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PROGRESS ON COMBUSTION MECHANISMS OF SOLID PROPELLANTS

N00014-89-J-1923

October 1991 - March 1992

E. W. Price

The goal of this project is to determine the mechanisms that control the combustion of heterogeneous solid propellants, with particular emphasis on propellants with new ingredients. The principal methods include: a) laser pyrolysis of ingredients to determine decomposition behavior of a surface heated at the high rates characteristic of propellant burning (10^5 ° C/sec); b) measurement of the burning of two-dimensional propellants (sandwiches of oxidizer and binder); c) experimental and computational studies of the leading edge portion of the gas phase oxidizer-fuel flame; and d) combination of the results into both phenomenological and rigorous computational models for steady and nonsteady burning of heterogeneous solids (propellants). A short term goal is to gain early characterization of the combustion behavior of several new energetic ingredients such as NMMO, CL-20 and ADN.

The status of the phases a - d in October 1991 was as follows:

a) The CO₂ laser pyrolysis facility was operational (Ref. 1,2), but in only limited use because of staff shortage due to funding shortage.

b) The studies of sandwich burning have progressed to evaluation of several binders, several catalysts (Ref. 2,3), and of inclusion of fine particulate AP in the binder lamina (with AP oxidizer laminae). The results have led to clarification of the dominant steps in combustion, and focussed attention on the importance of the leading edge portion of the O-F flamelets. The results with particulate AP in the binder have shown a suspected strong dependence of the qualitative nature of the O-F flame on oxidizer particle size (Ref. 4,5,6).

c) The studies of the gas phase O-F flame included a 2-D gas burner experiment that established the qualitative nature of the LEF (leading edge portion of the diffusion flame), including quantitative data on the flame location, heat release rate and temperature fields (using an air-methane flame). The computational phase (funded primarily by an IR&D contract from Thiokol) led to a computer program for 2-D, laminar flame (steady and nonsteady) (See Ref. 8,9). The program was used to compute the flame for air-methane for comparison with the

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experimental study. Results compared favorably at the qualitative level, and the computational results explained some unexpected results of the experimental study (See Ref. 10).

d) Progress in modeling of propellant combustion was confined to activities in a) - c) to clarify what aspects of the combustion process would have to be included, and to the modeling of the leading edge flame described in c). The convergence of these results is summarized in Ref. 10 and 11. Participation continued in Workshops aimed at achieving the goal of rigorous modeling of propellant combustion, in which the contributions of other investigators are dominated by research on chemical kinetics. In addition to that major area, several other areas need advances to achieve the goal of rational prediction of propellant combustion, e.g.,

- (i) Clarification and modeling of the physiochemistry of surface pyrolysis, in which condensed and vapor phase co-exist as a froth.
- (ii) Quantitative description of the passage, and effective velocity of a burning front in a heterogeneous solid, and how it depends on ingredient characteristics (for steady state burning).
- (iii) Detailed description of the combustion zone and burning surface (for use in calculating nonsteady burning and gas flow effects on rate).
- (iv) Advances in computational methods to reduce costs of rigorous description of combustion.
- (v) Development of phenomenological models of combustion (using both experimental and rigorous computational results) that are simple enough for engineering applications.

Progress during October 1991 - March 1992 is as follows:

a) Sandwich burning studies were started on particle-filled binder laminae between AP laminae in which the binders were PBAN, BAMO-THF, and NMMO and the particles were HMX and CL-20. The objective is to exploit the earlier sandwich burning results to learn something about the combustion behavior of new ingredients (and combinations) that are

available in such limited amounts that propellant combustion studies are limited. Preliminary results are encouraging (Fig. 1, 2), but there are problems with obtaining suitable and comparable particle sizes of different ingredients (e.g., Fig. 3 of ADN). As a further objective, consideration is being given to replacing the dry-pressed AP laminae with other oxidizers. However, this requires substantially more of the new ingredient, and requires barricading the press because of unevaluated hazard.

A parallel effort is in progress involving AP-PBAN sandwiches with both particulate AP and burning rate catalyst in the binder lamina (this supplements earlier studies with AP and catalyst added separately). The objective is to determine how the catalyst affects the combustion of small AP particles in the fuel-rich binder lamina. This is a critical issue because of the earlier finding that fine particles do not sustain individual diffusion flames at lower pressures (without catalyst), a property that affects both steady and nonsteady combustion in sandwiches (Ref. 6) and bimodal propellants (Ref. 5).

b) Rigorous computer modeling of the 2-D combustion problem has continued with the goals of

- (i) "speeding up" the computations,
- (ii) extending to chemical combinations more related to propellants,
- (iii) exploring the feasibility of obtaining oscillatory solutions,
- (iv) extending the computer program to encompass both gas and condensed phase.

These are all daunting goals that are approached incrementally. We have run the computer code with only one dimension, looking at the chemical reaction scheme of Guirao and Williams for AP. The results were not in satisfactory agreement with experimental data on AP self deflagration. We have worked on incorporation of adaptive gridding, but are not yet operational. We have compared results with different assumptions regarding the set of primary reactions (air methane, steady state). We have examined the effects of flow rate, of diluent concentration, and of fuel lamina thickness (air, methane, relatively complete kinetics). These latter results are being used to evaluate phenomenological models, and have been used to help understand results of the gas burner tests.

The most conspicuous result of the combination of the computational results and

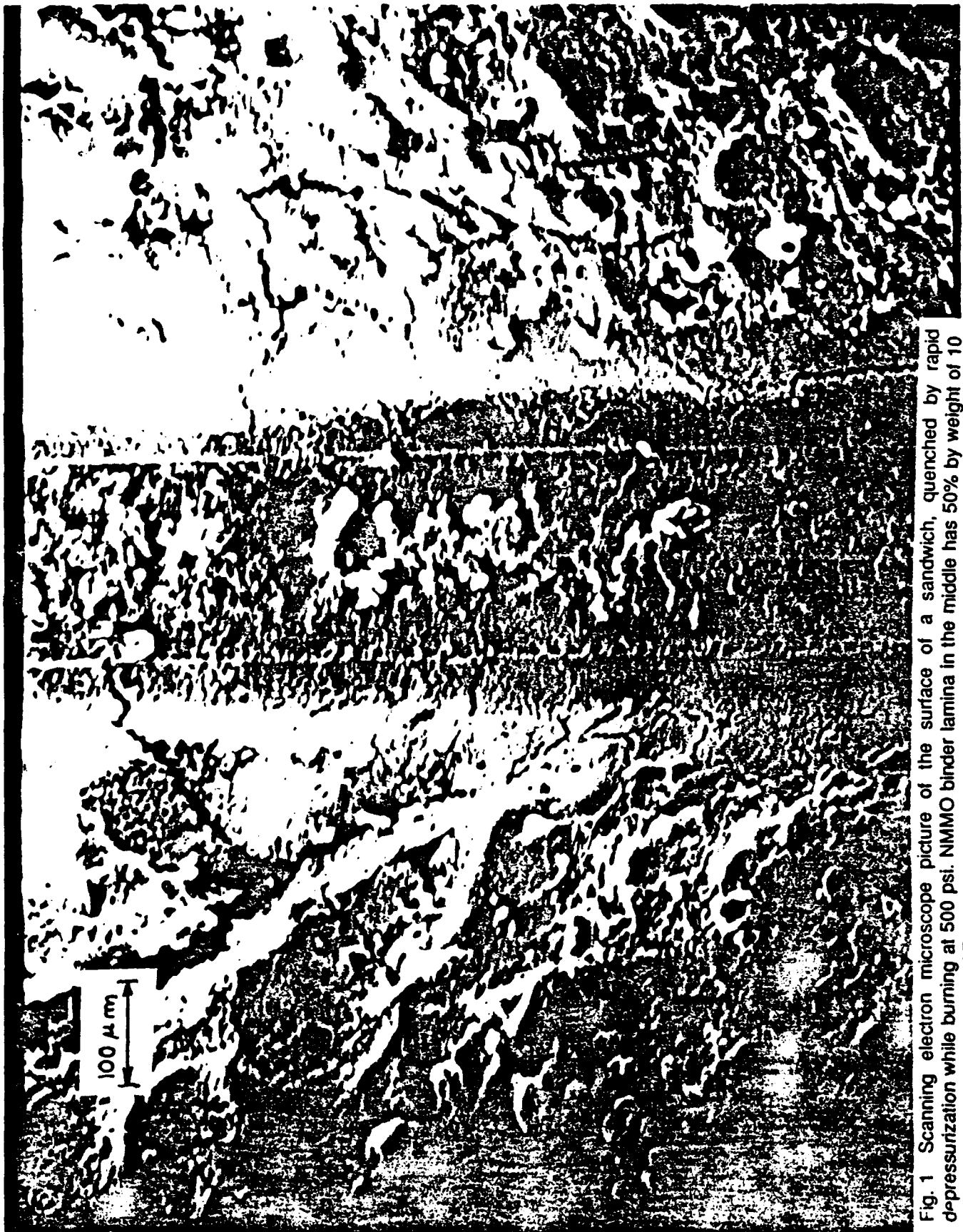


Fig. 1 Scanning electron microscope picture of the surface of a sandwich, quenched by rapid depressurization while burning at 500 psi. NMMO binder lamina in the middle has 50% by weight of 10 μm HMX. Outer laminae are AP.



Fig. 2 Similar to Fig. 1, but binder lamina has 80 μm CL-20 instead of HMX.



Fig. 3 Scanning electron microscope picture of an as-received particle of ADN.

experimental results was the observation of very high flame speeds in the LEF (up to 3 times the speed of a planar premixed flame of the same temperature). The computational results showed that this would be expected, and is due to flow divergence and slowing due to a small pressure peak at the location of the LEF due to extremely high heat release rate.

c) Work has begun on development of a phenomenological model of leading edge flames, using the gas burner results as an intuitive guide and means of validation, and using progressive reduction of the rigorous model as a guide to simpler models and as a means to systematically test the effect of assumptions.

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