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On The Partially Reacted Boundary Layer in Rate Sticks

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Abstract

Using our temperature dependent reactive rate (TDRR) reactive flow model to simulate detonation in a rate stick, we observe that a partially reacted layer (PRL) is being formed near the boundary. We are not aware that such a PRL has been observed in tests, and this is why we regarded it in the past as a numerical artifact. Assuming that such an artifact may be caused by the finite rise time of the detonation shock, we showed in [1] how it can be eliminated by delaying the outward boundary motion for a length of time comparable with the shock rise time. Here we revisit the PRL problem. We first show that it is not a numerical artifact but a real phenomenon. We do this by repeating the reactive flow run with a finer mesh. By looking at the PRL structure, we see that doubling the resolution affects the PRL only slightly. We then conjecture that the PRL formation has to do with the finite duration of the reaction process (or the finite extent of the reaction zone). By the time the boundary rarefaction reaches a cell near the boundary, it may still be only partially reacted, and its reaction process may be therefore cut off. To establish our conjecture, we show how the PRL structure changes with the reaction duration.

INTRODUCTION

When we simulate a rate stick test using our Temperature Dependent Reaction Rate (TDRR) reactive flow model, the result we usually get is that a thin layer near the boundary is only partially reacted. Using a pressure dependent reaction rate like in the Lee-Tarver Ignition & Growth model [2], we get an even more pronounced partially reacted layer near the boundary. We're not aware that such a partially reacted layer (PRL) has been observed experimentally. We therefore regarded it in the past as a numerical artifact. In [3] we proposed a way to eliminate the PRL from the simulations. We assumed there that the PRL is formed by the finite rise time of the detonation shock. Artificial viscosity usually smears the shock over a length of three mesh cells. By the time the rarefaction wave from the free boundary reaches the first and second cells near the boundary, the shock there has not fully built up yet, and the reaction there is quenched before it has a chance to develop. But in reality, this does not happen, as the shock rise time is of the order of a ns. To eliminate such an artifact, we proposed in [3] to artificially delay the boundary motion in the direction normal to itself for the shock rise time duration. But recently we repeated these rate stick simulations with finer meshes and realized that the PRL changed only slightly, even though the shock rise time was much shorter. We concluded that: 1) the formation of the PRL is probably real and not a numerical artifact, so that there is no point in eliminating it artificially; and 2) some other mechanism is responsible for the formation of the PRL.

In what follows we do rate stick simulations and show that the PRL is mainly an outcome of the reaction zone being of finite length (or finite duration). We also evaluate and show the structure of the PRL.

SIMULATIONS

The rate stick in the simulations is made of an insensitive high explosive (IHE), and has a diameter of 16mm. We monitor the detonation front at 60mm from the initiation boundary (almost 4 stick diameters), where the flow is about stationary. We use our reactive flow model with two mesh resolutions, 10 and 20 cells per mm. In figures 1 and 2 we show maps with lines of equal W (reaction progress parameter) from runs with the two resolutions, at 10 microseconds after initiations. From figures 1 and 2 we see that a PRL has been formed in both runs. We can also see that for the higher resolution run, the width of the PRL is only slightly narrower. To get a quantitative perception of the structure of the PRL, we show in figures 3 to 5 the maxima of pressure, reactant temperature, and the reaction parameter from the two runs along the radial direction, at 60mm down the stick.

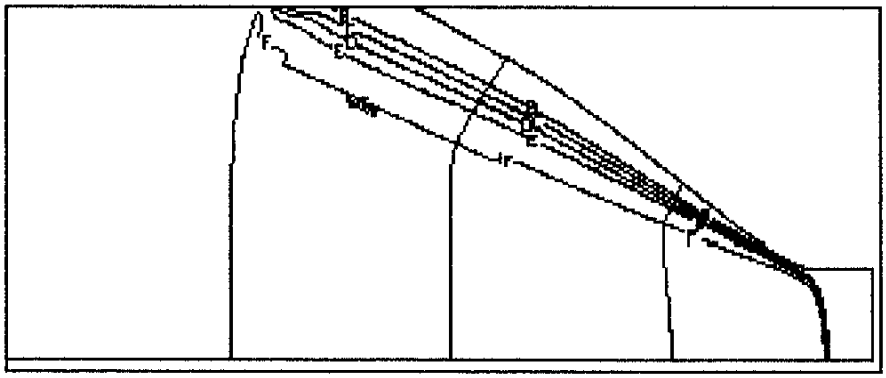


FIGURE 1. A map with lines of equal W (reaction progress parameter) at 10 microseconds after initiation, from the run with 10 cells per mm.

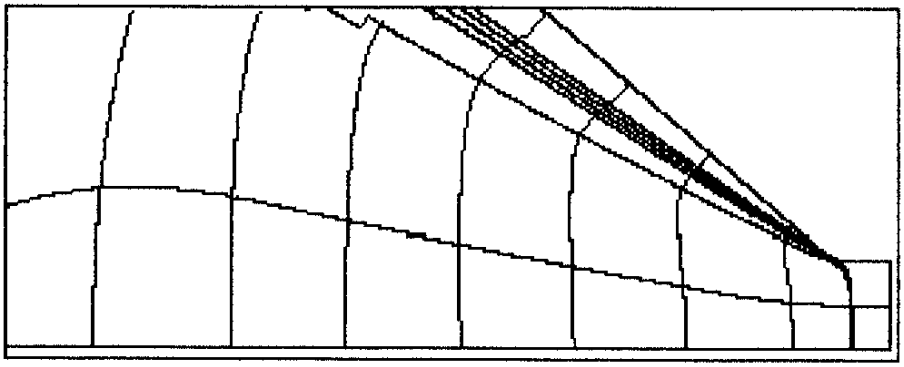


FIGURE 2. A map with lines of equal W (reaction progress parameter) at 10 microseconds after initiation, from the run with 20 cells per mm.

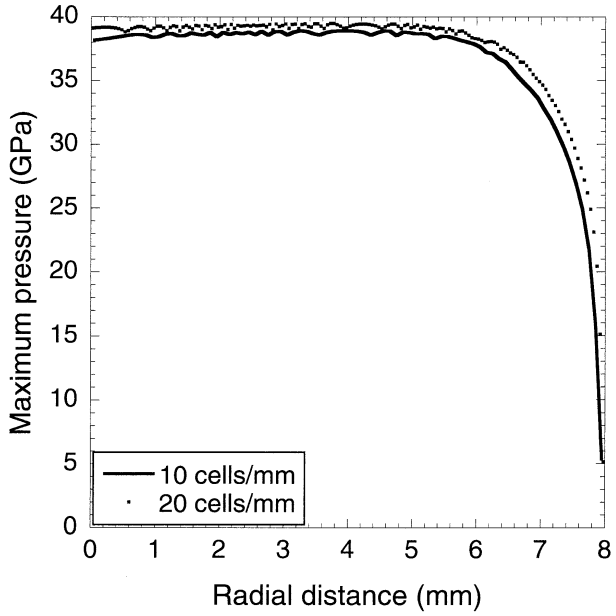


FIGURE 3. Pressure maxima along the radial direction at 60mm down the stick, with 10 and 20 cells per mm.

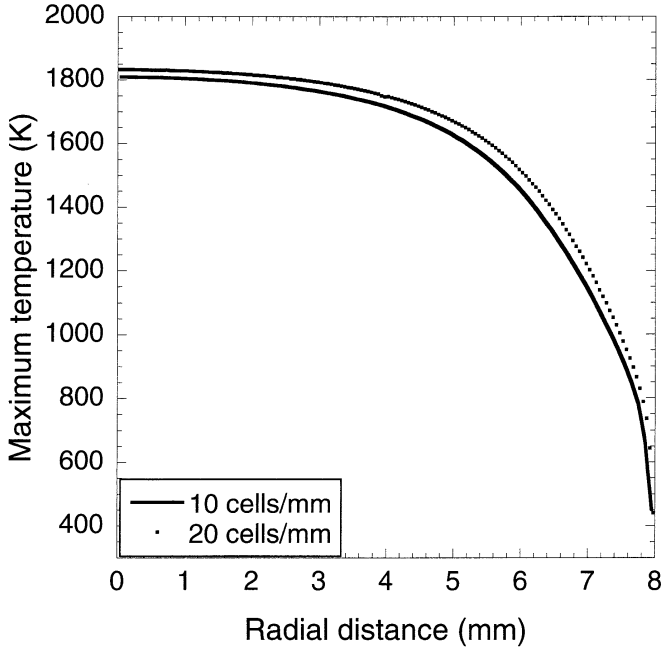


FIGURE 4. Reactant temperature maxima along the radial direction at 60mm down the stick, with 10 and 20 cells per mm.

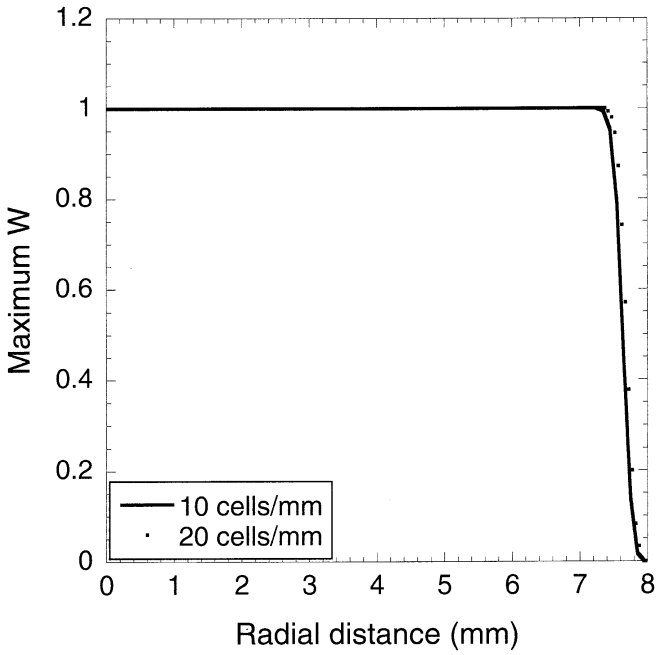


FIGURE 5. Reaction progress parameter maxima along the radial direction at 60mm down the stick, with 10 and 20 cells per mm.

From figures 3 to 5 we see that for a finer mesh the PRL at the boundary becomes narrower, but only slightly. From this and from additional runs not shown here we conclude that:

- The detonation shock rise time is not the main cause for the formation of the PRL.
- The main cause is probably the **finite duration of the reaction**. If the release wave from the boundary arrives at a certain cell before the reaction has time to develop to a significant extent, the reaction there is quenched down.

As mentioned above, we're not aware that a PRL has been observed in a rate stick test, or in any other detonation configuration. But nevertheless, we think that there is indirect evidence to its existence. In rate stick tests, the usual procedure is to photograph the front breakout from the far end of the stick with a smear camera along a diameter. From such a breakout curve one tries, among other things, to extract the boundary angle, which is important for DSD analysis. But usually, the edge of the breakout curve is somewhat blurred, and the extracted boundary angle has a sizable uncertainty. As a result, we find in the literature different values of the boundary angle for the same explosive. We suggest here that this uncertainty in the extracted boundary angle has to do with the existence of a PRL near the boundary.

To show that the PRL near the boundary is caused by the finite duration of the reaction, we made additional runs in which we artificially changed the duration of the reaction. The reaction rate in our reactive flow model TDRR is given by [1]:

$$\dot{W} = y(W) R_T \exp\left(-T^*/T_s\right) \qquad (1)$$

where y(W) is the Burn Topology Function, T_s is the reactant temperature, and R_T, T^* are material parameters calibrated from tests. We changed the reaction duration by changing the coefficient R_T. Increasing R_T by some factor decreases the reaction duration by the same factor.

In figures 6 and 7 we show the reaction progress parameter maxima along the radial direction near the boundary for three values of R_T and for two mesh resolutions. We see from figures 6 and 7 that:

- The PRL is thicker for longer reaction durations.
- The relation between the reaction duration and the PRL thickness is nonlinear.
- When R_T decreases by 25% (not shown here), the reaction is extinguished.
- From the nominal (middle) curve it can be seen that: 1) in the last cell near the boundary there is no reaction; 2) in the second cell from the boundary there is a minimal reaction extent; and 3) in the third cell from the boundary the extent of reaction is around 10%.

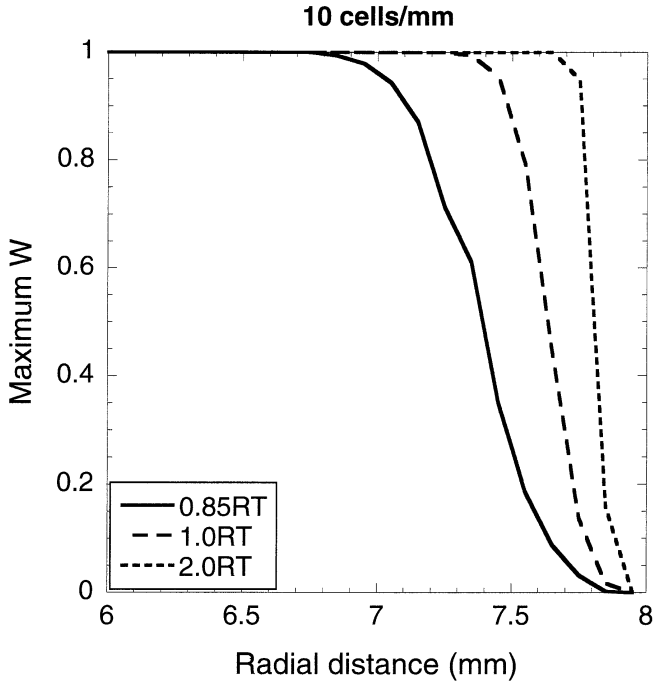


FIGURE 6. Reaction progress parameter maxima along the radial direction near the boundary, with 10 cells per mm, and with different values of R_T (or reaction duration).

SUMMARY

When simulating detonation in a rate stick with a reactive flow model, we get a partially reacted layer (PRL) near the boundary. In the past we regarded this PRL as a numerical artifact and proposed means to eliminate it. Recently we realized that the PRL obtained in simulations is not a numerical artifact. Performing the same simulations with a finer mesh shows that the PRL changes only slightly. From the simulations we conclude that the PRL near the boundary is caused by the finiteness of the reaction zone, or by the finite duration of the reaction. By the time that pressure in a cell near the boundary is released by the rarefaction wave from the boundary, the reaction there may have not yet advanced far enough before it dies out.

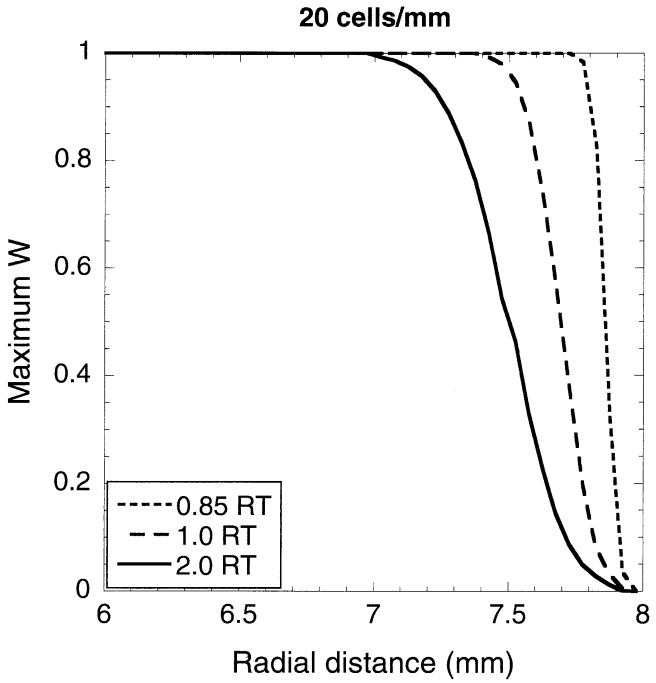


FIGURE 7. Reaction progress parameter maxima along the radial direction near the boundary, from a 20 cells per mm run, and with different values of R_T (or reaction duration).

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