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International Workshop

on

**MATHEMATICAL METHODS IN COMBUSTION**

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Final Technical Report

written by

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NOMENCLATURE

A	= nondim. function used in frequency response function theory
B	= nondim. function used in frequency response function theory
c	= specific heat, cal/g K
$E_{( )}$	= activation energy, cal/mole
$E_{( )}$	= $E_{( )}/R/T_{( )}$ , nondimensional activation energy
k	= thermal conductivity, cal/cm s K; also: ZN parameter (see section 9)
m	= mass burning rate, g/cm <sup>2</sup> s
n	= ballistic or pressure exponent in the steady-state burning rate law
$n_s$	= pressure exponent in the surface pyrolysis law
p	= pressure, atm
q	= energy flux intensity, cal/cm <sup>2</sup> s
Q	= heat release, cal/g (positive exothermic)
r	= ZN parameter (see section 9)
$r_b$	= burning rate, cm/s
R	= universal gas constant; 1.987 cal/mol K or 82.1 atm cm <sup>3</sup> /mol K
$R_p$	= propellant response to pressure fluctuations, nondimensional
$R_q$	= propellant response to external radiation fluctuations, nondimensional
t	= time coordinate, s
T	= temperature, K
$T_0$	= initial sample temperature, K
x	= space coordinate, cm

Greek symbols

$\alpha$	= thermal diffusivity, cm <sup>2</sup> /s
$\delta$	= ZN parameter (see section 9)
$\lambda$	= wavelength, $\mu$ m
$\mu$	= ZN parameter (see section 9)
$\nu$	= frequency, Hz; also: ZN parameter (see section 9)
$\rho$	= density, g/cm <sup>3</sup>
$\sigma_p$	= burning rate temperature sensitivity, 1/K
$\omega$	= $2\pi\nu$ , circular frequency, rad/s
$\Omega$	= $\omega \cdot \alpha_c / \bar{r}_b^2$ , nondimensional circular frequency

Subscripts and superscripts

c	= condensed-phase
g	= gas-phase
p	= pressure
q	= radiation
s	= burning surface
-	= steady-state value

Abbreviations

AP	= Ammonium Perchlorate (NH <sub>4</sub> ClO <sub>4</sub> )
BDP	= Beckstead-Derr-Price
DB	= Double-Base
FM	= Flame Modeling method
KTSS	= Krier-T'ien-Sirignano-Summerfield transient flame model
PDL	= Pressure Deflagration Limit
PU	= PolyUrethanes
QSHOD	= Quasi-Steady Homogeneous One-Dimensional
TF	= Transfer Function
ZN	= Zeldovich-Novozhilov method

### 1. TECHNICAL PROGRAM

The final program of the Workshop and list of participants is attached. Xerox copies of most presentations are available and were distributed to registered participants. In this final report, summarizing statements and basic discussions on specific topics are treated. References are mainly made to papers presented at this Workshop, but other papers from the open literature are mentioned when necessary.

### 2. BACKGROUND OF WORKSHOP

Combustion problems offer excellent opportunities to develop both analytic tools and numerical methods. But too often the two worlds interact only superficially. Mathematicians do not regard working on the needs from real world as professionally rewarding, while computer practitioners and engineers consider possible contributions from mathematicians too abstract, if not just useless. Both judgments are biased and this does not lead to productive interactions.

### 3. OBJECTIVES OF WORKSHOP

The overall objective of the Workshop was to try to improve communications and promote cross-fertilizations between applied mathematicians and computational scientists, by pointing out promising directions as well as effective means of interaction. Specific objectives of the Workshop were to critically compare analytic to numerical approaches, assess potentials and limitations of both, and hopefully foster new developments in combustion. To this end, a proper mix of formal lectures, specialized presentations, informal discussions, and constructive cross-criticism was implemented.

### 4. TOPICS SELECTED FOR DISCUSSIONS

The specific topics considered for discussions in this Final Technical Report on the Workshop are:

1. Synergism between analytic and numerical methods;
2. Numerical simulations and limitations;
3. Solid propellant combustion (as an example of problem).

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## 5. DISCUSSION PANEL

This Final Technical Report has been edited by the main investigator based on written inputs received by all co-authors and on discussions, held after the Workshop, mainly with Dr. E.S. Oran (Naval Research Laboratory, Washington, USA), Prof. M.Q. Brewster (Illinois University at Urbana-Champaign, USA), Prof. Novozhilov (Russian Academy of Sciences, Moscow, Russia), Prof. M.Kh. Strelets (State Institute of Applied Chemistry, Saint Petersburg, Russia), and Prof. V.E. Zarko (Russian Academy of Sciences, Novosibirsk, Russia).

## 6. SYNERGISM BETWEEN ANALYTIC AND NUMERICAL METHODS

In principle, analytic methods are applied at the initial stages of investigations of combustion problems. Further investigations to determine details of solutions are often performed by numerical methods. Thus, synergism between analytic and numerical methods plays an important role in combustion and sciences in general. However, problems of communications and mental attitude exist between the combustion theoreticians using analytic and numerical approaches. From the point of view of numerical scientists, a notable resistance was felt from traditional scientists to accept computer simulation as a tool for studying combustion. Historically, this is understandable since combustion is a relatively old discipline, in contrast for example with plasma physics which grew up with computers. While in the US this resistance has been slowly disappearing during last few years, in other countries traditional approaches still prevail.

In any event, real problems are too difficult for all combustion scientists and thus they should be strongly encouraged to use all weapons available from their arsenal to attack a given problem. Computational tools should be well integrated with analytic tools. Both methods seek approximations to the full solution, since explicit and exact solutions are only rarely available. Both methods provide different yet useful sorts of information to formulations of the problem less complex than the full problem. Numerical methods require a computational grid but provide complete knowledge about a discrete set of points, while analytic methods involve limiting cases or critical values of a parameter but provide parameter dependence. Synergism between the two approaches allows scientists to get more than just the sum of the two individual parts, and this is felt to be a key factor for future perspectives in sciences and engineering.

Papers properly exploiting the potential of this synergism were presented at the Workshop by Matkowsky on gasless combustion, Merzhanov on a variety of combustion problems ranging from thermal explosions to burning of heterogeneous systems, De Luca on solid propellant combustion, Oran on several reactive fluid dynamics problems, and others.



Another area of interaction is that of using analytic methods to improve numerical methods. This was mentioned by several speakers, but particularly emphasized by Matkowsky and Oran. Some examples of synergism include: how to optimize computational points, how to optimize numerical time steps, or even how to incorporate a Riemann solution into a solution of the coupled compressible continuity equation. This area is within the province of the computational scientist.

A third area of interaction concerns the use of an analytic solution as a benchmark, validation or a starting point for a simulation. This is perhaps the starting place for synergism between the computational scientist and traditional analyst. Such an interaction usually teaches everyone something: the computational scientist learns to use the computer program and the analyst learns more about the limits of validity of the theory.

Probably a less common idea, although one that is growing in recognition of what it can do, is to use a result from a simulation as a starting point for analysis of a system. In this sense, the simulation either produces a new phenomenon which may be further explained or whose existence can be justified by analysis or produces a data set that can be analyzed, much like an experiment. An example of the former is the unreacted pockets of material cut off by the interaction of transverse waves behind propagating detonations (see presentation by Oran). An example of the latter would be to use a computationally generated data set from a calculation of a mixing layer to look for attractors, chaos, or long-term mixing trends. An advantage here is that the computational data is relatively clean with conditions that are more controlled than what an experiment can produce.

With specific respect to this classical issue of analysis vs computation, Matkowsky remarked in the closure session of the Workshop that the enemy of computation is not analysis, and the enemy of analysis is not computation, but rather the enemy of both is the problem. Oran proposed to modify somewhat this statement: the problem is the challenge of both camps, and the enemy is our own limitation and mental rigidity. With these thoughts in mind, cooperation is worthwhile and stimulating for practitioners of both mathematical approaches; in combustion often synergism is already an accepted reality (see next section).

## 7. NUMERICAL SIMULATIONS IN COMBUSTION

Nine lectures were devoted to both the development of new numerical approaches and their application to combustion processes simulation. When analyzing the topics and contents of these lectures, two distinct features emerge, as revealed by the plenary lecture on "Limitations and Potentials of Numerical Methods for Simulating Combustion" given by Oran.

The first striking feature concerns the synergism, very promising and already progressing in combustion, between analytic and numerical approaches. This was the unifying theme of the Workshop and is discussed in Section 6.

The second striking feature concerns the fast increase of both computer capabilities and efficiency of numerical methods, an observation made in several presentations. This provides new qualitative possibilities to scientific and industrial users, permitting them to solve complicated, "real life" combustion problems involving multistage chemical kinetics, multi-dimensional fluid dynamics, and their interaction. Examples of such computations were given by Oran; Shur; De Michele, Pasini, and Tozzi; and Heiser.

New efficient numerical algorithms for simulation of combustion and detonation processes were presented by Di Blasi; Nekhamkina and Strelets; and Valorani and Di Giacinto. An original idea to describe chemical source terms in finite-difference schemes was presented by Continillo and Baruffo.

## 8. NUMERICAL LIMITATIONS

Consider the question of limitations of computational methods. The current limits are dictated by the: 1) computer speed and available memory, 2) algorithm efficiency, and 3) input data. In everything we do there are tradeoffs and balances. Concerning numerical limitations, the particular tradeoffs and balances depend very much on the problem being addressed.

Consider first the issue of computer speed and memory. The limits now are gigaflops and gigabytes, respectively, and this is increasing dramatically to the point where teraflops computers are expected in the next few years. Important conceptual breakthroughs that will allow this are parallel processing with distributed memories. Such computers make possible the direct numerical simulation of turbulent reacting flows, albeit in rather simplified geometries, or transient flows over complete airplanes. Even though not everyone has such computers available, the raw computational power generally attainable on a desktop is also exponentially increasing.

Algorithmic efficiency involves tradeoffs between such qualities as accuracy, speed, and robustness. This is very problem dependent and the balances can change quickly. What is optional for today's computers is not necessarily optimal for tomorrow.

Input data can always be a problem. Often it is not available in the form we need in a computation or we do not know the values in the right parameter regime. In such cases, we can use theoretical values, extrapolate experimental values, or simply guess and use the computation to determine reasonable ranges of values. This area requires constant interaction with experiments or more fundamental theories.

Finally, Oran draws the attention on a forefront area in numerical simulation, and that is the problem of treating complex geometries with moving bodies. The dream is to have simple, rectilinear structural grids with simple, vectorizable and parallelizable algorithms, that can accurately treat a problem as difficult as a manta ray moving through water (flexible body).

Unstructured, triangular or tetrahedral grids perhaps have optimal flexibility but are not easy to use or well suited to parallel computing. Hexahedral block-structured grids allow only moderately complex geometries but intrinsically have problems at corners and with distortions. New developments in globally structured rectilinear grids have the promise of being the most accurate and most suitable to parallel computations. However, they represent a back-step to less complexity that is often hard to accept, and they require some further development.

In summary and with respect to the limits of computation, these vary from problem type to problem type. However, over the last five years, the increase in scientific abilities to simulate flames, detonations, and reacting turbulent flows is enormous and has every promise of continuing to increase in such a dramatic fashion. This growth is accomplished by combining advances from many fields, ranging from experimental determination of input data (e.g., chemical rates) to advances in numerical algorithms, to advances in computers, and to advances in diagnostics (e.g., visualization).

## 9. SOLID PROPELLANT COMBUSTION

The following is an extract of the Final Technical Report (De Luca et al., 1990) on a previous Workshop held in Milan, Italy, 12-14 Nov 90, which was a convenient starting point for this specific theme at this Workshop.

"The most fully developed and utilized mathematical models employ a one-dimensional approximation that is rigorously applicable only to propellants that are homogeneous and burn with geometrically stable planar surfaces. It is also widely assumed that the dynamic response of the gas phase is quasi-steady. Within these assumptions, there are two independent approaches to analysis referred to here as the Zeldovich-Novozhilov (ZN) and the Flame Modeling (FM) approaches.

For quasi-steady gas phase, the basic assumptions and results of the approaches are the same. In principle, ZN is quicker while FM, being more complex, is also more informative. However, for fully transient burning, the gas phase has to be explicitly taken into account and, therefore, only FM can be implemented. ... "

The specific set of assumptions mentioned above is collectively referred to as the QSHOD assumptions. See Novozhilov, 1992 and Price, 1992 for a complete discussion on respectively ZN approach and QSHOD assumptions.

### 9.1 Nonlinear Modeling as an Example of Synergism

Several research groups developed nonlinear models (along numerical and sometimes analytic guidelines) of unsteady solid propellant combustion under a variety of assumptions, but primarily the QSHOD assumptions. The Italian group has focussed on the FM approach and its connections with ZN, while the US and Russian groups have thus far used the ZN approach. Some extension to consider in-depth (distributed) condensed phase reactions has also been reported.

Within the QSHOD framework, the Italian group performed a complete analysis of transient burning and combustion stability by properly combining analytic and numerical methods. The stability analysis requires the steady-state temperature profile corresponding to a given set of operating conditions to be explicitly known (static or uncoupled stability); in the case of a forced transition between two different sets of operating conditions, both the initial and final steady-state temperature profiles need to be explicitly known (dynamic or transitional or coupled stability). A first application of synergism lies right here: analytic methods conveniently provide steady thermal profiles only for the simplest configurations (for example, temperature - independent thermophysical properties), while numerical methods in principle can furnish any kind of thermal profile. It can be noted in this respect that the wanted steady thermal profile can also be obtained by experimental means and then mathematically described by any convenient approach. This stresses the possibility, and convenience, of a "full" synergism among analytic, numerical, and experimental techniques at least at this point of the whole procedure.

An integral analytic technique is then applied to the steady thermal profiles obtained either analytically or numerically. This technique implies the evaluation of a disturbance thermal layer thickness propagating in time and of the temperature just at the edge of this layer. Another form of synergism can be seen here: either analytic or numerical methods are applied according to the kind of steady thermal profile. An analytically defined function, called static restoring function, is then evaluated mainly by numerical means but resorting to analytic means when singularities are met. From this function, bifurcation diagrams are obtained for a wide range of operating conditions and for real world solid propellants. By cross-plotting bifurcation diagrams, stability diagrams are found for the wanted propellant and set of operating conditions.

The final results of this nonlinear transient burning and stability analysis can be checked by analytic techniques (mainly for uncoupled stability problems), numerical techniques (mainly for coupled stability problems), experimental techniques, or any combination of them. The point here is that a synergistic approach yields richer results and allows information to flow from one domain to another, thus permitting a constructive interaction and continuous improvement. Likewise, validation of a synergistic approach allows different techniques to be implemented, compared, and improved. It is underlined that the above analysis could not be carried out for any realistic application without a numerical support, and viceversa the numerical side would only be simulative without the analytic support.

Representative results reported at the Workshop (see the presentation by Pagani, Verri, and Salsa and that by De Luca) include "isolas" of stability, several bifurcation phenomena, existence and multiplicity of steady-state solutions, frequency of self-sustained oscillatory solutions, and so on. In particular, the complex interplay of diabaticity (positive or negative) of the burning sample with pressure (or any other operating condition) would be very cumbersome to understand by either numerical or experimental means. The variety of situations possibly arising from nonadiabatic and nonlinear burning is just too wide and too sensitive to initial conditions to be fully understood without a unifying interpretation. This can solely be provided through an analytic viewpoint.

An example is the behavior of a solid propellant burning, with different levels of diabaticity, near its pressure deflagration limit (PDL). This is a problem of static or uncoupled stability. The sheer existence of a PDL is experimentally known since 40 years; a computer simulation can detect but not explain the occurrence of a PDL; several analytic approaches attempted in the past could not justify the presence of a PDL. The combined analysis of PDL by analytic, numerical, and experimental means prompted the idea that PDL is reached when the self-sustained oscillatory solution, in turn triggered for decreasing pressure as an Hopf bifurcation, loses its stability. The frequency of the self-sustained oscillatory burning can be evaluated analytically, while its amplitude can be measured by numerical tests; by experimental means one can easily verify only frequencies. For diabaticity different from zero, the above picture is further complicated by: 1) the presence of a second, unstable steady-state solution for heat loss less than a critical value; 2) no steady-state solution for heat loss larger than this critical value; 3) one steady-state solution for heat input (of different nature for different values of heat input); 4) stable steady-state self-sustained oscillatory burning for heat input and pressure below some critical value; 5) stable steady-state time-invariant burning for heat input and pressure above this critical value. Details about this complex behavior were reported at the Workshop. The point here is simply that it would be very difficult to discriminate all of these overlapping trends without a well coordinated analytic and numerical efforts (synergism).

Another example is the dynamic extinction limit found when fast transients are imposed between two otherwise stable, time-invariant steady-state burning solutions. This is a problem of dynamic or transitional or coupled stability. The above nonlinear stability analysis is able to detect a critical value of burning rate under which extinction necessarily follows for monotonically decreasing pressure (for example), whereas numerical computations or experimental tests can only indirectly perceive the existence of this limiting value. This critical value corresponds to an unstable root of the perturbed energy equation. On the other hand, numerical computations can only prove the unstable or "repulsive" nature of this critical value of burning rate; even experimental methods are of marginal help in this instance, since unstable configurations cannot be directly observed. Again, the combined use of analytic, numerical, and experimental techniques allows a full understanding of phenomena otherwise intractable or at least puzzling by separate implementation of standard investigation techniques.

Other specific advances and developments in mathematical modeling of solid propellant combustion, which were reported at this Workshop, are summarized briefly. Although not discussed for a matter of space, different forms of synergism can be exploited for the following problems as well.

## 9.2 Equivalence of Linearized, Pressure-Driven ZN and FM Descriptions

Under the QSHOD assumptions, the ZN and FM descriptions of linearized, pressure-driven unsteady propellant combustion have previously been described as being equivalent within a somewhat limited scope of the descriptions (King, 1980; T'ien, 1984; De Luca et al., 1990; Beckstead, 1991). A more complete equivalence was shown (Son and Brewster, 1992) by formal extension to the 4th and last parameter in the descriptions (the Jacobian parameter in ZN) as follows:

$$A \text{ [FM nomenclature]} = \frac{k}{r} \text{ [ZN nomenclature]}$$

$$B \text{ [FM nomenclature]} = \frac{1}{k} \text{ [ZN nomenclature]}$$

$$n \text{ [FM nomenclature]} = \nu \text{ [ZN nomenclature]}$$

$$n_s \text{ [FM nomenclature]} = \frac{\delta}{r} \text{ [ZN nomenclature]}$$

where  $\delta = r\tau - \mu k$

being  $\nu = \frac{\partial n r_p}{\partial n p}$

$$\mu = \frac{1}{T_s - T_i} \frac{\partial T_s}{\partial n p}$$

$$k = (T_s - T_i) \frac{\partial n r_b}{\partial T_0}$$

$$r = \frac{\partial T_s}{\partial T_0}$$

It was noted by De Luca that there are computational difficulties, however, with using a value of  $n_s$  (or  $\delta$ ) other than zero for transient burning. Moreover, at present, there does not appear to be sufficiently accurate steady-state experimental data to warrant the use of non-zero  $n_s$  values.

### 9.3 Extension of Linearized, ZN and FM Descriptions to Radiation-Driven

The extension of the linearized ZN and FM theory to the radiation driven case was reported by Italian, Russian and US researchers at the Workshop. Similar results were reported by all groups, but minor differences could also be detected in the approaches. The US group presented results for both FM and ZN formulations; the Italian group also implemented both formulations but preferably uses FM, employing ZN mainly for comparison; the Russian group adopted the ZN formulation only.

In addition, the US group emphasized that, like in the pressure-driven case, the two FM and ZN approaches are equivalent if consistent parameter definitions are made. Between the US and Russian formulations of the ZN approach, there was also a difference in the way that the ZN parameters are defined. The US group considered the net radiant flux to the propellant surface,  $q$ , to be a third independent variable, in such a way that

$$r_b = r_b(p, T_0, q)$$

$$T_s = T_s(p, T_0, q)$$

The ZN parameters are thus defined as:

$$\nu^* \equiv \frac{\partial \ln r_b}{\partial \ln p}$$

$$\nu_q \equiv \frac{\partial \ln r_b}{\partial \ln q}$$

$$\mu^* \equiv \frac{1}{T_s - T_0} \frac{\partial T_s}{\partial \ln p}$$

$$\mu_q \equiv \frac{1}{T_s - T_0} \frac{\partial T_s}{\partial \ln q}$$

$$k^* \equiv (T_s - T_0) \frac{\partial \ln r_b}{\partial T_0}$$

$$r^* \equiv \frac{\partial T_s}{\partial T_0}$$

with  $\delta^* = \nu^* r^* - \mu^* k^*$

$$\delta_q = \nu_q r^* - \mu_q k^*$$

The Russian group invoked the equivalence principle, by which

$$r_b(p, T_0, q) = r_b(p, T_0^*, 0)$$

where

$$T_0^* = T_0 + \frac{q}{\rho_c r_b c_c}$$

This approach leads to ZN parameters defined as follows:

$$k^* \equiv (T_s - T_0) \left. \frac{\partial n r_b}{\partial T_0} \right|_{T_0^*}$$

$$r^* \equiv \left. \frac{\partial T_s}{\partial T_0} \right|_{T_0^*}$$

If the equivalence principle holds, then the Russian formulation seems preferable since it is simpler. However, Zarko expressed doubts about the validity of the equivalence principle; for details see Zarko, 1992. Brewster emphasized that the equivalence principle may still hold if consideration is taken of the fraction of radiation absorbed below the rate-controlling layer (cf Konev and Klevnoi, 1966; Ibricic and Williams, 1975).

#### 9.4 Transfer Function Between Linearized Radiation- and Pressure-Driven Response Functions

It has been widely recognized that it would be very advantageous if the general complex-valued, frequency-dependent transfer function

$$TF \equiv \frac{R_p}{R_q}$$

(for converting the easily measured linearized radiation-driven response function  $R_q$  to the linearized pressure-driven response function  $R_p$ ) could be reduced to a simple constant, namely the ratio of the steady-state burning rate sensitivities:

$$TF = \frac{\nu}{\nu_q} [\text{ZN nomenclature}] = \frac{n}{n_q} [\text{FM nomenclature}] .$$

In a previous study limited to negligibly small  $\bar{q}$  values (De Luca, 1976) it had been reported that the only condition, besides the inherent QSHOD assumptions, necessary for this simple relation to hold was the limit of surface absorption (opaque propellant). However, it has been recently found (Son and Brewster, 1992), and reported at this Workshop, that there is an effect of the mean radiant flux,  $\bar{q}$ , on the ZN or FM parameters ( $r, k, \nu, \mu$  or  $A, B, n, n_s$ ) that adds an extra restriction. Namely, for sufficiently large  $\bar{q}$  values there is a change in the steady-state parameters such that in general

$$\begin{aligned} r^* &\neq r, & \nu^* &\neq \nu, \\ k^* &\neq k, & \mu^* &\neq \mu \end{aligned}$$

where \* indicates  $q > 0$  and no \* indicates  $q = 0$ . In order for  $TF = \nu/\nu_q$  to hold, in addition to surface absorption, it is necessary for the mean radiant flux to be small enough that

$$\begin{array}{ll} r^* \rightarrow r, & \nu^* \rightarrow \nu, \\ k^* \rightarrow k, & \mu^* \rightarrow \mu. \end{array}$$

Since it is impossible to have an oscillating component of  $q$  with  $\bar{q} \rightarrow 0$ , and since surface absorption may be a difficult condition to achieve (even for what are ordinarily thought of as opaque material - wavelength combinations, e.g. AP - 10.6  $\mu\text{m}$ ), it remains to be seen whether or not these conditions can be achieved experimentally.

Nevertheless, it was emphasized at the Workshop that converting  $R_q$  data to  $R_p$  data is only a part of the potential benefit of the unsteady radiation - driven combustion technique. The ability to investigate the fundamental combustion mechanisms and test various combustion theories, which is afforded by the simplicity and versatility of this technique, is a benefit which perhaps surpasses that of direct  $R_p \rightarrow R_q$  conversion.

#### 9.5 Linear Stability Analysis of Radiation Augmented Combustion at Constant Pressure

Advances were also reported in linear stability analysis of radiation - augmented propellant combustion by several research groups. In general, it has been reported that external radiation ( $\bar{q} > 0$ ) tends to stabilize combustion (or increase the region of stable combustion) over the case without external radiation ( $\bar{q} = 0$ ). However, for a given level of external radiation, distributing the absorption of the radiant energy deeper in the propellant (reducing the propellant opacity) apparently decreases the domain of stability. The underlying physical reasons for these trends could not be discussed at the Workshop. It was also noted that stability is very sensitive to condensed phase heat release and activation energy parameters. These issues need to be further explored.

#### 9.6 Steady State Combustion Modeling: Negative Exponent Effect

The issue of negative exponent (mesa burning) was also discussed briefly at the Workshop. A presentation by Yin ascribed negative exponent in AP/PU propellants to melting and covering of AP particles by the binder on the propellant surface. A detailed model of the process based on the BDP model was presented.

In relation to negative exponent behavior in homogeneous propellants, Novozhilov speculated on a unique possible mechanism for the behavior. He suggested that the combustion may actually be microscopically oscillatory in the negative exponent region (with a reduced mean component of burning rate) due to the steady-state parameters ( $r, k$ ) crossing into the intrinsically unstable domain for this pressure range.

## 10. CONCLUSIONS

From this Workshop it appears as though a fruitful synergism between analytic and numerical methods already exists in several areas of combustion. This synergism looks capable of furthering our understanding of fundamental issues and providing reasonable guidelines for practical applications. A careful comparison of analytic to numerical developments, possibly together with experimental information for a conclusive validation, is an approach that stresses cooperative interaction (synergism).

Lack of communications between analysis and computation is a real fact due to different languages, backgrounds, professional interests, mental attitude, and finally just historical developments in sciences. But it should be overcome. Both analysis and computation benefit from each other. In principle, analytic methods are predictive but can only be applied to simplified problems, while numerical methods can afford very complex problems but are only simulative. Synergism will be more fruitful than just the sum of the two parts and is expected to trigger substantial progress in the current understanding of combustion and sciences in general.

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**MATHEMATICAL METHODS IN COMBUSTION**

**Final Program**

**Centro di Cultura Scientifica "A. Volta"**  
**Villa Olmo, Como, Italy**

**18-22 May 1992**

**International Workshop**  
on  
**MATHEMATICAL METHODS IN COMBUSTION**

**Centro di Cultura Scientifica "A. Volta"**  
**Villa Olmo, Como, Italy**

**18-22 May 1992**

**sponsored by**

Dipartimento di Energetica, Politecnico di Milano, Milano, Italy

Dipartimento di Matematica, Politecnico di Milano, U.O. del  
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**and under the auspices of**

The Italian Section of The Combustion Institute, Napoli, Italy

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## Mathematical Methods in Combustion

Monday, 18 May 1992 Villa Olmo, Room "Olimpo"

08.30 Registration

09.15 **L. De Luca, R. Reichenbach, V. Calarese**  
Introductory Remarks

### ANALYTICAL FUNDAMENTALS

**B.V. Novozhilov** chairman

09.30 **B.J. Matkowsky**  
Synergism of Analytical and Numerical Approaches in Combustion

10.30 **R. Natalini and A. Tesei**  
Blow-Up of Phenomena for Some Parabolic and Hyperbolic Models in Combustion Theory

11.00 *coffee break*

11.30 **A.G. Merzhanov**  
On the Role of Computer-Aided Calculations in Combustion Theory

12.00 **C.D. Pagani, M. Verri, and S. Salsa**  
Nonlinear Burning Stability of Solid Propellants: an Analytical Approach

12.30 **B.V. Novozhilov**  
On the Theory of Surface Spin Burning

13.00 **R. Dal Passo**  
On a Moving Boundary Problem Arising in Fluidized Bed Combustion

13.30 *lunch*

### MATHEMATICAL APPLICATIONS

**B.J. Matkowsky** chairman

14.30 **L. De Luca**  
Nonlinear Transient Burning of Solid Propellants: a Simple Example of Synergism between Analytical and Numerical Methods

15.00 **D. Grune and D. Hensel**  
Burning Behaviour of Solid Propellants at High Pressure and High Loading Density

15.30 *coffee break*

16.00 **N. Kidin**  
Acoustics and Control of Combustion Instabilities

16.30 **D.A. Goussis and S.H. Lam**  
Derivation of Simplified Models in Chemical Kinetics

17.00 Round Table Discussion

17.30 End of Session

Tuesday, 19 May 1992 Villa Olmo, Room "Olimpo"

8.50 **L. De Luca**  
Introductory Remarks

### NUMERICAL FUNDAMENTALS

M.K. Strelets chairman

09.00 **E.S. Oran**  
Limitations and Potentials of Numerical Methods for Simulating Combustion

10.00 **C. Di Blasi**  
Numerical Simulation of the Dynamics of Flame Spreading over Liquid Fuels

10.30 **M.Kh. Schur**  
Navier-Stokes Simulation of Supersonic Combustion in Continuous Wave HF-Chemical Lasers Based on *Compressibility Scaling Method*

11.00 *coffee break*

11.30 **G. Continillo and S. Baruffo**  
On the Approximation of Chemical Reaction Terms in Finite-Difference Calculations

12.00 **G. De Michele, S. Pasini, and A. Tozzi**  
Combustion Optimization in Power Station Boilers by Advanced Modeling Technology

12.30 **R. Heiser**  
A Navier-Stokes Solution of the Heat Transfer to Gun Barrels

13.00 **F. Magugliani**  
Computers in Science and Engineering Practical Applications

13.30 *lunch*

### DETONATION PROCESSES

E.S. Oran chairman

14.30 **O. Nekhamkina and M.Kh. Strelets**  
Application of Efficient Riemann Solver and TDV Scheme for Numerical Simulation of Detonation Waves in Hydrogen-Oxygen Mixtures

15.00 **M. Valorani and M. Di Giacinto**  
Numerical Analysis of Detonative Processes

15.30 *coffee break*

16.00 **H.E. Longtin and P. Clavin**  
Critical Conditions for Detonation Initiation by Non Uniform Hot Pockets of Reactive Gases

16.30 **A. Lunardi**  
Stability of Travelling Waves in Deflagration to Detonation Transition Models

17.00 Round Table Discussion: Assessment of Numerical Methods

17.30 End of Session

Wednesday, 20 May 1992 Villa Olmo, Room "Olimpo"

08.50 **L. De Luca**  
Introductory Remarks

### LINEAR COMBUSTION STABILITY

A.G. Merzhanov chairman

09.00 **B.V. Novozhilov**  
Combustion Stability of Solid Propellants ZN- and FM- Approaches

09.30 **P. Clavin**  
Acoustic Instabilities of Flames

10.00 **V.E. Zarko and A.B. Kiskin**  
Stability and Transient Radiation-Driven Solid Propellant Combustion

10.30 **J.Yin**  
Studies on Mathematical Models of Solid Propellant Combustion at Northwestern Polytechnical Institute, Xi'an, China

11.00 *coffee break*

11.30 **M.Q. Brewster and S. Son**  
Mathematical Modeling of Unsteady Combustion of Energetic Solids Subject to External Radiation

12.00 **F. Cozzi and L. De Luca**  
Radiation-Driven Frequency Response Function by Flame Models

12.30 Round Table Discussion: Linear Combustion Stability

13.30 *lunch*

### CLOSURE SESSION

L. De Luca chairman

14.30 **R. Reichenbach and V. Calarese**  
US Guidelines for Research Proposals

15.00 **B.J. Matkowsky, B.V. Novozhilov, and A. Lunardi**  
Future Perspectives in Analytical Methods

15.30 *coffee break*

16.00 **E.S. Oran, M.Kh. Strelets, and C. Di Blasi**  
Future Perspectives in Numerical Methods

16.30 General Discussion

17.15 **L. De Luca**  
Summary and Conclusions

17.30 Closure of Workshop

International Workshop  
on  
MATHEMATICAL METHODS IN COMBUSTION

List of participants

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18-22 May 1992

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