**REPORT DOCUMENTATION PAGE**

<table>
<thead>
<tr>
<th>REPORT NUMBER</th>
<th>GOVT ACCESSION NO.</th>
<th>RECIPIENT'S CATALOG NUMBER</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFSNTR-77-1277</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TITLE (and Subtitle)</th>
<th>TYPE OF REPORT &amp; PERIOD COVERED</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEADY STATE COMBUSTION OF NONMETALLIZED COMPOSITE SOLID PROPELLANTS</td>
<td>INTERIM 1 Jul 76 - 30 Sep 77</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUTHORS</th>
<th>CONTRACT OR GRANT NUMBER(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R L GLICK</td>
<td>F49620-76-C-0008</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PERFORMING ORGANIZATION NAME AND ADDRESS</th>
<th>PROGRAM ELEMENT PROJECT, TASK AREA &amp; WORK UNIT NUMBERS</th>
</tr>
</thead>
<tbody>
<tr>
<td>THIOKOL CORPORATION</td>
<td>230870 17A1</td>
</tr>
<tr>
<td>HUNTSVILLE DIVISION</td>
<td>61102F</td>
</tr>
<tr>
<td>HUNTSVILLE, ALABAMA 35807</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CONTROLLING OFFICE NAME AND ADDRESS</th>
<th>REPORT DATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NA</td>
<td>30 Sep 77</td>
</tr>
<tr>
<td>BLDG 410</td>
<td></td>
</tr>
<tr>
<td>BOLLING AIR FORCE BASE, D C 20332</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MONITORING AGENCY NAME &amp; ADDRESS</th>
<th>SECURITY CLASS. (OF THIS REPORT)</th>
<th>DISTRIBUTION STATEMENT (OF THIS REPORT)</th>
<th>DISTRIBUTION STATEMENT (OF THE ABSTRACT ENTERED IN BLOCK 20, IF DIFFERENT FROM REPORT)</th>
<th>SUPPLEMENTARY NOTES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UNCLASSIFIED</td>
<td>Approved for public release; distribution unlimited.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>KEY WORDS</th>
<th>ABSTRACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEADY-STATE COMBUSTION PERIOD PROPERTIES, DATA ANALYSIS, CORRELATION OF DATA BASES, COMBUSTION MODELLING</td>
<td>The combustion model including aluminum and iron oxide was employed to correlate data bases of Miller and Maykut. Results for additive free formulations were excellent for both rate and exponent; results for formulations with aluminum and aluminum plus iron oxide were poor. A new method for extracting particle size dependent information from rate/response function/formulation data was developed from the statistical methodology itself and employed to process the aforementioned data bases. Results were encouraging; Miller's additive free and aluminum plus iron oxide data correlated very well; Miller's aluminum data showed</td>
</tr>
</tbody>
</table>

**DD FORM 1473 EDITION OF 1 NOV 68 IS OBSOLETE**
that the increasing aluminum particle size increases interactions between oxidizer modes; Maykut's data base showed that aluminum induced interactions among oxidizer modes are decreased as iron content increases. Results elucidate mechanisms for rate, exponent, and response function control and show that the equal rate hypothesis employed in much combustion modeling is incorrect. A new approach for including the effects of transients introduced by particle size dependent rates in both steady and nonsteady combustion modeling was conceived.
STATISTICAL ANALYSIS OF STEADY STATE COMBUSTION OF NONMETALLIZED COMPOSITE SOLID PROPELLANTS

DR. R. L. GLICK
THIOKOL CORPORATION
HUNTSVILLE, ALABAMA 35807

REPORT, CONTRACT F49620-76-C-0008

JULY 1, 1976 - SEPTEMBER 30, 1977

PREPARED FOR:
DEPARTMENT OF THE AIR FORCE
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFSC)
BOLLING AIR FORCE BASE, D. C. 20332

Approved for public release; distribution unlimited.
FOREWORD

This is a report covering the work completed under Contract F49620-76-C-0008 for the period 1 July 1976 through 30 September 1977. Publication of this report does not constitute Air Force approval of the findings or conclusions contained herein. It is published only for the exchange of data and stimulation of ideas.

APPROVED BY:

G. F. Mangum
Project Director

C. C. Lee
Director, Programs

AIR FORCE OFFICE OFサイオティIC RESEARCH (AFSC)
NOTICE OF TECHNICAL TO DOD
This technical report has been reviewed and is approved for public release IAW AFR 190-12 (7b). Distribution is unlimited.
A. D. Blose
Technical Information Officer
Figures (continued)

8. Exponent: Calculated vs Experimental for Miller's Additive Free Data Base (SD-III-88) 20

9. Burning Rate: Calculated vs Experimental for Miller's 18% 24-micron Aluminum Data Base (SD-I-88) 21

10. Burning Rate Exponent: Calculated vs Experimental for Miller's 24 micron Aluminum Additive Data Base (SD-I-88) 22

11. Burning Rate: Calculated vs Experimental for Miller's 90 micron Aluminum Additive Data Base (SD-IV-88) 23

12. Burning Rate Exponent: Calculated vs Experimental for Miller's 90 micron Aluminum Additive Data Base (SD-IV-88) 24

13. Burning Rate: Calculated vs Experimental for Miller's 6 micron Aluminum Additive Data Base (SD-V-88) 25

14. Exponent: Calculated vs Experimental for Miller's 6 micron Aluminum Additive Data Base (SD-V-88) 26

15. Burning Rate: Calculated vs Experimental for Miller's Extended Solids Data Base (SD-VI-90) 27

16. Burning Rate Exponent: Calculated vs Experimental for Miller's Extended Solids Data Base (SD-VI-90) 28

17. Burning Rate: Calculated vs Experimental for Miller's 24 micron Aluminum/Iron Oxide Data Base (SD-VII-88) 29

18. Exponent: Calculated vs Experimental for Miller's 24 micron Aluminum/Iron Oxide Data Base (SD-VII-88) 30

19. Variation of Modal Rates with Modal D_{43} (microns) for Miller's Additive Free Data Base (SD-III-88) 31

20. Effect of Volume Mean Diameter on Burn Rate, Miller's Data Base (SD-VII-88) 32

21. Effect of Volume Mean Diameter on Exponent, Miller's Data Base (SD-VII-88) 33

22. Schematic Illustrating Arrangement of Pseudopropellants 34
ABSTRACT

The combustion model including aluminum and iron oxide was employed to correlate data bases of Miller and Maykut. Results for additive free formulations were excellent for both rate and exponent; results for formulations with aluminum and aluminum plus iron oxide were poor. A new method for extracting particle size dependent information from rate/response function/formulation data was developed from the statistical methodology itself and employed to process the aforementioned data bases. Results were encouraging; Miller's additive free and aluminum plus iron oxide data correlated very well; Miller's aluminum data showed that increasing aluminum particle size increases interactions among oxidizer modes; Maykut's data base showed that aluminum induced interactions among oxidizer modes are decreased as iron content increases. Results elucidate mechanisms for rate, exponent, and response function control and show that the equal rate hypothesis employed in much combustion modeling is incorrect. A new approach for including the effects of transients introduced by particle size dependent rates in both steady and nonsteady combustion modeling was conceived.

Goals of embedding Williams/Guirao AP decomposition model and Cohen nitramine model in the combustion model were not reached.
INTRODUCTION

Increasing emphasis on low visible exhaust signature in tactical applications of solid rocket motors has virtually eliminated significant amounts of condensed phases from the products of combustion. This has created a number of problems.

1. At equal total solids contents replacement of metal additive with AP reduces specific impulse.

2. Replacement of metal additive with oxidizer alters the relationship among rate, formulation, and environment.

3. Replacement of metal additive with oxidizer increases the probability of combustion instability because particle damping is absent.

The upshot is that propellant formulation is more difficult in the low signature area; all constraints imposed on a high signature formulation must be met at a higher total solids loading (if equivalent energetics are demanded) with greatly enhanced probability of combustion instability plus a new constraint—signature.

Propellant formulation has long proceeded in largely empirical channels. However, deviations of low signature formulations from the rate/formulation/environment relations established largely for metallized propellants over the past two decades, introduction of ingredients outside the historical data base (nitramines, ultra fine aluminum oxide, etc), and the importance of combustion instability have all contributed to increasing cost and risk of low signature propellant development efforts relative to those for similar high signature propellants. The economics of an empirical approach are strongly related to the cost of gathering data. With high signature systems only passing attention was paid to combustion stability; this is not the case for low signature systems. As a result, determination of propellant properties related to combustion stability accounts for a substantial portion of the aforementioned cost/risk differential.

Theory shows that steady and nonsteady combustion phenomena are related for homogeneous propellants when the frequency is not too high. On phenomenological grounds a steady/nonsteady relation must also exist for composite propellants. However, it is not that for homogeneous propellants. Since a steady/nonsteady relation means that propellant stability properties can be computed from steady-state data, it would be of considerable economic importance for low signature composite propellant development programs. Unfortunately, the empirical path followed by propellant developers virtually prohibits any possibility for discerning the aforementioned steady/nonsteady relation.
The overall objective of this work is to construct an analytical model describing steady-state combustion of composite propellants. This is both a worthy goal in itself (propellant constraints relate to steady-state properties) and a necessary step to understanding nonsteady phenomena.
Combustion Modeling

Reference 3 presents mathematical developments for a steady-state combustion model of composite propellant with additives. Basically, a statistical procedure is employed to account for oxidizer particle size and additives are divided into either active or passive categories. In the former category, the additive modifies the kinetics of the deflagration process; in the latter the additive acts solely as an inert heat sink. In this program this model has been transformed into an operational computer code and employed to correlate experimental data.

The data bases of Miller\(^{(4)}\) and Maykut\(^{(5)}\) have been employed to test the model. Miller's data base includes additive free, aluminum additive, and aluminum plus iron oxide additives. Maykut's data base includes aluminum and varying amounts of iron oxide. Both data bases are for HTPB/AP formulations and have similar total solids contents.

The correlation process proceeded as follows. First, basic parameters were adjusted to give a "best" fit with Miller's additive free data. Second, with these parameters, rates and exponents were predicted for Miller's 24 micron aluminum additive formulations (no additional parameters are required to account for passive additives). Third, parameters associated with the iron oxide catalyst were adjusted to give a best fit to selected rate vs catalyst data in Maykut's data base. Fourth, rates and exponents were predicted for the formulations in Miller's 24\(\mu\) aluminum plus 1% iron oxide data base and the remainder of Maykut's data base.

Results for Miller's additive free data are reported elsewhere.\(^{(6)}\) The correlation was superb for both rate and exponent. The standard error of estimate of the correlation was roughly 6 percent. This is of the same order as errors in the burning rate measurements themselves. Consequently, the correlation is essentially as good as the data itself.

Figures 1 and 2 present the correlation of Miller's 24 micron aluminum data (formulation set SD-I-88). It is clear that appreciable scatter exists. Examination of the outliers* shows that, in general, they are formulations possessing a "wide" distribution. Consequently, the present model seems adequate only for metallized propellants with narrow distributions. As Miller has pointed out elsewhere\(^{(7)}\), the addition of aluminum causes interactions to occur among particles of differing size. As presently constituted, the combustion model does not include interactions.

*Numbers associated with the formulations are the formulation numbers assigned by Miller.\(^{(4)}\)
Figures 3 and 4 present the correlation of Miller's 24 micron aluminum plus 1% iron oxide data (formulation set SD-VII-88). There is considerable scatter in this correlation. However, when contrasted with the aforementioned aluminum additive data the scatter does not appear to relate to wide and narrow distributions. Indeed, it appears that there is a systematic error in the predicted exponents (refer to the dashed correlation line) and that propellants with rates below 1 in/sec systematically deviate from the above 1 in/sec correlation. The latter behavior was evident in correlations of the same data presented by Beckstead.\(^\text{(8)}\)

Figures 5 and 6 present the correlation of Maykut's HTPB/AP/30\(\mu\) Al/iron oxide data base. As before, there is appreciable scatter. However, the character of the scatter differs from that of Miller's 24\(\mu\) Al plus iron oxide data base. Here the outlyers are largely those with wide distributions. Moreover, the rate correlation possesses a systematic deviation (dashed line) while the exponent correlation doesn't.

In summary, correlation of these systematic data bases has shown that the basic additive free model appears to be adequate while the model for additives is inadequate. It is clear that metal additives cannot be treated as simple heat sinks. However, problems with the present treatment of catalysts are confounded with aluminum effects. An extensive catalyst data base without metal additive is required to adequately define inadequacies in the catalyst model.

Analysis of Data With the Statistical Framework

The aforementioned results show that the present combustion model is, at present, inadequate for \textit{quantitative} calculations with propellants containing additives. In the combustion model errors can arise from two sources (a) the statistical framework and (b) the unit combustion model. One suspects that the statistical framework is more accurate than the unit combustion model. Therefore, effort was expended to explore use of the basic statistical framework to correlate data.

Correlation of Miller's additive free data had shown that best correlation occurs when the pseudo-propellant oxidizer/fuel ratios are all equal. Thus, \(\kappa_{\text{os,}k}^\circ = \kappa_{\text{os}}\) so that the basic rate equation

\[
\bar{m}_k = \left(\frac{\varepsilon}{K}\right) \sum_{k=1}^{M} \alpha_{\text{os,}k} \frac{F_{\text{os,}k}}{D} \, \frac{dD}{d}
\]

becomes

\[
\bar{m}_k = \kappa_{\text{os}}^{-1} \sum_{k=1}^{M} \alpha_{\text{os,}k} \left(\frac{\varepsilon}{K}\right) \frac{F_{\text{os,}k}}{D} \, \frac{dD}{d}
\]

The integral in the latter equation is the mean mass flux from the pseudo-propellant containing the kth oxidizer mode. Therefore, Eq. (2) can be
rewritten as

$$\bar{m}_k = \sum_{k=1}^{M} \alpha_{ox, k} \bar{m}_k$$

(3)

which leads to

$$\bar{m}_k = \sum_{k=1}^{M} \alpha_{ox, k} \bar{m}_k$$

(4)

since $\alpha_{ox, D} = \alpha_{ox}$. Differentiation of Eq. (4) leads to

$$d\bar{F}_k = \sum_{k=1}^{M} \alpha_{ox, k} \bar{F}_k d\bar{F}_k / \bar{F}_k$$

(5)

Therefore, algebraic manipulation yields

$$\bar{m}_k = (\alpha_{ox, k})^{-1} \sum_{k=1}^{M} \alpha_{ox, k} \bar{F}_k \bar{m}_k$$

(6)

$$\bar{F}_k = (\alpha_{ox, k})^{-1} \sum_{k=1}^{M} \alpha_{ox, k} \bar{F}_k \bar{F}_k$$

(7)

$$\bar{R}_k = (\alpha_{ox, k})^{-1} \sum_{k=1}^{M} \alpha_{ox, k} \bar{R}_k \bar{F}_k$$

(8)

These equations assert that the ballistic properties of composite propellants should be expressible in terms of modal properties. On the other hand, experimental data can be analyzed to determine these modal properties. That is, if ballistic data from at least $N$ formulations with the same chemical composition but differing median oxidizer size were available, the $\bar{F}_k$, $\bar{m}_k$, etc. ($k = 1, N$) could be computed from that data. Once these $\bar{F}_k$, $\bar{m}_k$, etc. ($k = 1, N$) were known, the ballistic properties of any formulation with that chemical composition could be computed. Consequently, ballistic properties of all members of a bimodal family with fixed chemical composition but differing particle size could be defined from ballistic data for just two members; a trimodal family would require data from three members.

In short, it appears that the statistical framework offers some exciting possibilities for generalizing experimental ballistic data. In addition, the modal pseudo-propellant properties demonstrate the effects of particle size and additives at a level much closer to the unit combustion model. Therefore, the "statistical framework approach" also offers some exciting possibilities for assisting the theoretical modeling.

To test the "accuracy" of the statistical framework for correlating ballistic data a computer code for extracting the best, in a statistical sense,
from any data set was developed. Appendix B presents the code and a sample case illustrating input and output. Figures 7 and 8 present the correlation of Miller's additive free rate and pressure exponent data while Table I presents the best fit $\overline{F}_k$ and $\overline{n}_k$. Correlation in all cases is superb.

Figures 9 and 10 present the correlation of Miller's 24 micron aluminized propellant data while Table I presents the best fit $\overline{F}_k$ and $\overline{n}_k$. The presence of aluminum degrades the correlation. However, data scatter is much less than that shown by Figures 1 and 2. Therefore, an appreciable portion of the inaccuracy in the theoretical model must be attributable to the unit combustion model. It is important to note that the data outliers are generally associated with formulations possessing wide oxidizer distributions. Consequently, there is every reason to believe that if interaction effects were included in the statistical framework the outliers would be brought into the fold.

Figures 11 to 14 present correlations for Miller's 6 micron and 90 micron aluminized propellant data while Table I presents the best fit $\overline{F}_k$ and $\overline{n}_k$. Comments pertinent to the individual data correlation are essentially the same as those for the 24 micron data. However, when Figures 9, 11, and 13 are viewed in sequence it is obvious that the correlation degrades with increasing aluminum particle size. This trend is also evident in the standard error of estimate data of Table 1. Thus, interaction effects must increase with increasing aluminum particle size.

Figures 15 and 16 present correlations for Miller's 24 micron plus 1 percent iron oxide propellant data while Table I presents the best fit $\overline{F}_k$ and $\overline{n}_k$. Correlation of this data is superb. Clearly, as Miller has noted, the addition of 1% iron oxide has suppressed (or compensated for) interactions among the oxidizer particles.

Table II presents modal rates and exponents and statistical measures of the correlation of Maykut's data base. Several trends are noted. First, the correlation improves as pressure decreases. This suggests that interactions are related to transport property effects since kinetics become of increasing importance as pressure decreases. Second, the correlation improves as catalyst content increases. This shows that catalyst progressively cancels (or compensates) interactions. Note that in Miller's data 1% catalyst eliminated interactions while 2% catalyst is required here. Third, note that catalyst has little effect on the 16$\mu$m mode; effects appear to be concentrated in the coarse and fine modes.

The above results show that the correlation methodology possesses excellent capabilities for extracting modal properties under circumstances when interactions are small. Data from these situations may be employed to elucidate particle dependent combustion phenomena. Figure 19 presents the variation of modal burning rate with volume mean particle size for Miller's additive free formulations. It is clear that burning rate depends strongly upon oxidizer particle size and that variation is pressure dependent. Note that at 500 psi there is little variation of rate with particle size for particles.
below 10μ. This indicates that small particle rates are kinetic rather than diffusion limited. Note that this situation alters as pressure increases.

Figure 20 compares the diametral dependence of burning rate with formulation for Miller's data base. The addition of aluminum substantially degrades the burning rates of fine material while producing relatively little effect on the coarse modes. The addition of catalyst causes substantial increases in the burning rate of both fine and coarse AP modes but little effect in the 50 to 100μ range. Figure 21 illustrates the dependence of modal exponent on volume mean diameter of the mode for several formulations in Miller's data base. For the additive free formulation exponent increases to unity as diameter decreases. This indicates that as diameter approaches zero rate control shifts to a kinetic mechanism. The surprising result is the tendency for exponent to increase for very coarse oxidizer modes. The mechanism for this increase is not known. However, the combustion model predicts this trend. The effect of both aluminum and catalyst is primarily to suppress high exponents at small particle sizes.

The modal property trends shown in Figures 20 and 21 explain many formulation trends. For example, rate is sensitive to the amount of coarse material because rate is weighted solely by mass fraction. However, exponent is much less sensitive to the amount of coarse material because the exponent is weighted by both mass fraction and rate and the modal rates of coarse material are low. Thus, rate tends to be controlled by both coarse and fine while exponent is largely controlled by the fine fraction. With the data in hand it is clear that high exponent (n > 0.7) formulations with significant metal content are highly improbable in a HTPB/AP/Al/Iron Oxide system; the modal exponents are all low. On the other hand, high exponent can be readily achieved in an additive free system simply by incorporating small diameter fines.

It appears that inert additives act to suppress both rate and exponent of fine AP. Rate can be restored with a catalytic additive, but exponent apparently cannot. This suggests that inert additives should provide means for reducing exponent independent of particle size control while a mixture of inert/catalytic additives should provide means for controlling both rate and exponent independent of particle size control.

The functional similarity of Eqs. 6 and 8 and the fact that \( n_{p_t} \) approaches \( n_t \) as frequency approaches zero suggests strongly that techniques for exponent control should carry over into control of pressure coupled response. From the arguments presented above it is seen that propellants formulated with significant amounts of coarse AP should possess both low exponent and low pressure coupled driving. Moreover, inert additives should be excellent stability additives. These trends have substantially been borne out. (10) The efficacy of inert additives has generally been laid at the doorstep of particle damping. However, the above suggests that part of the observed effects may be attributed to reduced pressure coupled driving.

It is important to note that the \( R_{p_t}n \) "analogy" is definitely not exact. The reason is that the frequency where the response function peaks varies with
the thickness of the subsurface energy store which varies locally with rate. What this means is that dynamic effects cloud the issue. Therefore, the above formulation generalizations will probably vary with frequency.

It is unfortunate that available data bases do not usually contain either temperature sensitivity or response function information (Miller's data base will eventually supply limited response function information). Without systematic data in these areas we are simply working in the dark.

Strategy for Inclusion of Nonsteady Phenomena in Combustion Modeling

Combustion phenomena in composite propellants is inherently nonsteady at the single particle level. That is, even when the environment is quiescent 
\[
r = r(x,t)\]
where \(x\) denotes position on the burning surface. This, in turn, implies that \(T_S = T_S(x,t)\) and \(q''_S = q''_S(x,t)\). However, all steady-state combustion models are functionally equivalent to the assumption that \(q''_S\) and \(T_S\) are not functions of time. This is justified by assuming that transient phenomena cancels in the summation to a mean state. If the mean state is to be one of the accessible physical states, this assumption is generally false; the magnitude of the error introduced by this assumption is unknown.

The success of the steady-state models in dealing with Miller's additive free formulations suggests (but does not prove) that when the environment is quiescent these errors are small. However, in models that employ the equal rate hypothesis \(r(D) = r(D+\Delta D)\) surface temperature, subsurface energy store, and surface heat flux are equivalent for all particles. Consequently, for low and midfrequency response where the chemically reactive zones behave quasi-steadily, the response function should possess characteristics similar to those of a homogeneous propellant (single relative maximum). On the other hand, if \(r(D) \neq r(D + \Delta D)\) surface temperature and heat flux are not unique. Therefore, the possibility of a multi-relative maximum response function exists. The factor that distinguishes among these possibilities is the subsurface temperature profile.

In existing nonsteady models approximations have been introduced. Condon and Glick(2) have assumed that each monodisperse pseudo-propellant in the set representing the composite propellant possesses its equilibrium subsurface temperature profile. Cohen(9) has introduced the particle diameter as a length scale and thereby assumed the characteristic thermal thickness is proportional to particle size. Results depend strongly upon these assumptions.(2)

The major difficulty with current approaches to the condensed phase heat transfer aspects of the composite propellant combustion problem is that they are deterministic when the physical problem has a probabilistic character. For steady-state probabilistic phenomena probabilities in the spatial domain at fixed time are equivalent to probabilities in the temporal domain at fixed spatial coordinates. Thus, in a one-dimensional sense the propellant can be viewed as a super Dagwood sandwich of the monodisperse pseudo-propellants (refer to Figure 22). As the monodisperse pseudo-propellants all possess
the same bulk thermal properties in the mean, these properties are common to the sandwich layers. Therefore, the temperature field is governed by

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial y^2} - \sigma \frac{\partial T}{\partial y}$$

(6)

The initial condition is clearly

$$T(-\infty, y) = T_0$$

(7)

Following Z-N\(^{(1)}\) appropriate boundary "conditions" that enable computation of \(r(t)\) are

$$r = r(q''_{\infty}, p, D)$$

(8)

$$T_s = T_s(q''_{\infty}, p, D)$$

(9)

$$p = p(t)$$

(10)

In conventional Z-N strategy \(r\) and \(T_s\) are not functions of particle diameter because conventional Z-N strategy applies solely to homogeneous propellants. Since deflagration occurs through a layered medium here the additional independent variable must occur.*

The Z-N boundary conditions can be derived from any steady-state source since the Z-N form of the boundary conditions is independent of time as long as the reactive regions are quasi-steady. The obvious source is from a detailed combustion model. However, by employing the aforementioned methodology to extract modal properties from experimental data a source much closer to basic experimental data may be available. The latter approach is in the original spirit of Z-N methodology which was aimed at circumventing need for combustion modeling.

The last question to be answered is how are the pseudo-propellant layers arranged. The answer of course is randomly such that the probability of finding pseudo-propellant with \(B \Delta D \Delta D\) is equivalent to the volume fraction of that pseudo-propellant in the propellant recipe. This is the probabilistic aspect of the problem.

The output of this approach for a small sinusoidal environment variation will be both the mean burning rate and the small signal response to that variation (pressure coupled response function). In addition, mean rates and small signal response functions for each pseudo-propellant should be recoverable.

*The methodology can also account for velocity coupling.(1)
REFERENCES


Figure 1. Burning Rate: Calculated versus Experimental for Miller's 24 micron Aluminum Additive Data Base (SD-I-88)
Figure 3. Burning Rate: Calculated versus Experimental for Miller's 24 micron Aluminum plus 1% Iron Oxide Data Base (SD-VII-88)
Figure 4. Burning Rate Exponent: Calculated versus Experimental for Miller's 24 micron plus 1% Iron Oxide Data Base (SD-VII-88)
Figure 5. Burning Rate: Calculated versus Experimental for Maykut's Data Base
Figure 6. Burning Rate Exponent: Calculated versus Experimental for Maykut's Data Base
Figure 7. Burning Rate: Calculated versus Experimental for Miller's Additive Free Data Base (SD-III-88)
Figure 8. Exponent: Calculated Versus Experimental for Miller's Additive Free Data Base (SD-III-88)
Figure 9. Burning Rate: Calculated versus Experimental for Miller's 18% 24-micron Aluminum Data Base (SD-1-88)
Figure 10. Burning Rate Exponent: Calculated versus Experimental for Miller's 24 micron Aluminum Additive Data Base (SD-I-88)
Figure 11. Burning Rate: Calculated versus Experimental for Miller's 90 micron Aluminum Additive Data Base (SD-IV-88)
Figure 12. Burning Rate Exponent: Calculated versus Experimental for Miller's 90 micron Aluminum Additive Data Base (SD-IV-88)
Figure 13. Burning Rate: Calculated Versus Experimental for Miller's 6μ Aluminum Data Base (SD-V-88)
Figure 14. Exponent: Calculated Versus Experimental for Miller's 6µ Aluminum Data Base (SD-V-88)
Figure 15. Burning Rate: Calculated versus Experimental for Miller's Extended Solids Data Base (SD-VI-90)
Figure 16. Burning Rate Exponent: Calculated versus Experimental for Miller's Extended Solids Data Base (SD-V1-90)
Figure 17. Burning Rate: Calculated Versus Experimental for Miller's 24μ Aluminum/Iron Oxide Data Base (SD-VII-88)
Figure 18. Exponent: Calculated Versus Experimental for Miller's 24μ Aluminum/Iron Oxide Data Base (SD VII-88)
Figure 19. Variation of Modal Rates with Modal $D_{43}$ (microns) for Miller's Additive Free Data Base (SD-III-88)
Figure 21. Effect of Volume Mean Diameter on Exponent, Miller's Data Base
Figure 22. Schematic Illustrating Arrangement of Pseudopropellants
### Table 1

**Modal Properties for Miller's Data Base (1000 psi)**

<table>
<thead>
<tr>
<th>Formulation Designation</th>
<th>Modal Rates, in/sec</th>
<th>Modal Exponents</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( f_{400} )</td>
<td>( f_{200} )</td>
<td>( f_{90} )</td>
</tr>
<tr>
<td>SD-III-88</td>
<td>.953</td>
<td>.190</td>
<td>.536</td>
</tr>
<tr>
<td>SD-I-88</td>
<td>0.000</td>
<td>.215</td>
<td>.524</td>
</tr>
<tr>
<td>SD-IV-88</td>
<td>.000</td>
<td>.319</td>
<td>.643</td>
</tr>
<tr>
<td>SD-V-88</td>
<td>.044</td>
<td>.257</td>
<td>.541</td>
</tr>
<tr>
<td>SD-VI-90</td>
<td>.029</td>
<td>.406</td>
<td>--</td>
</tr>
</tbody>
</table>

- Subscripts denote nominal diameter of mode in microns.
- SE** Standard Error of Estimate
TABLE II
MODAL PROPERTIES FOR MAYKUT'S DATA BASE (1000 psi)

<table>
<thead>
<tr>
<th>p psia</th>
<th>Iron Oxide</th>
<th>r&lt;sub&gt;200&lt;/sub&gt;</th>
<th>r&lt;sub&gt;16&lt;/sub&gt;</th>
<th>r&lt;sub&gt;1.7&lt;/sub&gt;</th>
<th>Rate SEE**</th>
<th>n&lt;sub&gt;200&lt;/sub&gt;</th>
<th>n&lt;sub&gt;16&lt;/sub&gt;</th>
<th>n&lt;sub&gt;1.7&lt;/sub&gt;</th>
<th>Exponent SEE</th>
</tr>
</thead>
<tbody>
<tr>
<td>700</td>
<td>0.5</td>
<td>0.000</td>
<td>0.907</td>
<td>1.273</td>
<td>.125</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>0.75</td>
<td>0.021</td>
<td>0.839</td>
<td>1.665</td>
<td>.080</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>2.0</td>
<td>0.137</td>
<td>1.050</td>
<td>1.611</td>
<td>.026</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>0.5</td>
<td>0.000</td>
<td>1.109</td>
<td>1.531</td>
<td>0.156</td>
<td>0.826</td>
<td>0.586</td>
<td>0.404</td>
<td>0.159</td>
</tr>
<tr>
<td>1000</td>
<td>0.75</td>
<td>0.000</td>
<td>.936</td>
<td>2.211</td>
<td>0.137</td>
<td>0.365</td>
<td>0.546</td>
<td>0.417</td>
<td>0.147</td>
</tr>
<tr>
<td>1000</td>
<td>2.0</td>
<td>0.179</td>
<td>1.215</td>
<td>2.158</td>
<td>0.020</td>
<td>0.331</td>
<td>0.433</td>
<td>0.593</td>
<td>0.018</td>
</tr>
<tr>
<td>2000</td>
<td>0.5</td>
<td>0.000</td>
<td>1.548</td>
<td>2.340</td>
<td>0.295</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2000</td>
<td>0.75</td>
<td>0.000</td>
<td>1.355</td>
<td>2.183</td>
<td>0.184</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2000</td>
<td>2.0</td>
<td>0.156</td>
<td>1.671</td>
<td>3.057</td>
<td>0.087</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Subscripts denote nominal diameter of mode in microns.
**Standard Error of Estimate
APPENDIX A

NOMENCLATURE

D  particle diameter
E  error
$F_{\text{ox}, k}$  distribution function for the $k$th oxidizer mode
$m$  mass flux
$M$  number of oxidizer modes
$n$  pressure exponent
$N$  number of formulations
$p$  pressure
$q_s$  heat flux at the burning surface in the condensed phase
$r$  burning rate
$R_p$  pressure coupled response function
$t$  time
$T$  temperature
$y$  spatial coordinate
$\alpha$  oxidizer mass fraction
$\sigma_p$  temperature sensitivity at constant pressure
**Subscripts**

- **D** denotes particles with \( D \leq D < D + \Delta D \)
- **j** denotes jth formulation
- **k** denotes kth oxidizer mode
- **n** denotes exponent
- **o** denotes initial conditions
- **ox** denotes oxidizer
- **r** denotes rate
- **s** denotes conditions at burning surface
- **t** denotes total propellant

**Special**

- (\( \bar{\cdot} \)) bar over denotes a mean value
APPENDIX B
MODAL PROPERTIES CODE

This computer program extracts modal properties from multi-modal propellant ballistic data according to the equations

\[ F_k = \frac{\sum_{k=1}^{M} \alpha_{k,1} \bar{F}_{k,1}}{\alpha_{k}} \quad B-1 \]

\[ \bar{m}_k = \frac{\sum_{k=1}^{M} \alpha_{k,1} \bar{u}_{k,1}}{(\alpha_{k})} \quad B-2 \]

where \( M \) is the number of oxidizer modes; \( \alpha_{k,1}, \bar{F}_{k,1}, \bar{m}_k \) are oxidizer mass fraction (mass ox/mass propellant), modal burn rate, and modal exponent respectively; \( \alpha_{t} \) is the total oxidizer content; and \( \bar{F}_{t} \) and \( \bar{m}_t \) are the measured burning rate and pressure exponent respectively.

A nonlinear optimizer (PATSH) is employed to extract the "best" modal parameters \( \bar{F}_{k,1}, \bar{m}_k, k = 1, M \) from a chemically consistent set of experimental data \( \bar{F}_{t,j}, \alpha_{k,j}, \bar{m}_k,j, j = 1, N \) where \( N \geq M \). A chemically consistent data set is one where all \( N \) formulations have the same chemical composition (variables are modal recipe and environment). The "best" \( \bar{F}_{k,1}, \bar{m}_k \) is that which produces the smallest

\[ E_F = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \left( \frac{F_{t,j} - \bar{F}_{t,j}}{F_{t,j}} \right)^2} / N \]

for the \( \bar{F}_{k,1} \) and the smallest

\[ E_{m} = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \left( \frac{m_{k,j} - \bar{m}_{k,j}}{m_{k,j}} \right)^2} / N \]

for the \( \bar{m}_k \).

Here \( \bar{F}_{t,j}, \bar{m}_{k,j} \) refers to test data and \( \bar{F}_{t}, \bar{m}_{k} \) to calculated (by Eqs. B.1 and B.2) results for the jth formulation. The "search" for the \( \bar{F}_{k} \) begins with \( \bar{F}_{k} = \bar{F}_{k+1} = \bar{F}_{t,1} \) and \( \bar{m}_{k} = \bar{m}_{k+1} = \bar{m}_{t,1} \).

The input format consists of two major units. The first card defines the number of oxidizer modes, the number of formulations with these modes, the number of pressures at which data was obtained, and those pressures. Subsequent cards tabulate recipe, rate, and exponent for each formulation and pressure in the sequence. Figure B.1 illustrates a typical data set.
Output consists of the standard error of estimate of the fits and the $r_{ik}$, $n_k$, $k = 1, M$. Figure B. 2 illustrates results obtained from the Figure B. 1 data set. Figure B. 3 lists the Fortran IV code.
**MILLER DATA SET SD-III-1, -25 (ZERO ADDITIVE)**

<table>
<thead>
<tr>
<th>Data</th>
<th>.3158</th>
<th>.3158</th>
<th>.3158</th>
<th>.3158</th>
<th>.3158</th>
<th>.3158</th>
<th>.3158</th>
<th>.3158</th>
</tr>
</thead>
<tbody>
<tr>
<td>0821031000.500 2000</td>
<td>.1368</td>
<td>.2421</td>
<td>.3158</td>
<td>2421</td>
<td>.3158</td>
<td>2421</td>
<td>.3158</td>
<td>2421</td>
</tr>
<tr>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
</tr>
<tr>
<td>.3158</td>
<td>.2421</td>
<td>.3158</td>
<td>.2421</td>
<td>.3158</td>
<td>.2421</td>
<td>.3158</td>
<td>.2421</td>
<td>.3158</td>
</tr>
<tr>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
<td>.5579</td>
<td>.3158</td>
</tr>
<tr>
<td>.4211</td>
<td>.4526</td>
<td>.4211</td>
<td>.4526</td>
<td>.4211</td>
<td>.4526</td>
<td>.4211</td>
<td>.4526</td>
<td>.4211</td>
</tr>
<tr>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
</tr>
<tr>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
<td>.3158</td>
</tr>
</tbody>
</table>

**Figure B.1 - Input Format for Code**
### Miller Data Set SD-111-1475 (Zero Additive)

**Mixing Fraction Data**

<table>
<thead>
<tr>
<th>WOOF 1</th>
<th>WOOF 2</th>
<th>WOOF 3</th>
<th>WOOF 4</th>
<th>WOOF 5</th>
<th>OCEC 1</th>
<th>OCEC 2</th>
<th>OCEC 3</th>
<th>OCEC 4</th>
<th>OCEC 5</th>
<th>ODF 1</th>
<th>ODF 2</th>
<th>ODF 3</th>
<th>ODF 4</th>
<th>ODF 5</th>
<th>ODF 6</th>
<th>ODF 7</th>
<th>ODF 8</th>
<th>ODF 9</th>
<th>ODF 10</th>
<th>ODF 11</th>
<th>ODF 12</th>
<th>ODF 13</th>
<th>ODF 14</th>
<th>ODF 15</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.3158</td>
<td>3.0</td>
<td>3.0</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td>0.3158</td>
<td>0.3158</td>
<td>0.1368</td>
<td>0.1368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure B.2 - Sample Output**
## Table: Miller Data Set 59-111-1-25 (Zero Additive)

### Table: Computed Mean Rates, in/sec

| RPM | RM2 | RM3 | RM4 | RM5 | RM6 | RM7 | LEF | LFL | UFL | UFL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| -0.0525 | 0.1896 | 0.3358 | 0.6227 | 1.6735 | 1.5172 | 1.3554 | 1.9486 | 0.8593 | 0.1526 | -0.0884 | 0.4352 | 0.5576 | 1.7054 | 0.8743 | 0.4950 |

### Table: Comparison Theory/Experiment

<table>
<thead>
<tr>
<th>AC</th>
<th>ERR</th>
<th>AC</th>
<th>ERR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1650</td>
<td>1.2266</td>
<td>-0.0530</td>
<td>0.9160</td>
</tr>
<tr>
<td>1.1660</td>
<td>1.3886</td>
<td>0.0390</td>
<td>0.6890</td>
</tr>
<tr>
<td>1.1660</td>
<td>1.0690</td>
<td>0.0848</td>
<td>0.7970</td>
</tr>
<tr>
<td>0.8790</td>
<td>0.8963</td>
<td>-0.0303</td>
<td>0.9280</td>
</tr>
<tr>
<td>1.1660</td>
<td>1.1674</td>
<td>-0.0064</td>
<td>0.6210</td>
</tr>
<tr>
<td>1.0660</td>
<td>1.1964</td>
<td>-0.0916</td>
<td>0.6920</td>
</tr>
<tr>
<td>1.0080</td>
<td>1.0381</td>
<td>-0.0450</td>
<td>0.7710</td>
</tr>
<tr>
<td>0.9010</td>
<td>0.6654</td>
<td>0.0355</td>
<td>0.8410</td>
</tr>
<tr>
<td>1.0100</td>
<td>1.0207</td>
<td>0.0090</td>
<td>0.6170</td>
</tr>
<tr>
<td>0.9780</td>
<td>0.9144</td>
<td>0.0650</td>
<td>0.6130</td>
</tr>
<tr>
<td>0.7060</td>
<td>0.7118</td>
<td>-0.0557</td>
<td>0.6930</td>
</tr>
<tr>
<td>0.5610</td>
<td>0.5929</td>
<td>0.0568</td>
<td>0.4510</td>
</tr>
<tr>
<td>0.6340</td>
<td>0.6049</td>
<td>0.0325</td>
<td>0.4740</td>
</tr>
<tr>
<td>0.7100</td>
<td>0.7190</td>
<td>0.0001</td>
<td>0.4670</td>
</tr>
<tr>
<td>0.7090</td>
<td>0.7540</td>
<td>0.0395</td>
<td>0.5290</td>
</tr>
<tr>
<td>0.5390</td>
<td>0.5818</td>
<td>-0.0787</td>
<td>0.6100</td>
</tr>
<tr>
<td>0.3500</td>
<td>0.3312</td>
<td>-0.0038</td>
<td>0.4350</td>
</tr>
<tr>
<td>0.5240</td>
<td>0.4896</td>
<td>0.0657</td>
<td>0.4530</td>
</tr>
<tr>
<td>0.4490</td>
<td>0.4864</td>
<td>0.0370</td>
<td>0.4630</td>
</tr>
<tr>
<td>0.5360</td>
<td>0.5391</td>
<td>0.0059</td>
<td>0.4490</td>
</tr>
<tr>
<td>0.4450</td>
<td>0.4203</td>
<td>0.0556</td>
<td>0.5280</td>
</tr>
</tbody>
</table>

---

Figure B.2 - Sample Output (continued)
HILLER DATA SET SD-III-1, 25 (ZERO ADDITIVE)

\[ P = 300.0 \text{ PSI} \quad \text{RATE STD ERR} = 4.7113F-02 \quad \text{EXPONENT STD ERR} = 6.1590E-02 \]

<table>
<thead>
<tr>
<th>COMPUTED LOCAL RATES, IN/SFC</th>
<th>COMPUTED MODEL EXPONENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R2</td>
</tr>
<tr>
<td>-0.0276</td>
<td>0.1434</td>
</tr>
</tbody>
</table>

**COMPARISON THEORY/EXPERIMENT**

<table>
<thead>
<tr>
<th>R</th>
<th>NC</th>
<th>ERR</th>
<th>N</th>
<th>NC</th>
<th>EPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4270</td>
<td>0.6795</td>
<td>-0.0694</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6830</td>
<td>0.8207</td>
<td>0.0685</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6322</td>
<td>0.6018</td>
<td>0.0678</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6712</td>
<td>0.4730</td>
<td>-0.0492</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7370</td>
<td>0.7412</td>
<td>-0.0057</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6018</td>
<td>0.7274</td>
<td>-0.0094</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6318</td>
<td>0.6136</td>
<td>0.0270</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5990</td>
<td>0.4868</td>
<td>0.0304</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6760</td>
<td>0.6676</td>
<td>0.0124</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6370</td>
<td>0.5996</td>
<td>0.0587</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6490</td>
<td>0.4708</td>
<td>-0.0486</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6070</td>
<td>0.4249</td>
<td>-0.0441</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6610</td>
<td>0.5799</td>
<td>0.0434</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5210</td>
<td>0.5169</td>
<td>0.0079</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5360</td>
<td>0.5301</td>
<td>0.1110</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3660</td>
<td>0.4613</td>
<td>-0.0904</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7460</td>
<td>0.2343</td>
<td>0.2213</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3790</td>
<td>0.3480</td>
<td>0.0719</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3320</td>
<td>0.3520</td>
<td>-0.0601</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3930</td>
<td>0.3899</td>
<td>0.0079</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3940</td>
<td>0.2961</td>
<td>0.0256</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure B.2- Sample Output (continued)
**MILLER DATA SET SD-111-1-25 (ZERO ADDITIVE)**

| $P$  | RATE STO ERR | 4.4093E-02 | EXPONENT STO ERR | 5.159E-02 |

- COMPUTER 

<table>
<thead>
<tr>
<th>initial</th>
<th>final</th>
<th>exp.</th>
<th>exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1396</td>
<td>0.1732</td>
<td>0.3480</td>
<td>0.3000</td>
</tr>
</tbody>
</table>

- COMPARISON THEOREY/EXPERIMENT

<table>
<thead>
<tr>
<th>$a$</th>
<th>$RC$</th>
<th>$ERP$</th>
<th>$N$</th>
<th>$NC$</th>
<th>FBA</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.2140</td>
<td>2.2071</td>
<td>0.0031</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.2910</td>
<td>2.3729</td>
<td>0.3577</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.9090</td>
<td>1.8733</td>
<td>0.0185</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.7080</td>
<td>1.6695</td>
<td>0.0085</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.7440</td>
<td>1.6945</td>
<td>0.0165</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.7960</td>
<td>1.9656</td>
<td>0.0067</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.8220</td>
<td>1.7852</td>
<td>0.0625</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.6440</td>
<td>1.9240</td>
<td>0.0499</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5890</td>
<td>1.9622</td>
<td>0.0169</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.4400</td>
<td>1.3050</td>
<td>0.6711</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1640</td>
<td>1.3050</td>
<td>0.6711</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7610</td>
<td>0.7960</td>
<td>0.0470</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1500</td>
<td>1.2630</td>
<td>0.0274</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.9550</td>
<td>0.9760</td>
<td>0.0255</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1160</td>
<td>1.0631</td>
<td>0.0474</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.8560</td>
<td>0.8790</td>
<td>0.0268</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.4360</td>
<td>0.4586</td>
<td>0.0515</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7080</td>
<td>0.6498</td>
<td>0.0172</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6300</td>
<td>0.6288</td>
<td>0.0019</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7520</td>
<td>0.7080</td>
<td>0.0128</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6520</td>
<td>0.6220</td>
<td>0.0004</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure B.2 - Sample Output (concluded)
C COMPUTE ALFAIJ
C
0020   DO 67 J=1, JJ
0021   ALFAIJ = 0.0
0022   DO 68 J = 1, JJ
0023      ALFAIJ = ALFAIJ + FAT(J) + ALFAIJ)
0024   CONTINUE
0025   67 CONTINUE
C
C FIND W11,(K) FOR EACH (K)
C
0026   DO 20 K = 1, K1
C
C SET INITIAL W11,(K)
C
0027   DO 20 J = 1, JJ
0028      W11(J) = (1.0)
0029   END
0030   20 CONTINUE
C
C FIND OPERATIONAL W11,(K)
C
0031   CALL PAT(M,N,F1,,F1,1,1,5.0,0.001,50.0,1.0) MP11(K)
0032   DO 90 J = 1, JJ
0033      W11(J) = MP11(K)
0034   END
0035   90 MP11(K)
C
C NEED FIND W111 ?
C
0036   IF(KPRINT .EQ. 2) GO TO 100
C
C FIND OPERATIONAL W111
C
0037   CALL PAT(M,N,F2,,F2,1,1,5.0,0.001,50.0,1.0) MP211
C
C OUTPUT COMPUTED RESULTS THIS (K)
C
0038   100 WRITE(6, 110) MEAS
0039   110 FORMAT(1H4, 20A4)
0040   WRITE(6,110) PK1, ERR1, ERR2
0041   115 FORMAT(1H5, 20A4)
0042   WRITE(6,110) X, F1, F2, F3, F4, F5, F6, F7, F8, F9, F10
0043   WRITE(6,110) X, F1, F2, F3, F4, F5, F6, F7, F8, F9, F10
0044   120 FORMAT(1H5, 20A4)
0045   WRITE(6,110) X, F1, F2, F3, F4, F5, F6, F7, F8, F9, F10
0046   130 FORMAT(1H5, 20A4)
0047   WRITE(6,110) X, F1, F2, F3, F4, F5, F6, F7, F8, F9, F10
0048   140 FORMAT(1H5, 20A4)
0049   WRITE(6,110) X, F1, F2, F3, F4, F5, F6, F7, F8, F9, F10
0050   150 FORMAT(1H5, 20A4)
0051   WRITE(6,110) X, F1, F2, F3, F4, F5, F6, F7, F8, F9, F10
0052   160 FORMAT(1H5, 20A4)

Figure B.3 - Computer Code (continued)
Figure B.3 - Computer Code (continued)
Figure II. 1 - Computer Code (continued)
SUBROUTINE PAPSH(PSI, SS1, DELS, DELT, ILIM, ITLP, WPARY)
C
C THIS VERSION OF PAPSH HAS BEEN ALTERED FROM THE WLTOS2 VERSION TO
C CONFORM TO THE CALLING SEQUENCE OF THE ORIGINAL CODE (Isfortnit
C
C COMMON/OPTN, DELS, DLIM, TLT, ITL, IPT
C
C IFTMNSH RC 22, FTMT 7, FTMT 3, FEIMS
C
C DATA PARS /F
C
C DATA ML,FW/1.02/
C
C F(SA)=S=55,APS(SIS)=.,G001=.G
C
C THE IFTLICE PARAMETER ADDED BY WLTOS2 HAS BEEN SPECIFIED MS CF

C
C IFTLICE=1
C
C ITLICF=0
C
C DEL=DELS
C
C IF (ITP.GE.0) WRITE(IPR,604) DEL,DLIM,TLT,ILIM,ITLP
C
C DO 10 I=1,N
C
C 705 XFGF(I)=I
C
C 110 ITER=0
C
C 101 CUL=1
C
C 102 CALL WRIT4(PSI, SS1)
C
C 103 SSITST=F(SS)
C
C 104 SSSI
C
C 105 NPAR=N
C
C 106 DO 101 I=1,N
C
C 110 PPAR(I)=PSI(I)
C
C 111 ICALL=I
C
C 112 IF (ITP.LT.0) GO TO 150
C
C 113 WRITE(IPR,599) ITER
C
C 114 WRITE(IPR,600) (PSI(J),J=1,N)
C
C 115 WRITE(IPR,601) S,DEL
C
C 116 GO TO 150
C
C 117 150 IF(SL,LT,SSITST) GC FT 200
C
C 118 DEL=DELS(I)
C
C 119 IF (ITP.LE.0) GC FT 100
C
C 120 IF (ITP.GE.0) WRITE(IPR,704)
C
C 121 IF (OUT.LT.51) GC TO 702
C
C 122 CALL WRIT4(GL, SP)
C
C 123 IF (ITP.GE.0) WRITE(IPR, 707)
C
C 124 IF (ITP.GE.0) WRITE(IPR, 704)
C
C 125 IF (ITP.GE.0) WRITE(IPR, 701)
C
C 126 CALL WRIT4(C1, C1)
C
C 127 DEL=DELS
C
C 128 OUT=0
C
C 129 GOTO 90
C
C 200 SSITST=F(SS)
C
C 300 SSITST=F(SS)
C
C 310 ITER=ITER+1
C
C 320 NPAR=NPAR+1
C
C 330 IF (ITP.LE.0) GC FT 700
C
C 340 IF (ITP.LT.0) GO TO 203
C
C 350 WRITE(IPR,599) ITER
C
C 360 WRITE(IPR,599) NPAR
C
C 370 WRITE(IPR,599) WPARY(I)
C
C 380 WRITE(IPR,600) (FMT(I),I=1,12)
C
C 390 WRITE(IPR,601) SS,DEL
C
C 400 IF (ITP.LT.100) GC TO 203
C
C 410 IF (IPPAR.LT.11) GC TO 203
C
C 420 IMPS=IPART
C
C 430 IMPR=IMPS
C
C 440 IMPR=IPAT
C
C 450 CALL WRIT4(PSI, SP)
C
C 460 IMPR=IMPS
C
C 470 IMPR=IPAT
C
C MAKE PATTERN MOVE
C
C Figure B.3 - Computer Code (continued)
FORTRAN IV G LEVEL 21

0054  203 GC 201 I=1,N
0055  TMT(i)=PS(i)
0056  PSL(i)=PSL(i)
0057  2C1 PHI(i)=PHI(i)*ALFA*(PHI(i)-TMT(i))
0058  CALL WRITE(PS(i),10)
0059  2C0 IF(IP(I),10,20) GC TO 732
0060  WRITE(IIP,620) PHI(i),L=1,N
0061  WRITE(IIP,620) SPI,CEL
0062  2C2 ICALL=2
0063  C MAKE EXPL MVES
0064  GO TO 150
0065  C IS PRESENT VALUE < RASET VALVE
0066  260 IF(SLI,SLT,STY) GO TO 200
0067  GO TO 100
0068  C
0069  C
0070  150 GO 100 L=1,N
0071  PHI=PHI(i)
0072  STEP=PHI(10)+0.5
0073  IF(STEP=EQ.0.5) STEP=0.5
0074  IF(STEP=EQ.0.5) STEP=0.5
0075  PHI=PHI(i)+STEPM
0076  PHI=PHI(i)-STEPM
0077  IF(IP(I),10,20) GC TO 729
0078  CALL WRITE(PS(i),10)
0079  IF(IP(I),10,20) GC TO 729
0080  CS=PS(i)
0081  IF(IP(I),10,20) GC TO 729
0082  CS=PS(i)
0083  179 CS=PS(i)
0084  180 CONTINUE
0085  GO TO 116,260,ICALL
0086  C
0087  C
0088  C
0089  700 IF (IP(I),10,20) WRITE(IIP,701)
0090  701 IF (IP(I),10,20) WRITE(IIP,701)
0091  702 IF (IP(I),10,20) WRITE(IIP,701)
0092  703 IF (IP(I),10,20) WRITE(IIP,701)
0093  704 IF (IP(I),10,20) WRITE(IIP,701)
0094  705 IF (IP(I),10,20) WRITE(IIP,701)
0095  706 IF (IP(I),10,20) WRITE(IIP,701)
0096  707 IF (IP(I),10,20) WRITE(IIP,701)
0097  708 IF (IP(I),10,20) WRITE(IIP,701)
0098  709 IF (IP(I),10,20) WRITE(IIP,701)
0099  710 IF (IP(I),10,20) WRITE(IIP,701)
0100  711 IF (IP(I),10,20) WRITE(IIP,701)
0101  EN

Figure B.3 - Computer Code (concluded)