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A MATHEMATICAL MODEL FOR DEFINING EXPLOSIVE YIELD
AND MIXING PROBABILITIES OF LIQUID PROPELLANTS

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Summary

This paper describes how a mathematical model can be constructed to fit theoretical or experimental data on yield and spill of liquid propellants. It shows how these primary quantities can be separated, how probability distributions can be found for each, and how probability confidence regions and confidence limits can be established.

The fundamental function of this very general mathematical model, based upon four independent parameters, and the characteristics of the resulting probability surface are discussed in detail.

The mathematical model, programmed for an IBM 709 computer, is applied to some spill test data of liquid propellants for which the necessary information is available and then with a minimum number of assumptions to missile failure yield estimates.

Introduction

The yield from liquid propellant explosions as a result of missile failures is of extreme importance in assessing the hazards to astronauts, launch support personnel, launch support facilities and surrounding structures.

To prepare against the effects from such liquid propellant explosions, methods must be found by which the most probable expected yield can be predicted.

Unfortunately many of the physical phenomena involved in producing the yield are little understood, making the prediction of the expected yield difficult and complex.

One approach to this problem for the prediction of the overall effects by means of a mathematical model is suggested in this paper. The mathematical model developed here allows for a well balanced procedure of theoretical and experimental investigations with the theory guiding the experimentation which in turn modifies the theory.

The mathematical model suggested in this paper is very general in nature, being able to satisfy a wide range of either theoretical information or experimental data and has the required statistical characteristics to make it possible to separate the yield and spill functions, giving probability distributions, confidence limits, confidence regions, etc.

With this model it is then possible to extract a maximum amount of information from extremely sparse data and to guide future experimental programs. This procedure furthermore allows the conducting of small scale,

relatively inexpensive experiments to define the model and to reduce the large scale, expensive experiments to very few in number. The large scale tests serve as check points to validate or modify the model.

In this manner it is possible to develop a valid scaling law for liquid propellant explosions through a well planned program with theory guiding the experimental procedure and to do this in the shortest possible time and at minimum cost.

Theory of Approach

The basis of the development of the mathematical model is the fundamental characteristic of the sparse experimental data giving information on the yield and spill of liquid propellants. Work is under way to extend this data by developing theoretical yield-spill relationships.

With the above information it is possible, as is shown in this paper, to develop a very general mathematical model which can express presently available data and is flexible enough to incorporate future information as it becomes available. It also satisfies the statistical requirements providing for valid estimating procedures of the parameters involved and allows the separation of the individual characteristics of the yield function and the spill function. The model may be referred to as a modified Dirichlet bivariate surface.

The Yield and Spill Functions

The primary quantities used in formulating the mathematical model are the yield function and the spill function.

The yield function is preferably defined as the fraction of maximum theoretical yield potential of the on board liquid propellants (also utilizing the oxygen of the atmosphere, where applicable). It can also be expressed in terms of TNT equivalency, presently a common method of reporting the data.

The spill function is the fraction of the total on board propellants which are spilled, or actually mixed, at the time of reaction between fuel and oxidizer. In either case it is a time dependent variable different for each missile configuration and mode of failure.

In the formulation of the model it is assumed that the relationship between the yield function and the spill function is available. Information of this type can be found in literature, but only in very small quantity, representing liquid propellant spill tests. Preliminary investigations are

now under way to extend this data both theoretically and experimentally and the indications are that the resulting yield functions and spill functions will have lower values in most cases than those reported in literature based upon tests which were designed to give a high degree of mixing.

The Mathematical Model

With the relationship between the yield function (y) and the spill function (x) establishing either theoretically or by experiment, the model can be formulated resulting in a statistical function which is capable of incorporating the above x - y relationship and is able to provide for valid estimating procedures of the parameters involved. Details of the development of this mathematical model are left to the references ^{1,7} and only the high points are presented here.

The relationship between the yield function and the spill function can be expressed in terms of three parameters a , b , and c as shown in equation (1).

$$y = \frac{b}{b+c} x^d \quad (1)$$

From this a statistical function can be developed capable of incorporating physical information over a rather wide range and which satisfies the theoretical requirements for statistical analysis. It is a modified Dirichlet bivariate surface having four parameters a , b , c and d , making it extremely flexible. This statistical surface is expressed mathematically as equation (2).

$$f(x,y) = \frac{d \Gamma(a+b+c)}{\Gamma(a) \Gamma(b) \Gamma(c)} x^d (1-x^d)^{a-1} y^{b-1} (x^d-y)^{c-1} \quad (2)$$

where Γ is the Gamma function
The only restrictions on this function are that

$$y > 0, \quad x > 0, \quad y \leq x^d, \quad d \neq 0$$

To fully define the above function for a specific class of information it is necessary to evaluate the parameters a , b , c and d on the basis of the particular yield function - spill function relationship describing the physical phenomena.

Evaluation of the Parameters a , b , c and d

To evaluate the parameters a , b , c and d for the modified Dirichlet bivariate surface the following statistical estimating procedure is used.

Defining

$$u_i = 1 - x_i^d \quad (3a)$$

$$v_i = \frac{y_i}{x_i^d} \quad (3b)$$

four simultaneous estimation equations can be written for the four parameters a , b , c , d .

$$\overline{\ln v} = \Psi(b) - \Psi(b+c) \quad (4a)$$

$$\ln \bar{v} = \ln(b) - \ln(b+c) \quad (4b)$$

$$\overline{\ln u} = \Psi(a) - \Psi(a+b+c) \quad (4c)$$

$$\ln \bar{u} = \ln(a) - \ln(a+b+c) \quad (4d)$$

Where a bar over an expression indicates the average value of all available values

\ln indicates the natural logarithm (base e)

Ψ is Euler's Digamma Function

The mathematical model is now ready to be applied to theoretical information or experimental data. Evaluation of the parameters a , b , c , and d gives the model its characteristic configuration and analysis of the resulting statistical surface produces a wealth of new information.

Characteristics of the Mathematical Model

The parameters a , b , c , and d give the mathematical model, expressed by the function of equation (2) its characteristics, which can be brought out by proper mathematical analysis. Some of the most significant ones with regard to this investigation are the

- A. Probability Distribution of the Yield, P_y
- B. Probability Distribution for the Spill, P_x
- C. Confidence Regions for the Yield and Spill
- D. Confidence Limits for the Yield Function
- E. Confidence Limits for the Spill Function

A detailed discussion of how these characteristics can be extracted from the above mathematical model follows.

A. Probability Distribution for the Yield,

P_y

To obtain the probability distribution for the yield function it is necessary to determine the ordinate for the probability distribution for each value of y .

This ordinate for a particular value of y is represented by the area of the cross-section of the mathematical model at this value of y and perpendicular to the x - y plane. This area can be obtained graphically or by integration requiring a large scale computer.

The integral representing the probability ordinate is

$$P_y(y) = \int_y^1 f(x,y) dx \quad (5)$$

The lower limit of equation (5) is the value at which $f(x,y)$ becomes positive for the chosen value of y . The function $f(x,y)$ is given in equation (2).

B. Probability Distribution for the Spill,

P_x

To obtain the probability distribution for the spill function the procedure is the same as in the above paragraph except that the variables x and y are interchanged so as to obtain the integral

$$P_x(x) = \int_0^{x^d} f(x,y) dy \quad (6)$$

Here the upper limit is the value of y at which $f(x,y)$ becomes negative for a chosen value of x .

C. Confidence Regions for Yield and Spill

To obtain probability regions for spill (x) and yield (y) it is necessary to determine the volume under the probability surface and then divide this volume into slabs of desired sub-volumes.

In this manner regions are obtained representing the intersections of planes, the sub-volumes, with the statistical surface. These intersections projected as regions simulate contour lines on a topographical map representing the various elevations.

The above analysis can be made by building a physical model of the mathematical function (using clay, putty, wood, etc.) and by determining the total volume and sub-volumes by submersion into liquid, or it can be done by double integration, again necessitating a large scale computer to solve integrals like

$$V_{x,y} = \int_0^1 \int_0^{x^d} f(x,y) dy dx \quad (7)$$

for the total volume and with different limits for the sub-volumes. The limits of the integrals have to give the required sub-volumes to include the desired percentages of x and y surface values.

D. Confidence Limits for the Yield

To obtain confidence limits for the yield function it is necessary to work with fractional areas under the yield probability distribution.

The peak of this curve represents the statistically most probable value. The fraction of the total area under the probability distribution lying between two values of y represents the fraction of all values in this interval. If the highest statistically expected yield is desired with a confidence, let us say of 95%, then the value of y has to be found for which 95% of the area under the probability distribution curves lie to the left of it. Many other questions of this type can be answered in this manner.

E. Confidence Limits for the Spill

The same information regarding the spill probabilities can be obtained as were described above for the yield. The procedure is the same except that the spill probability distribution curve is used in this case.

Information, in addition to the above, can be extracted from the mathematical model by sectioning it and sub-sectioning it physically or mathematically in various ways.

The calculation procedures A through E were computerized¹ and quantitative results are presented as examples for

- I. The Mathematical Model Applied to Available Experimental Data.
- II. The Mathematical Model Applied to Available Experimental Data and Missile Failure Yield Estimates.
- III. The Mathematical Model Applied to Available Missile Failure Yield Estimates.

A comparison of the results, obtained by the mathematical model defined here by a minimum of data, from these three examples and the actual observations, will give better insight into the workings and characteristics discussed above. With more representative, and better data, this mathematical model could be defined with greater statistical confidence, and the reliability of the numerical results presented increased.

I. The Mathematical Model Applied to Available Experimental Data

In this section the mathematical model, which was developed as described above, is

applied to test results which contain the necessary information to make this application possible. These are the results presented in Table I. They may or may not be representative of actual missile failures, but they certainly exhibit fundamental characteristics of liquid propellant explosions.

Table I
Experimental Data of Liquid Propellant Explosions

1. (D,H) _{max} Test Series	y = 0.78	x = 1.00
2. J ₁ Test	0.47	0.846
3. J ₂ Test	0.165	0.348
4. J ₃ Test	0.186	0.252

This very sparse experimental data is presented in Fig. 1 graphically. Applying standard curve fitting procedures the x-y functional relationship is obtained as also shown in this figure.

The estimating procedure, as outlined above, using equations (3a) through (4d) results in numerical values for the parameters a, b, c, and d. These values are

$$a = 3.1, \quad b = 4.0, \quad c = 1.1, \quad d = 1.5$$

The values of the parameters substituted into equation (2) define the mathematical model as controlled by the input as shown. The resulting function becomes a three dimensional configuration as seen in Fig. 2. It has steep sides and a flat body, best described as simulating a "Shark Fin".

Analysis of this surface gives much information about the original data, which was used in describing this surface, which could not have been obtained in any other way.

Evaluation of equation (5), using the above values for the parameters a, b, c, and d results in the yield probability distribution shown in Fig. I-1. Closer inspection of this distribution indicates that the most probable yield value for these experiments, as predicted by the model, is about 0.43, and analysis to obtain confidence limits indicates that, for instance, 95% of all yield values fall statistically below 0.8. From this yield probability distribution, other confidence limits can be obtained as desired.

Evaluation of equation (6) results in the probability distribution for the spill function. It is graphically presented in Fig. I-2. Using the same analysis procedures as above, the most probable spill value, as predicted by the model, is about 0.8, and 95% of all spill values lie below a spill value of 0.94. Again other confidence regions can be obtained as desired.

Confidence regions for both yield and spill can be obtained from the model by solving integrals of the type of equation (7) for the total volume and the required

sub-volumes with the results as shown in Fig. I-3. In this figure, all x-y values fall into an approximate triangular region bounded by points (0,0), (0.1), and (1,1); 80% of all x-y values fall into the next smaller region; 60% into the next smaller region; and so on. The peak point of the surface is also indicated.

Other relationships and information could be obtained by sectioning the mathematical model in different ways.

II. The Mathematical Model Applied to Available Experimental Data and Missile Failure Yield Estimates

The mathematical model is next applied to both the available experimental data and actual missile failure yield estimates. Unfortunately no actual missile failures have been instrumented thus far to provide the required information. For this reason a basic assumption had to be made before the missile failure information could be used. This assumption is that the relationship between the quantity of propellants mixed and the resulting yield is a fundamental characteristic of liquid propellant explosions. Preliminary investigations now under way seem to support this assumption.

The results presented in this section are based upon the data presented in Table I, the estimates of Table II, and the above stated basic assumption.

Table II
Yield Estimates and Data of Missile Failures^{3,4,5,6}

5. Atlas 9-C	y = 0.18	
6. Atlas 48-D	0.08	
7. Atlas	0.06	
8. Titan 1	~ 0.02	
9. Titan 1	~ 0.01	
10. Atlas	0.0088	
11. Centaur	0.029	Quad. 0.089, 0.017, 0.007, 0.003
12. Jupiter #9 (Impact)	0.11	
13. S-IV Failure	0.01	
14. S-IV Test (Pyro)	0.03 - 0.06	

Evaluating the parameters a, b, c, and d for the new input information in the same manner as for section I gives

$$a = 21, \quad b = 4.0, \quad c = 1.1, \quad d = 1.5$$

Comparing the new values with those obtained in section I shows that only the value for parameter a changed, the others remained the same. Again more and better data would determine these parameters with greater accuracy defining the mathematical model with greater statistical reliability.

The results for the above numerical set of parameter values are presented graphically in Fig. II-1, the yield probability distribution; Fig. II-2, the spill probability distribution; and Fig. II-3, the confidence regions for yield and spill.

From these results the most probable yield value as predicted by the model is now about 0.13 with 95% of all yield values falling below a yield value of about 0.29.

The most probable spill value as predicted by this model is about 0.32 with 95% of all spill values falling below about 0.48.

The yield-spill confidence regions are much smaller than before, as can be seen by comparing Fig. I-3 and II-3, and are much closer to the origin. Again the regions containing 100%, 80%, 60%, 40% and 20% of all x and y values are shown.

III. The Mathematical Model Applied to Available Missile Failure Yield Estimates

Applying the mathematical model as developed above to the data shown in Table II and the assumption made in Section II, the parameters take on the following values:

$$a = 70, \quad b = 4.0, \quad c = 1.1, \quad d = 1.5$$

The statistical surface described by these new parameter values gives, when analyzed, the results presented in Fig. III-1, the yield probability distribution; Fig. III-2, the spill probability distribution; and Fig. III-3, the confidence regions for yield and spill.

This analysis shows the most probable yield value, as predicted by this model, centers around a value of about 0.04 with 95% of the yield values falling below about 0.11.

The most probable spill function value, as predicted by this model, is about 0.16 with 95% of all spill values falling below about 0.27.

The yield-spill confidence regions are now getting quite small and so only the 100% and the 80% regions are shown. The peak point of the statistical surface has now moved rather close to the origin.

A Possible Scaling Law as Suggested by the Mathematical Model

Closer scrutiny of the numerical results presented here shows that for the information used, only parameter a changed between sections I, II, and III.

One of the major differences underlying the data of these sections is the quantity of propellants involved.

This fact, and that the parameter a was the only thing that had to be changed to redefine the model to make it applicable to the various sections, suggests that its variation with quantity of propellants involved may constitute the basis for a "Scaling

Law".

Expressing the parameter a as a function of the scale (s)

$$a = F(s) \quad (8)$$

which is an exponential relationship for the data and estimates presented here, and substituting this relationship into equation (2), gives the mathematical model described in terms of the scale (s) and the previous parameters b, c, and d.

Analysis of the mathematical model as described by equations (2) and (8) give the required scaling law for liquid propellant explosions.

Closure

From the work discussed and presented in this paper it is seen how a mathematical model can be constructed based upon the general characteristics of theoretical and experimental results of liquid propellant explosions, how this model can be applied to experimental results and the wealth of information which can be obtained in this manner.

The mathematical model developed and used here is very general in nature containing four controlling parameters and can therefore satisfy a wide range of data. It is not overly sensitive to changes in these parameters.

To demonstrate how this model can be used it was applied to the very sparse experimental data available and with a basic assumption, that the yield-spill relationship is a fundamental characteristic of liquid propellant explosions, to actual missile yield estimates.

The quantitative results predicted by this analysis such as probability distributions, confidence regions, confidence limits, etc. should be considered preliminary since the model used here was defined by very little data even though the obtained results are in general agreement with the limited actual experience.

The results obtained from the mathematical analysis of the model seem to suggest the parameter a as a "scaling factor" allowing the prediction of the characteristics of liquid propellant explosions as a function of scale, or quantities of propellants involved.

The reliability of the model should be improved for prediction purposes by better theoretical information and better experimental results, which describe and define the model more precisely by giving better values to the parameters.

In conclusion it may be well to say again that the mathematical model presented here, and others like it can help in guiding future experimental program, indicating what information is needed and where, and in reducing the cost of these programs by reducing the number of expensive test necessary. Furthermore the approach through a mathematical model may well indicate the most direct route

to follow to obtain a valid scaling law for yield prediction for liquid propellant explosions.

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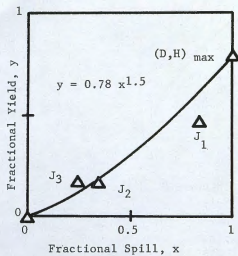


Figure 1 Yield Function -
Spill Function Relationship



Figure 2 Mathematical Model
Represented by a Statistical
Surface (Shark Fin)

The Mathematical Model, $a = 3.1$, $b = 4.0$, $c = 1.1$, $d = 1.5$

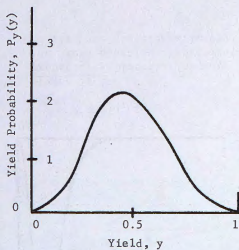


Figure I-1
Probability Distribution for
the Yield Function
(Experimental Results)

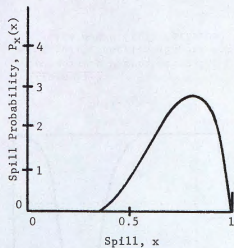


Figure I-2
Probability Distribution for
the Spill Function
(Experimental Results)

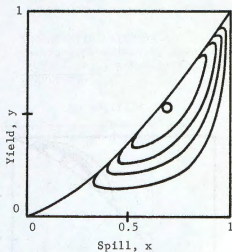


Figure I-3
Yield - Spill Probability
Regions
(Experimental Results)

The Mathematical Model, $a = 21$, $b = 4.0$, $c = 1.1$, $d = 1.5$

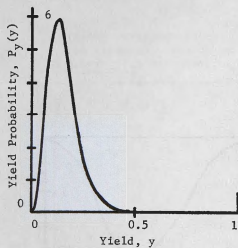


Figure II-1
Probability Distribution for
the Yield Function (Experimental
Results and Missile Failures)

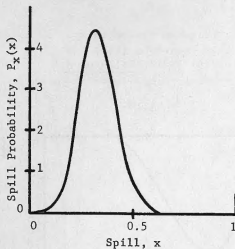


Figure II-2
Probability Distribution for
the Spill Function (Experimental
Results and Missile Failures)

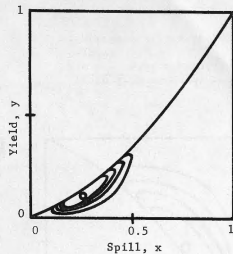


Figure II-3
Yield - Spill Probability
Regions (Experimental Results
and Missile Failures)

The Mathematical Model, $a = 70$, $b = 4.0$, $c = 1.1$, $d = 1.5$

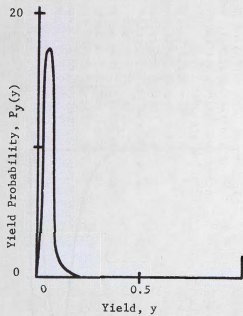


Figure III-1
Probability Distribution for
the Yield Function (Missile
Failures)

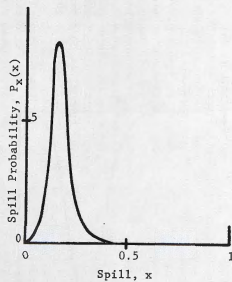


Figure III-2
Probability Distribution for
the Spill Function (Missile
Failures)

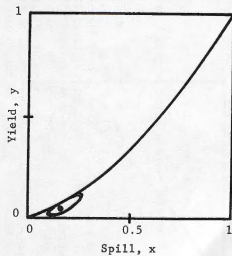


Figure III-3
Yield - Spill Probability
Regions (Missile Failures)