Transport Phenomena for Nonshock Initiation Processes

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2.1 An Overview of Transport Theory in Explosives Problems

A useful explosive material is, of course, stable under reasonable environmental conditions. It will neither release energy nor produce gas without some kind of thermal stimulus. The possible stimuli include impact, spark, friction, boundary heat, or shock. These processes raise the temperature of the explosive material, either in a localized volume, or throughout its entire volume, to a point where the exothermic, gas-producing reaction becomes self-sustaining (ignition). We refer to the events leading to self-sustaining reaction as the pre-ignition regime, and the behavior after self-sustaining reaction commences as the post-ignition regime. We further generally characterize the post ignition regime by either laminar nonviolent deflagration; violent, convectively driven explosion; or the process may undergo a transition to detonation (DDT).

Transport phenomena are inherent to the nonshock initiation process and post-ignition behavior. Specifically, transport phenomena are the movement of heat (energy), molecular species, and momentum under the influence of temperature, species concentration, pressure, and velocity gradients. The theory of these phenomena, together with the production of gas and heat from chemical reactions (kinetics and thermodynamics), in principle fully describe the processes that occur prior to ignition (preignition) and what happens after (post-ignition). In practice, the theory has only been applied to very simple situations due to the complexity of the integrated problem.

The stimuli listed above all serve to raise the temperature of the explosive either within a volume small with respect to the charge (impact, spark, friction, shock) or globally (boundary heat). Each of these stimuli will be discussed in detail in other chapters of this text. As these are the initial drivers for the ignition process, we briefly introduce them here. Impact leads to localized heating when deformation becomes concentrated, where the material fails by cracking, or when the yield strength is exceeded and causes shear localization and concentration of energy along shear bands (Chap. 10). Spark energy
is localized along the spark channel (Chap. 11). Friction (Chap. 9) localizes heat between moving surfaces or at specific locations, where, for example, foreign matter (grit) becomes trapped between the surfaces (the latter has been implicated in accidents.) A shock wave compresses material along its leading edge and causes heat generation directly by adiabatic compression of the material itself, by collapsing void space, or by grain boundary interactions. Boundary heat, as the phrase implies, is heat applied to the outer surfaces of an explosive charge, or its container, and the most common source is fire, and ignition by this method is commonly called “cookoff” (Chap. 7).

Chapter 3 discusses reaction kinetics and thermodynamics. We mention them here in the context of heat transport because, of course, exothermic chemical reaction becomes the driving force for the ignition and combustion process once one (or more) of the ignition stimuli meet a critical criterion. To a first order, the general Arrhenius expression provides an illustration of the rate of gas production as a function of temperature and some reactive state, \( f(X) \), of the explosive (e.g., reaction extent, density, concentration of reactive species, available surface area, etc.):

\[
\dot{N} = A \cdot \exp \left( -\frac{E}{RT} \right) \cdot f(X). 
\]  

(2.1)

The product of enthalpy change (per mole converted) and the rate of gas production reveal the rate of heat production:

\[
\dot{Q} = \dot{N} \cdot \Delta h. 
\]  

(2.2)

These expressions illustrate the sensitivity of the process to temperature in the exponential term and the dependence of some reactive state of the explosive. When one (or more) of the listed stimuli is applied with sufficient intensity to raise the temperature to a value where significant heat production occurs, ignition may occur. The specific ignition threshold is crossed when the rate of heat production in a volume exceeds the rate of heat removal from that volume by a heat transport process (conduction, convection, or radiation). For combustion to spread, energy must be fed back from the combustion zone to regions of unreacted material at a sufficient rate to maintain combustion. These are central concepts of ignition and propagation theory and will be discussed throughout the book. As described, ignition and reaction spread arise from the specific interplay of heat transport behavior, reaction kinetics, and the thermodynamics of the involved reactions.

Heat transport theory has played a central role in determining the factors that lead to ignition. The critical conditions for ignition are determined by applying the principle of energy conservation on the stimulated volume, balancing heat production by chemical reaction and heat loss by conduction or convection. In conjunction with carefully constructed experiments, the application of heat transport theory has also provided a tool to help deduce