PREFACE

Great challenges still exist in the area of propellant and combustion research 100 years after the passing of Alfred B. Nobel, who deserves to be called the "father of propellant science." Among Nobel's many breakthroughs and patented inventions, his development of ballistite, the first double-base propellant, has had a profound and lasting impact upon the propellant field. To commemorate Nobel's pioneering and innovative contributions to the development of explosives, pyrotechnics, and propellants, the Fourth International Symposium on Special Topics in Chemical Propulsion: *Challenges in Propellants and Combustion 100 Years After Nobel*, was held in Stockholm, Sweden, from the 27th through the 31st of May, 1996. The Symposium highlighted the substantial advancements made in propellant and combustion science during the last several decades, and also allowed for the exchange of information about current and future developments and research topics.

The International Symposium had several major objectives. These were: 1) to promote communication between researchers, designers, and manufacturers regarding state-of-the-art approaches in the field of propellants and combustion; 2) to discuss new and improved safety techniques in the combustion of energetic materials; and 3) to recommend future directions for research in combustion and chemical reaction systems. The Symposium also addressed several pressing global issues: a) the resolution of environmental issues in the combustion of energetic materials; b) the need for economical utilization of finite fuel resources; c) the production of power using existing or newly synthesized energetic materials; and d) the development of adequate techniques for disposal of surplus propellants and explosives for demilitarization purposes.

The Symposium was attended by 167 participants from 21 countries. In total, there were 127 technical papers, including 83 oral presentations and 44 poster papers. Of these, 100 (including the historical lecture on Nobel) were selected for publication in this edited book. All papers were reviewed using the same comprehensive procedures employed by respected journals in this field. Therefore, this volume should be considered an edited book of carefully reviewed and selected technical papers, rather than a collection of Symposium proceedings. The recent advances, future directions, and special challenges in each of the eight technical areas covered in this book are described below.

Area 1: Chemical Kinetics of Propellant Combustion. Major advancements have been made in the past decade in the use of detailed kinetics to model the combustion processes of various energetic materials. Incorporation of elementary reactions with specific rate constants is a common practice in the simulation of gas-phase reaction processes. The determination of rate constants for many elementary reactions between fragmented and decomposed species from propellant ingredients is a major task for propellant chemists. For the condensed phase, the diagnostics are much more limited than those for the gas phase. Theories for condensed phase reactions contain many more uncertainties. As kinetics for both the gaseous and condensed phases become available, it may be possible to understand and control transient events, such as ignition and combustion instability, at the molecular level.

Area 2: Environmental Considerations in Combustion of Solid and Liquid Propellants. Significant progress has been made towards the modeling of combustion products and phenomena which may affect the environment at both the ground and atmospheric levels. In many cases, the practical solution to combustion-related environmental hazards has been to design propellants in such a way as to avoid the generation of ecologically harmful ingredients. This is usually not a simple matter, as the formulator must identify substitute ingredients which not only create no hazardous products themselves, but also possess the chemical and physical properties necessary to deliver the required performance. The most serious concern in recent years, the generation of hydrochloric acid (HCl) by solid propellants, has been lessened by the partial substitution of either nitramine crystals (HMX or RDX) or ammonium nitrate for ammonium perchlorate crystals. In both cases, the generation of HCl has been significantly reduced, but these substitutions result in greater production of NO_2, which is thought to be of comparable toxicity to HCl. The task confronting "environmentally-minded" propellant designers is indeed challenging, since a favorable balance of performance and environmental safety cannot be easily achieved.

Area 3: Recycling of Energetic Materials. Since the end of the Cold War, disarmament of nuclear and conventional munitions has produced hundreds of millions of pounds of surplus propellants, explosives, and pyrotechnics worldwide. Historically, surplus energetic materials have been disposed of by open burning/open detonation (OB/OD). The disposal of these materials by OB/OD is becoming unacceptable due to public concerns and increasingly stringent environmental regulations. The proposed recycling of energetic materials as chemical feedstocks for the production of higher value chemicals potentially represents a "win-win" situation, since liabilities (surplus munitions) are converted to assets (useful products), sparing the environment the burden of present destructive disposal practices. The recycling of energetic materials will also play an important role in the formulation of new propellants and explosives. The goal is to demonstrate that pollution from the destruction of surplus propellants can be reduced by as much as 90% using life-cycle assessment methodologies and suitable recycling technologies.

Area 4: New Techniques and Improved Safety in Combustion of Energetic Materials. Due to demilitarization and the extension of lives of propulsion systems, the study of hazards and safety of energetic materials has become more important during the past decade. The ignition, decomposition, and mechanical damage of energetic materials can result in hazards such as explosions, deflagration-to-detonation transition (DDT), cook-off, and delayed detonation by unknown mechanisms (XDT). Incidents caused by these hazards have resulted in the loss of lives and the destruction of billions of dollars worth of propulsion equipment. The international community has performed significant research in the areas of DDT, XDT, cook-off, decomposition, ignition, electrostatic discharge, combustion and damage-induced reactions. These studies are intended to improve, mitigate and predict the overall safety of various propulsion systems. In order to reduce the probability of system hazards, future trends in the development of propulsion systems should incorporate design considerations for mechanical protection and thermal insulation of new and existing devices.

Area 5: Commercial Application in the Combustion of Energetic Materials. The advent of airbag technology and the widespread popularization of fireworks displays in many countries has led to an increase in the commercial use of propellants and pyrotechnics. The public's awareness of the use of such energetic materials has grown significantly with these and other commercial applications. In private industry, however, there is a lack of communication about important technological problems, largely due to the perceived need for corporate secrecy. One solution is to increase cooperation between academic institutes and industry, so that program managers and engineers in private industry will become more aware of the potential of advanced technologies, related background research, and the benefits of information exchange.

Area 6: Ignition and Combustion Performance of Propellants for Rocket Propulsion. Knowledge of the performance of propellants and their ingredients is very important for the proper design and utilization of chemical rocket propulsion technologies. Current and near-future trends in this area include: a) further characterization of propellants using new energetic ingredients, such as ADN, CL-20, BAMO, GAP, and Alex (ultra-fine aluminum particles made by plasma explosion processes); b) extension of theoretical models to simulate combustion processes of propellants containing these new ingredients; c) further modification of models for simulation of the combustion and agglomeration of aluminum additives in solid propellants; d) development of more reliable models for the study of dynamic and unstable burning phenomena of solid propellants; e) extension of boundary-layer type of erosive burning models to include propellants containing new ingredients; f) the use of PolyNIMMO (3-Nitratomethyl-3-methyloxetane) polymer as an energetic binder in ramrocket gas-generator propellants; and g) the effect of chemically induced stresses on the ignition and combustion of solid propellants.

Area 7: Combustion Diagnostics. The development of new diagnostic techniques and the utilization of existing advanced instruments for the study of propellant flames and combustion phenomena in motors and engines continue to challenge the combustion community. Propellant flames often involve short residence times, large temperature and species concentration gradients in both condensed and gas phases, high pressures, and elevated temperatures. The data obtained from intrusive and non-intrusive techniques are crucial for several reasons. First, it is desirable to acquire a thorough fundamental understanding of the combustion behavior of energetic materials through in-depth data interpretation and mechanistic studies. Second, efforts at several institutions in the U.S. and abroad are underway to develop and validate comprehensive models describing the complex processes of heat transfer and finite-rate chemical kinetics during ignition and steady deflagration of energetic materials. To validate such models, data from carefully conducted experiments are needed for a broad range of test conditions. Recent advances and applications of non-intrusive diagnostic methods include multi-channel IR, tunable laser, UV/visible and X-ray absorption spectroscopy, and CARS and LIF spectroscopic techniques.

Area 8: Theoretical Modeling and Numerical Simulation of Combustion Processes of Energetic Materials. With the advent of the digital computer, the numerical simulation of physicochemical processes has become increasingly important in the design of combustion systems and prediction of combustion processes. The increased reliance upon computer-based predictions in design is largely the result of economic pressures. Not only is numerical simulation more economical than experimentation, but also the cost of performing a given calculation has decreased significantly over the years. This is mainly due to tremendous increases in computer speed and memory capacity with limited increases in overall computer costs. Numerical CFD simulations involving full sets of chemical reactions have now become possible. Whenever it is presently not economical or practical to utilize full numerical simulation free of empiricism, phenomenological models have been adopted to make possible numerical predictions of complex processes in various combustion devices. Therefore, modeling and numerical simulation are indispensable to the prediction of combustion processes of energetic materials.

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Symposium Chairman
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