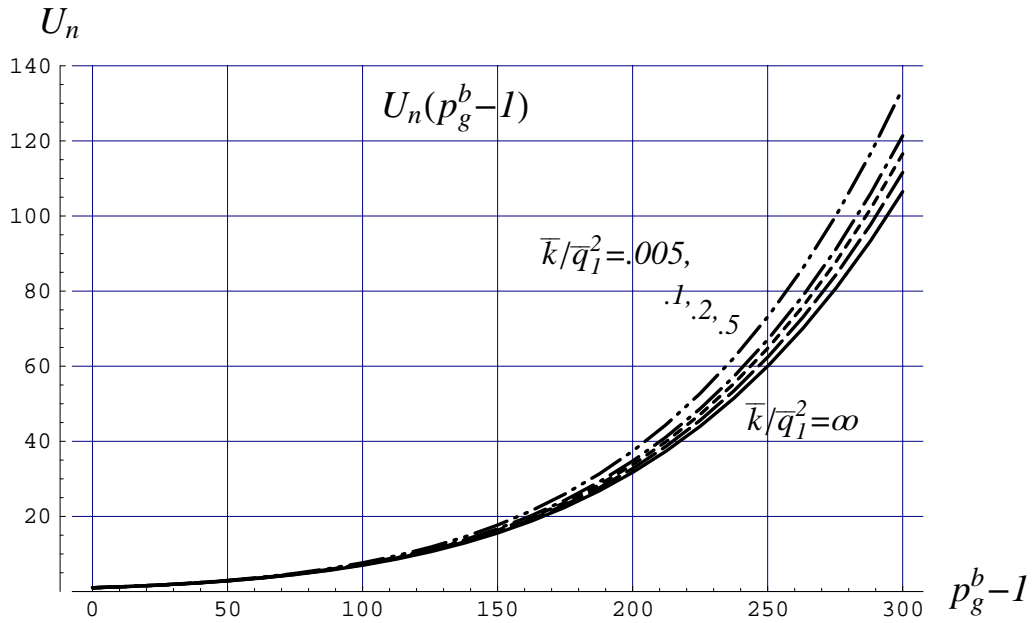


Figure 3. Representative “two-term” approximation of the normalized deflagration velocity  $U_n$  as a function of the overpressure  $p_g^b - 1$ . The curves correspond to various values of a normalized interphase heat-transfer coefficient  $\bar{k}/\bar{q}_1^2$ . Increased resistance to interphase heat transfer leads to a decrease in the burning-rate eigenvalue, and hence to an increase in the propagation speed. The behavior of  $U_n$  as the overpressure increases reflects the often-observed transition from a conduction-dominated regime to one in which convection plays a significant role.

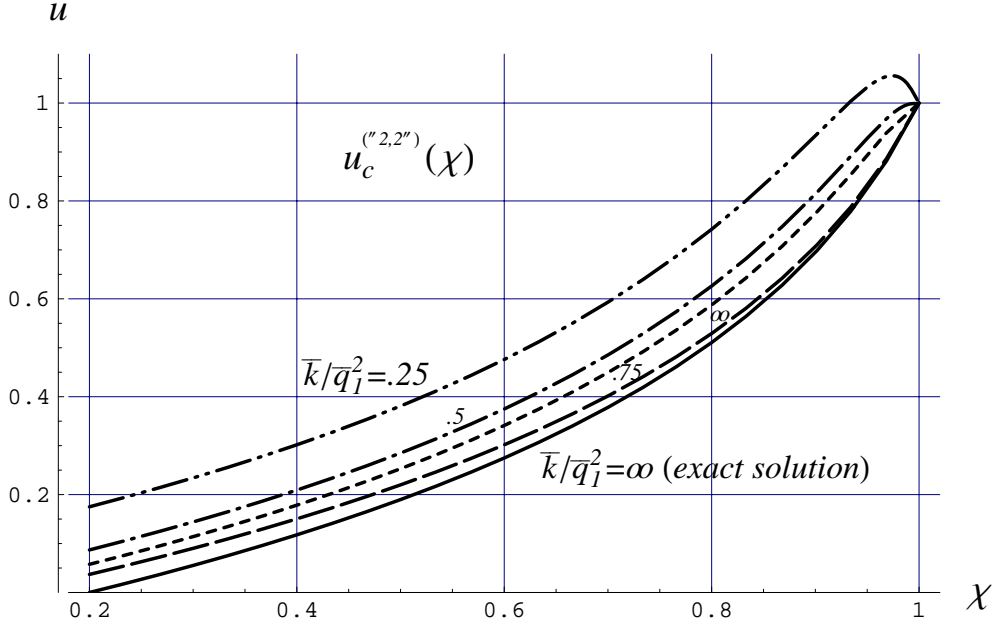


Figure 4. The “two-term” composite approximation for the liquid-temperature variable, denoted by  $u_c^{(“2,2”)}$ , for representative parameter values. The exact solution for  $\bar{k} = \infty$  is represented by the solid curve. As described in the paper [6], the approximation at this order of matching satisfy the boundary condition at  $\chi = 1$  exactly, and possess an  $O[\bar{l}^2(-\ln \bar{l})^{-1}]$  error at  $\chi = \alpha_s$ , where  $\bar{l}$  is the gas-to-liquid thermal-conductivity ratio used as the small expansion parameter.