Strategies for Understanding the Deflagration-to-Detonation Transition

AUTHOR(S): Blaine W Away, LANL, M-8

SUBMITTED TO: Fundamental Physics and Chemistry of Combustion, Initiation, and Detonation of Energetic Materials

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution or to allow others to do so for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.
The deflagration-to-detonation (DDT) phenomenon has been studied for many years. However, no comprehensive model of the DDT process is available. It is important to understand the mechanism by which an explosive will detonate when the source of ignition is a weak shock or flame, and to be able to predict this response. We have identified several key areas of the DDT problem which need to be understood before any such prediction can be made, and have established a modest program to obtain a more fundamental understanding of the behavior of explosive under the conditions that can lead to DDT.
Strategies for Understanding the Deflagration-to-Detonation Transition

Blaine Asay
Explosives Applications, M-8
Los Alamos National Laboratory
DDT, SDT, XDT: What Are They?

• **DDT**: Deflagration to Detonation Transition
  - Source of ignition can be flame, weak shock, or compression
  - Confinement very important
  - Widely used in initiation systems (e.g. detonators)

• **SDT**: Shock to Detonation Transition
  - Source of ignition is typically strong shock
  - Used for main charge initiation

• **XDT**: Unknown(X) to Detonation Transition
  - Source of ignition unknown; occurs during shotgun tests
  - Most likely subset of DDT
Why is DDT of Interest?

- Safety of Stockpile
  - If sympathetic detonation is to occur, it will probably be caused by fragments
  - Donor fragments in credible accident scenarios are too small to cause SDT
  - Therefore, cause of accidents involving weapons will most likely be DDT

- Rocket Motor Accidents

- General High Explosive Safety

Los Alamos
DDT Has Been Studied for Many Years

- Early Theoretical and Fundamental Work
  - Andreev (1944), Kistiakowsky (1948), Macek (1959)

- Navy-Funded Programs on Propellants
  - High Energy Propellant Safety (HEPS), 1975
  - Hazard Assessment of Rocket Propellants (HARP), 1983

- LANL
  - Campbell (1980), McAfee et al. (1989, 1991)

- Extensive Literature- Several Reviews
  - Bernecker (1985), Meilor et al. (1988)

Los Alamos
DDT is Much More Difficult to Study Than SDT.

- Shock Initiation
  - Problem: Initiate detonation by only one mechanism
  - Question: Will shock of certain shape and duration cause initiation?

Los Alamos
DDT is Much More Difficult to Study Than SDT (cont.)

- SDT: Time and Space Scales Typically Well-Defined
  - Times are usually 1-10 μs
  - Distances are usually 1-50 mm

- DDT: Scales Can Vary by Orders of Magnitude
  - Times can range from 1 μs to 100 ms
  - Distances can range from mm to many cm

- Character of DDT Problem Very Different
  - In SDT, waves are supersonic, small confinement dependence
  - In DDT, process begins as subsonic and ends as supersonic, large confinement dependence
DDT Initiation

- Problem: Initiation of detonation is caused by various mechanisms.
- Question: Will a potential source of ignition, when coupled with the necessary damage and the required confinement, cause initiation?

- Ignition can be caused by weak shock, compaction wave, flame, hot fragment, strongly divergent shock, ...
- Damage can take the form of cracks, rubble, granules, deconsolidation, ...
- Sufficient confinement can be supplied by explosive itself, case walls, ...

Los Alamos
DDT Is a Function of Many Variables

- **Particle Size**
  - Small particles contribute large fraction of surface-to-volume, but small fraction of total mass
- **Density**
- **Permeability**
- **Ignitor System**
  - Piston
  - gasless
  - gas producing
- **Length and Diameter**
  - Lengthening of confinement tube caused decrease in transition distance in one case
- **Kinetics/Energetics of Explosive**
- **Temperature**

Los Alamos
These Difficulties Have Important Ramifications

- **Modeling:**
  - Widely varying temporal and spatial scales cause serious problems with choice of mesh size and time step control
  - Equation-of-state information required on fracture behavior, particle size effects, etc.
  - Three-dimensional effects can be significant
  - Regional importance of two-phase treatment

- **Experiments:**
  - Different scales cause serious problems with choice of placement and timing of diagnostics
  - Large number of diagnostics required to observe transition from one stage to another

Los Alamos
Role of Convective Transport

• Convection is Important During Early Phases of DDT

• When and Where it is Important is Unclear

• Must Exercise Caution When Defining Role
  - Results previously ascribed to convective combustion were reevaluated and found to be "completely associated with increasing $P_i$ values [higher shock reactivity] and not with... convective combustion." (Bernecker, 1985)
  - "...descriptions of DDT phenomena which cite 'conductive-to-convective burning... not whole story" (Graham and Sewell)
  - "Convective combustion is a meaningless misnomer... " (HEPS Final Report, 1987)
Role of Convective Transport Not a Trivial Issue

- **Two-Phase Model**
  - Separate conservation equations for each species (with six equations in 1D, eight in 2D, and ten in 3D)
  - Phase interaction terms for mass, momentum, and energy transfer between phases
  - Separate equations of state and constitutive relations for each isolated phase
  - A closure statement for the phase fraction (i.e., the alpha in the P-α relation)
  - The phase quantities are primitive and the mixture quantities are auxiliary
  - The minimum numbers of equations for a two-phase theory (not including the constitutive relations) are seven in 1D, nine in 2D and eleven in 3D. In a 1D model, up to 20 constitutive constants need to be provided.

Los Alamos
Role of Convective Transport Not a Trivial Issue (cont.)

- **Single-Phase Model**
  - Conservation equations for mass, momentum, and energy of the mixture (three equations in 1D, four in 2D and five in 3D)
  - No phase interaction terms
  - An equation of state and a constitutive relation for the mixture
  - A closure statement for phase fraction (the alpha in the P-\(\alpha\) relation). In a rate formulation this accounts for one equation
  - Mixture quantities are primitive
  - The minimum numbers of equations for a single-phase theory (not including constitutive relations) are four in 1D, six in 2D and seven in 3D. In a 1D model perhaps as few as seven constitutive constants need to be provided

Los Alamos
Recommendations from the Literature for Future Studies (Mellor et al.)

- Dynamic and Quasi-Static Compaction for Real and Model Systems
- Permeability Measurements at Higher Re Numbers
- Solid Phase Reaction Kinetics: Slow Heating Tests or Steady State Are Not Applicable. Transient Kinetics a Must (R≠bp^n)
- Study Each Step Separately, Then Merge
- Must Prove Models Against Experiments
- Understand Mechanisms for Damage
- Test Systems With Real, Not Simulated, Damage
- Need More Studies With Simple (Model) Systems
- Use Better Instrumented Tests To Follow Thermochemical Processes: Need To Follow Temperature and Species Concentrations
- Measure All Processes From t=0, Not Just Near Transition

Los Alamos
Program Requirements

- Tightly Coupled Experimental/Modeling Efforts
  - Experiments drive theory and vice versa

- Avoid Unnecessary Complexity
  - Incorporate in model only those quantities that can be experimentally determined (e.g., \( x(t) \))
  - Cannot now measure gas-phase pore pressure, solid pressures, phase interaction parameters, microstructural behavior

- Initially Work on Single, Well-Defined Model System

- Unified Approach- Strong Collaboration

- Final Product is Predictive Model

Los Alamos
Major Thrust Areas Were Defined

- **Fundamental Studies**
  - Burn rate as function of porosity and pressure, shock acceleration
  - Shock formation in porous systems, coalescence of stress waves
  - Compaction behavior, low levels of reaction
  - Gap and wedge test data at low pressures
  - Ignition front, permeability, role of convective transfer

- **Applied Studies**
  - Bullet impact
  - Sympathetic detonation

- **Theory/Modeling**
  - Evaluation of complexity required and existing models
  - Equation-of-state

Los Alamos