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TITLE: Strategies for Understanding the Deflagration-to-Detonation Transition

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MASTER

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Strategies for Understanding the Deflagration-to-Detonation Transition

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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.

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DDT, SDT, XDT: What Are They?

- **DDT: D**eflagration to **D**etonation **T**ransition
  - Source of ignition can be flame, weak shock, or compression
  - Confinement very important
  - Widely used in initiation systems (e.g. detonators)

- **SDT: S**hock to **D**etonation **T**ransition
  - Source of ignition is typically strong shock
  - Used for main charge initiation

- **XDT:** Unknown(**X**) to **D**etonation **T**ransition
  - 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**

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 Assesment of Rocket Propellants (HARP), 1983

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

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

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?

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

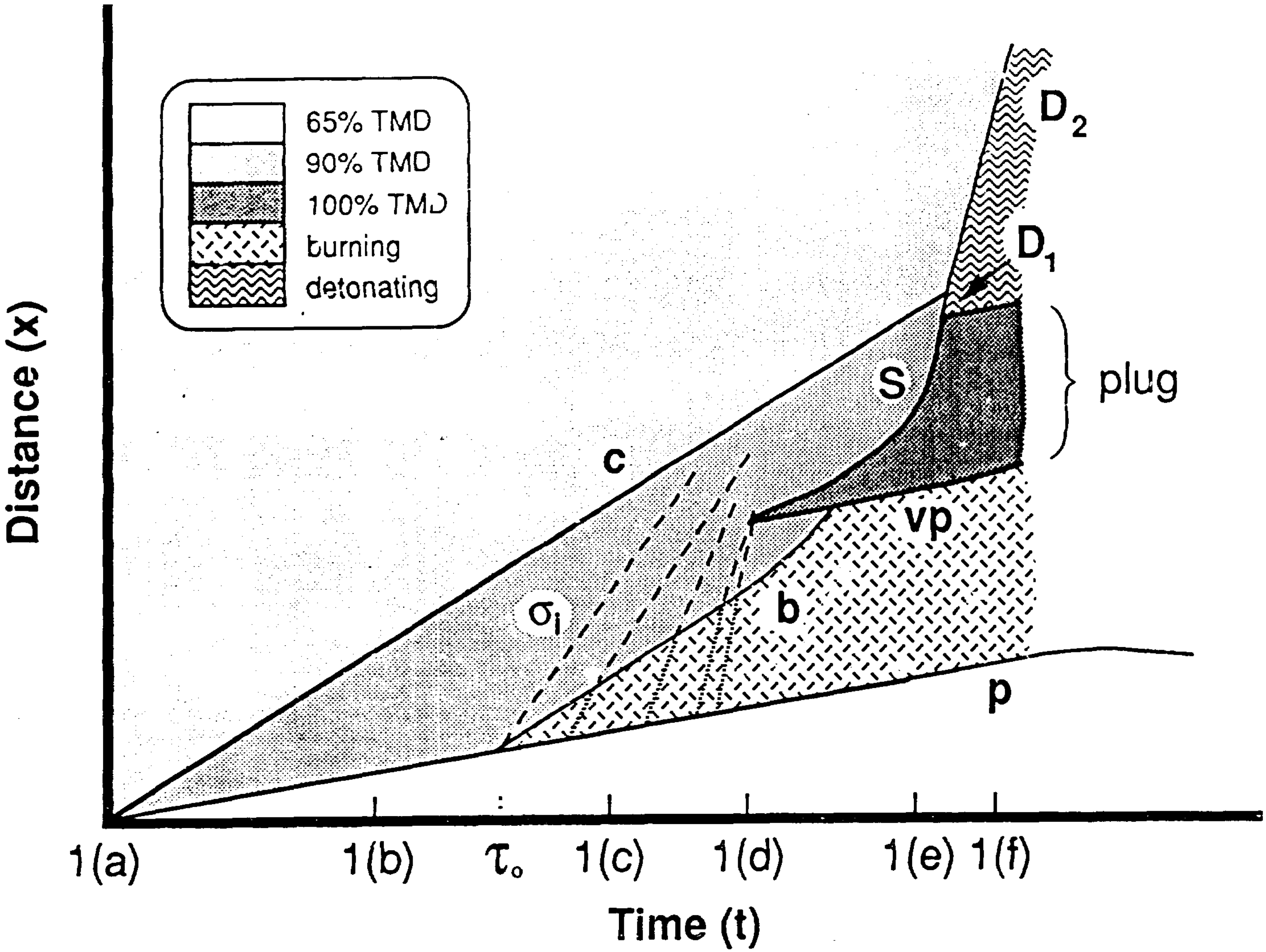
- **Character of DDT Problem Very Different**
  - In SDT, waves are supersonic, small confinement dependence
  - In DDT, process begins as subsonic and ends as supersonic, large confinement dependence

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

- **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, ...



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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**

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

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.

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 -α 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

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 ($R \neq bp^n$)
- 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

Program Requirements

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

- **Avoid Unnessary 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, microstuctural behavior

- **Initially Work on Single, Well-Defined Model System**

- **Unified Approach- Strong Collaboration**

- **Final Product is Predictive Model**

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