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MEMORANDUM REPORT NO. 2729

COMPARISON OF PREDICTIONS OF THREE TWO-PHASE FLOW CODES

Carl W. Nelson

February 1977

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USA BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER MEMORANDUM REPORT NO. 2729	2. GOVT ACCESSION NO.
	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (*and Subtitle*) Comparison of Predictions of Three Two-Phase Flow Codes	5. TYPE OF REPORT & PERIOD COVERED BRL Memorandum Report
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(*s*) Carl W. Nelson	8. CONTRACT OR GRANT NUMBER(*s*)
9. PERFORMING ORGANIZATION NAME AND ADDRESS USA Ballistic Research Laboratory Aberdeen Proving Ground, MD 21005	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 1W161102AH43
11. CONTROLLING OFFICE NAME AND ADDRESS USA Materiel Development & Readiness Command 5001 Eisenhower Avenue Alexandria, VA 22333	12. REPORT DATE February 1977
	13. NUMBER OF PAGES 36
14. MONITORING AGENCY NAME & ADDRESS(*if different from Controlling Office*)	15. SECURITY CLASS. (*of this report*) Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (*of this Report*)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (*of the abstract entered in Block 20, if different from Report*)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (*Continue on reverse side if necessary and identify by block number*)

two phase flow, flame spreading, solid propellant, guns, interior ballistics, computer codes

20. ABSTRACT (*Continue on reverse side if necessary and identify by block number*) ssv/4589

Three different two-phase flow codes (University of Illinois, Calspan, Gough) have been compared by application to a 155mm howitzer high zone charge with input data derived from independent measurements or analysis. Code predictions were compared with firing test values and with a lumped parameter code. Quantitative comparisons are reported for pressure difference waves, peak breech pressure, rise time and travel at peak pressure, flame spreading rate, and CPU time. The major findings were that (1) each code predicts different pressure waves, (2) pressure wave predictions are insensitive to the presence of the central core igniter, and (3) nominal data are inadequate for quantitative predictions.

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LIST OF SYMBOLS

A	particle surface area
C	particle specific heat
D	particle drag
d_m	effective particle diameter
f	drag coefficient
g_c	gravitational constant
q_t	heat absorbed at ignition
Q	heat flux to solid
t_{ig}	particle ignition time
T_b	particle bulk temperature
T_o	particle initial temperature
T_s	particle surface temperature
u	gas velocity
u_p	solid velocity
V_i	particle volume
α	thermal diffusivity
λ	thermal conductivity
ρ	particle density
ϕ	porosity

I. INTRODUCTION

There now exist several numerical codes to predict the two-phase interior ballistics of solid propellant guns. The debate on the correctness of the governing equations should seek the practical effects of their differences. This report will compare the predictions of three such codes for the interior ballistic performance of a 155mm howitzer with a high zone charge.

The codes to be compared are those of the University of Illinois, Calspan, and Gough. Differences in the theoretical approach have been described by Kuo[1] elsewhere. A comparison of the key differences is shown in Table I.

Table I. Comparison of Features

	Illinois	Calspan	Gough
Igniter Flow Rate	Specified	Computed	Specified
Bed Compaction	None	Elastic	Inelastic
Ignition Criteria	Bulk Temp	Surface Temp	Surface Temp
Area of Igniter	Ignored	Considered	Ignored
Effective Particle Diameter	6V/S	$\sqrt[3]{6V/\pi}$	6V/S
Internal Boundaries	None	Implicit	Explicit

The common data are the best independent estimates of the required input for the codes. To the extent possible, code peculiarities were not considered in selecting the input data. Physical measurements, burning rate and ignition experiments, shell pushing test experiments, and thermodynamic calculations provided input without a posteriori adjustment to improve code-test agreement. Constants for empirical correlations for viscous drag and heat transfer were those suggested by the original correlations. Arbitrary assignment of other constants was made usually on the code author's recommendation.

This task has the limited goal of comparison of the predictions. It does not firmly establish the roots of any differences nor does it attempt to simulate gun firings by manipulation of terms and parameters. The approach is to identify the a priori prediction capability with independent input. One exception was an arbitrary increase in bore resistance to match peak bore resistance and peak chamber pressure with test values for the gun when peak pressure was under predicted as has been the usual experience with interior ballistics codes. Even though only one problem has been run, some semblance of generality has been retained.

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[1] *Kuo, K. K., "Report on the JANNAF Workshop on Theoretical Modeling and Experimental Measurements of the Combustion and Fluid Flow Processes in Gun Propellant Charges," 13th JANNAF Combustion Meeting, Monterey, CA, September 1976. Proceedings to be published.*

II. EXPERIMENTAL

The Problem

The 155mm howitzer with a charge of 11.8kg of M30 propellant has been observed to be prone to pressure waves under certain ignition conditions[2]. The charge-in-chamber configuration has been approximately simulated by considering a uniformly tapering chamber holding a bore size charge with a one inch standoff from the breech.

Input data are given in Table II. About the physically measurable data there should be no debate. About the other data there are definite uncertainties because they can only be indirectly determined.

Table II. Input Data

Initial Temperature	294 K
Speed of Sound in Packed Bed	442 m/sec
Settling Porosity of Nominal Composition	0.424
Left Hand Boundary of Propellant	2.5 cm
Right Hand Boundary of Propellant	79 cm
Mass of Propellant	11.8 kg
Density of Propellant	1.58 g/cm^3
Number of Perforations	7
Outside Diameter of Grain	1.05 cm
Inside Diameter of Grain	0.081 cm
Length of Grain	2.41 cm
Burning Rate Coefficient	0.012 cm/s /(MPA)$^{.67}$
Burning Rate Exponent	0.67
Ignition Temperature	450 K
Chemical Energy of Propellant	4420 J/g
Molecular Weight of Propellant Gas	23.46
Specific Heat Ratio	1.24
Covolume	0.945 cm^3/g
Chemical Energy of Igniter	3450 J/g
Mass of Projectile	43.6 kg

Igniter flow rates needed for the Illinois and Gough models were derived from experiments by White, et al[3]. Flow from the base pad is assumed to occupy the first 2.5cm from the breech. Although the real base pad is only about 0.6cm thick, numerical considerations dictate that the source extend over a longer distance. In Gough's code, instability results when the igniter flow does not occupy the entire standoff gap.

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[2] *Clarke, E. V., May, I. W., "Subtle Effects of Low Amplitude Pressure Wave Dynamics on the Ballistic Performance of Guns, 11th JANNAF Combustion Meeting, CPIA Pub 261, p 141-156, September 1974.*

[3] *White, K. J., Price, C. F., May, I. W., "Black Powder and Clean Burning Igniter Train Studies," 13th JANNAF Combustion Meeting, Monterey, CA, September 1976. Proceedings to be published.*

Bore resistance is computed from an expression proposed by Pilcher[4]:

$$P_{res} = f(z)\left(\frac{1+a\dot{z}}{1+b\dot{z}}\right)$$

where $\dot{z}$ is the projectile velocity, a and b are constants, f(z) is the static friction pressure. For this problem, f(z) is shown in Figure 1 where is also shown some results of using the formula. After the nominal values allowed an under-prediction of peak chamber pressure, values for the constants were decreased to give a better match to resistance measurements for low zone charges[5]. The ratio between the two was kept constant. The shaded area in Figure 1 includes all the peaks of resistance vs travel functions for the low zone firings. That they do not occur at the peak static resistance distance shows a deficiency in either the formula or the test data. The short table on Figure 1 shows the effect on maximum pressure of changing the constant a from its nominal value (a_o). P_{max} values in MPa.

The Illinois and Gough codes use the formula 6V/S(where V is the particle volume and S the wetted surface) for an effective spherical particle for drag computation. Surface is the burning surface including the perforations. The Calspan code uses the cube root of the particle volume ignoring the perforations. Random orientation of the particles makes the internal passages mostly unavailable for axial gas flow. To the gas they appear as solid right circular cylinders. For the particle dimensions on this problem the three approaches yield the following estimates for effective diameter initially and after 20% of the web has burned:

	Initial	20% Web Burned
Calspan	13mm	12mm
Illinois; Gough	9mm	7mm
Solid Cylinders	13mm	12mm

The larger effective diameter translates to a proportionately lower drag estimate. In trials with an earlier version of the Gough code, the revised formula caused the predicted first reverse pressure gradient to fall by about one third. As the grain burns the disparity ratio grows although the effect on the flow probably decreases. In this comparison problem the Illinois and Calspan codes have been run with the original formulation; the Gough code has used the solid cylinder formula.

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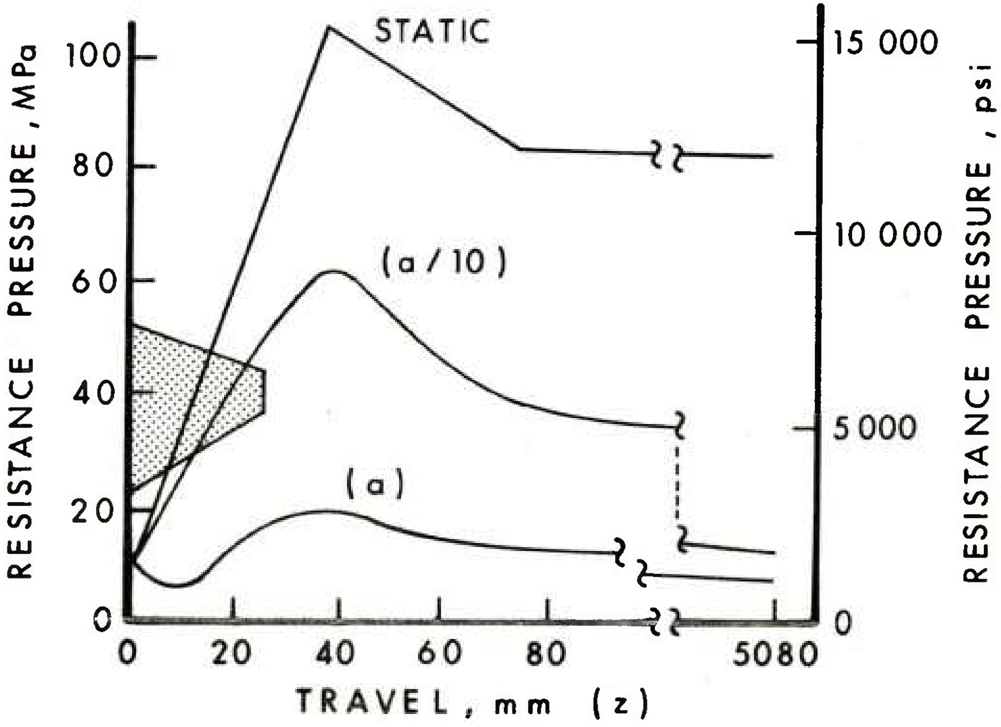
[4] *Pilcher, J. O., Wineholt, E. M., "Analysis of the Friction Behavior at High Sliding Velocities and Pressure for Gilding Metal, Annealed Iron, Copper and Projectile Steel," BRL Report (in press), 1976.*

[5] *DeLorenzo, J., Vallado, A. C., "Compilation of Traces and Tabulation of Round to Round Data for the 155mm XM211 Program (Phase I) Conducted at Picatinny Arsenal 12-23 April 1976," unpublished, Picatinny Arsenal, May 1976.*

$$P_{RES} = \underset{\text{(static)}}{f(z)} \underset{\text{(dynamic)}}{\left[\frac{1.+a\dot{z}}{1.+b\dot{z}}\right]}$$



a/a_o	P_{MAX}
3.5	250
1.0	272
0.1	321

Figure 1. Bore Resistance

Because one of the main purposes for development of these codes is finding the effect of igniter variations, two configurations have been computed. The first was a nominal base pad plus center core; the second was base pad only.

Inputs peculiar to each code are discussed in the section on that code.

A. Illinois Model

The Illinois model has been documented in three articles[6,7,8] which describe the approach and some results; the coding has not been published. Of note are the diffusion terms in the momentum and energy equations, the use of a solid phase energy equation, the bulk temperature ignition concept, and the treatment of the gas phase pressure gradient. Potential users of the model should be aware that there are a few differences between the documented equations and the coding. The only serious difference is that the coding uses a convective derivative for a coordinate system expanding at the projectile velocity as does Gough's code.

Bulk Ignition Temperature is a concept peculiar to this code whereby ignition is assumed to occur when the solid phase has absorbed a specified amount of energy. An implicit assumption is made that the ignition energy is independent of rate of heating. No experimental data are offered to estimate an input value.

To be consistent with the other two codes where surface temperature is the ignition criterion, a bulk temperature must be computed that gives ignition at about the same time. For a unit volume, the heat exchange from hot gas to solid at a constant heating rate is

$$(1-\phi_o)\ \rho C(T_b-T_o) = QA\ t_{ig}(1-\phi_o)/V_i \tag{1}$$

from which the ignition time is

$$t_{ig} = \frac{\rho C(T_b-T_o)V_i}{QA} .$$

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[6] *VanTassell, W., Krier, H., "Combustion and Flame Spreading Phenomena in Gas Permeable Explosive Materials," Int J Heat and Mass Transfer 18 pp 1377-1386 (1975).*

[7] *Krier, H., Rajan S., VanTassell, W., "Flame-Spreading and Combustion in Packed Beds of Propellant Grains," AIAA J 14 (3), p 301-309 (1976).*

[8] *Krier, H., Gokhale, S. S., "Predictions of Vigorous Ignition Dynamics for a Packed Bed of Solid Propellant Grains," Intl J Heat and Mass Transfer, 19, p 915-923, 1976.*

The surface temperature of a semi-infinite solid can be taken from Carslaw and Jaegar[9]

$$T_s = T_o + \frac{2Q}{\lambda} \sqrt{\frac{\alpha t_{ig}}{\pi}} \tag{2}$$

from which the ignition time can be extracted and equated to the bulk ignition time and the resulting equation solved for the Bulk Ignition Temperature rise.

$$T_b - T_o = \frac{\lambda A}{4QV}(T_s - T_o)^2 \ . \tag{3}$$

For the values used in this problem the expression reduces to

$$T_b - T_o = 705/Q \ .$$

The Illinois code predicts a heat flux varying from 50 to 300 cal/cm^2/sec with an average value of 180. The resultant bulk temperature rise is then

$$T_b - T_o = 4°K \ .$$

An alternative approach is to consider the data of Summerfield et al[10] [Fig. 16, p. 105] which gives ignition time as a function of heating rate

$$t_{ign} = bQ^a \ . \tag{4}$$

Applying the data reported to the formulation and assuming a constant heating rate

$$q_t = 0.9\ Q^{-0.2}$$

Substituting Q_t for Q_{tig} in Equation (1) yields an estimate

$$T_b - T_o = 3.3°K \ .$$

That the two estimates are close to each other is satisfying enough to use 4°K as the bulk ignition temperature rise for this problem. Krier et al have used a series of temperature rises ranging from 5 to 25°K as an arbitrary input parameter.

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[9] *Carslaw, H. S., Jaeger, J. C., "Conduction of Heat in Solids," Oxford University Press, London, 1959.*

[10] *Summerfield, M., Caveny, L. H., Ohlemiller, T. J., DeLuca, L., "Ignition Dynamics of Double Base Propellants," in BRL Report 1707 (ed by I. W. May and A. W. Barrows), April 1974, AD #919315L.*

Heat feedback to the solid phase during combustion continuously increases the solid phase temperature. As suggested by VanTassel and Krier the "heat of vaporization" is taken as 10% of the total energy release in combustion. A difficulty arises in adding the heat of vaporization as a sensible heat effect when it nominally represents a phase change. The payoff comes at burnout when there is no sink for the stored sensible heat in the solid phase. Program execution stops before burnout.

The code has been applied to two other problems. Beckstead et al[11] found it a useful tool in DDT analysis of a simulated rocket motor grain. Krier and Gokhale[8] modeled a propellant bed ignited by a detonating pellet. In the latter application, the detailed results from a typical page of output showed some anomalous values. Gas temperatures were reduced well below the initial temperatures in the forward portion of bed while the particle temperature was rising - a violation of the second law of thermodynamics. Gas temperatures in several cells at the breech were well above the flame temperature of the pressurizing gases even though no external work is done on the bed. A porosity minimum of 0.25 was arbitrarily assigned even though the assumption of no particle interaction has long been invalid by the time the porosity drops to that value. At that point porosity gradients become arbitrary.

B. Calspan Model

The Calspan artillery code has been used to simulate several guns. Fisher et al[12,13] reported simulation of a 155mm howitzer with coding adapted to the 155mm configuration.

Input for this code is more extensive than for the other two. Details are required for the igniter train to include igniter burning rate function, thermal properties, geometry of base pad and/or central core,

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[11] *Beckstead, M. W., Peterson, N. L., Pilcher, D. T., Hopkins, B. D., Krier, H., "Convective Combustion Modeling Applied to Deflagration-to-Detonation Transition," 12th JANNAF Combustion Meeting, CPIA Publication 273, 1975.*

[12] *Fisher, E. B., Graves, K. W., Trippe, A. P., "Application of a Flame Spread Model to Design Problems in the 155mm Propelling Charge," 12th JANNAF Combustion Meeting, CPIA Pub 273, p 199-219, December 1975.*

[13] *Fisher, E. B., Graves, K. W., "Propellant Ignition and Combustion in the 155mm Howitzer," Calspan Corp Report VQ-5524-D-2, January 1975.*

equation of state, and ignition temperature. Comparing references[12-16] shows that no single set of values for black powder has been used in Calspan's applications. For this test problem input values were a combination of references[13-17]. Key values are shown in Table III.

Table III. Black Powder Properties

Parameter	Value	Source
Ignition Temperature	550K	Ref.17
Heat of Explosion	670 cal/g	Ref.17
Density	1.8 g/cc	Ref.17
Burning Rate Coefficient	$1.2\ \text{cm/sec/atm}^{.24}$	Ref.18
Burning Rate Exponent	0.24	Ref.18

Other constants for computing the thermodynamic properties of the black powder and the product gas were as used by Calspan.

Calspan's simulation of the 155mm howitzer[12] used arbitrary values for shot start and particle drag to force a match between predicted and observed values of peak pressure and pressure wave amplitudes. Nominal values are used in this study.

Three different drag laws have been used in the various applications of the code. For this case the law used is that supplied with the code:

$$D = \frac{2f}{g_c d_m} \left(\frac{1-\phi}{\phi}\right) \rho (u-u_p) \left| u-u_p \right| \tag{5}$$

where $f \simeq 1$. (Note that in Ref. 12, $f=5$.)

A distinctive feature of this code is that igniter input is computed rather than specified. When the black powder charge configuration is specified, ignition and gas production and flow from the igniter are coupled to the main bed computation. For computer time considerations the sequence is artifically speeded by assuming the base pad is already

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[14] *Fisher, E. B., Trippe, A. P., "Development of a Basis for Acceptance of Continuously Produced Propellant," Calspan Report No. VQ-5163-D-1, November 1975.*

[15] *Fisher, E. B., Trippe, A. P., "Mathematical Model of Center Core Ignition in the 175mm Gun," Calspan Report VQ-5163-D-2, March 1974.*

[16] *Fisher, E. B., "Propellant Ignition and Combustion in the 105mm Howitzer," Calspan Corp. Report No. VQ-5524-D-1, January 1975.*

[17] *Gough, P. S., "Fundamental Investigation of the Interior Ballistics of Guns," Space Research Corporation SRC-R-75, August 1974 (also IHCR 75-3, Naval Ordnance Station).*

ignited by the primer. Variations have been run with the propellant also ignited near the base of the charge and with the entire black powder charge ignited. To make the Calspan code more like the other codes, one could specify a completely ignited black powder charge with propellant at ambient temperature.

C. Gough Model

The Gough model has been under continual revision since the first version[17]. A major revision[18] added internal boundaries to handle the gas/bed interfaces, especially for Army propelling charges. A second revision[19] added the treatment of an irreversible constitutive law for particle-particle stress, an unsteady boundary layer, and unsteady combustion.

Peculiar input is needed for the filler element between the front end of the charge and the projectile, for the decay constant for sound speed in the packed bed. Adiabatic inelastic compression of air in front of a 0.25kg salt bag was assumed as a first approximation. Inelasticity is a compromise to permit stable calculation at the boundary. Some support for the adiabatic compression is found in the data of East and McClure[20].

This code provides the most complete description of the mechanical aspects of the bed dynamics. With explicit representation of boundaries between regions separated by discontinuities, numerical smearing of the boundaries is eliminated. Increased friction and stress transmission as compaction increases permits more accurate computation of gradients within the bed.

To retain a degree of commonality in this study, the most recent code developments have not been used. Neither transient combustion nor the Shelton type boundary layer analyses has been exercised or analyzed enough to permit confidence in the results.

III. RESULTS

The computed predictions of each code are compared in Table IV with test data and with the prediction of the Baer-Frankle lumped parameter code with the same input. Values in parenthesis are for the base pad only igniter configuration.

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[18] *Gough, P. S., "Numerical Analysis of a Two Phase Flow with Internal Boundaries," Paul Gough Associates PGA-TR-75-4, November 1975.*

[19] *Gough, P. S., "Numerical Analysis of a Two Phase Flow Model of Interior Ballistics," Paul Gough Associates PGA-TR-76-1, April 1976.*

[20] *East, J. L., McClure, D. R., "Experimental Studies of Ignition and Combustion in Naval Guns," 12th JANNAF Combustion Meeting, CPIA Publication 273, p 221-257, December 1975.*

Table IV. Comparison of Predictions - Nominal Input (Base Pad Only)

	Experiment	Illinois	Calspan	Gough	Lumped Parameter
Pressure Diff (MPa)					
First Trough	-6(-100)	-43(-26)	-8(-4)	-6(-8)	
Second Peak	14(150)		14(10)	24(24)	
Max Breech Pressure(MPa)	312(450)		251(240)	272(270)	268
Time (P_{1000}-P_{max}) (ms)	6		7.7(8.0)	6.5(6.7)	6
Muzzle Velocity (mps)	830(860)		787(730)	785(790)	793
Travel at P_{max}(m)			1.0(1.1)	0.6(0.6)	0.5
Flame Spread Rate (mm/μs)		0.2(0.2)	0.2→0.5	0.2→0.5	
CPU Time (min)		*	16**	11	0.1

* Halted at 26 min
** Estimated Equivalent 1108 Time

Of first, but not surprising, note is that peak pressure and muzzle velocity predictions are lower than firing test values. Also not surprising is that these codes take at least 100 times more computer time than a lumped parameter code.

Figure 2 examines the predictions of pressure wave behavior for nominal igniter. The shaded area is a composite of ten firing tests[21]. The time scale is translated for each case to align all the curves at the first negative pressure difference. Qualitative differences are obvious in magnitude of the waves. The Illinois code predicts a large first negative but was stopped from running further because the time increment was too small to allow competitive calculations. Only the Gough code followed the observed gun behavior. The dip between 6 and 7 milliseconds in the Gough prediction derives from a strange dip in breech pressure immediately after its maximum.

Figure 3 shows pressure wave behavior for a base pad only igniter. The shaded area represents a composite of five firings with only 10.9kg of propellant [sequence A20, Ref. 21]. Two similar waves have been seen in 11.8kg charges [Rd A127, 165, Ref. 21] that are presumed to be due to base ignition. One case is known of catastrophic pressure wave. Values shown as experimental in Table IV represent typical values. The Illinois code predicted a smaller first reverse difference. The Calspan and Gough codes predicted no substantial change. None approached a catastrophic condition.

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[21] *Firing Record P82415 Aberdeen Proving Ground, March 1974.*

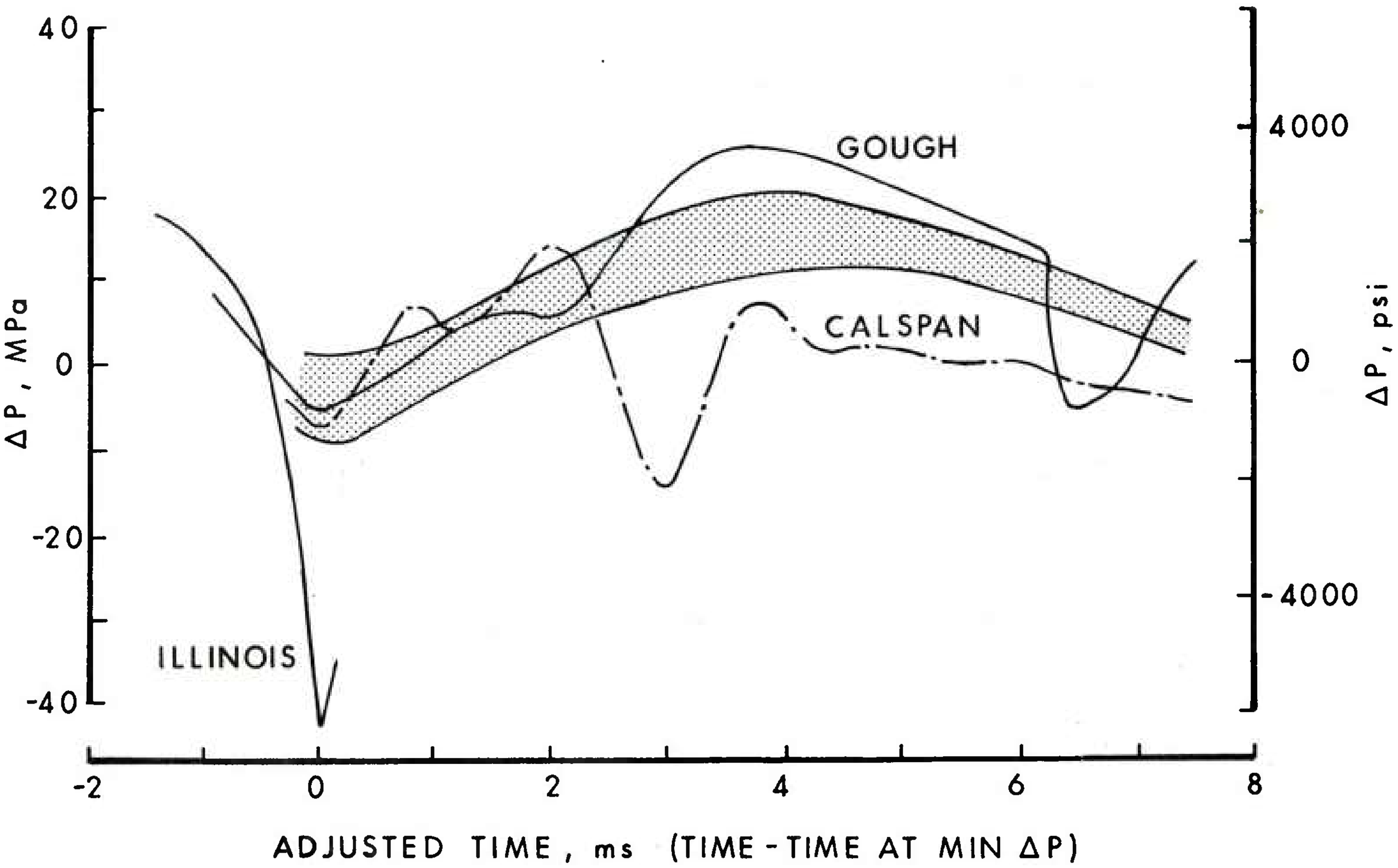

Figure 2. Pressure Differences, Nominal Input Data

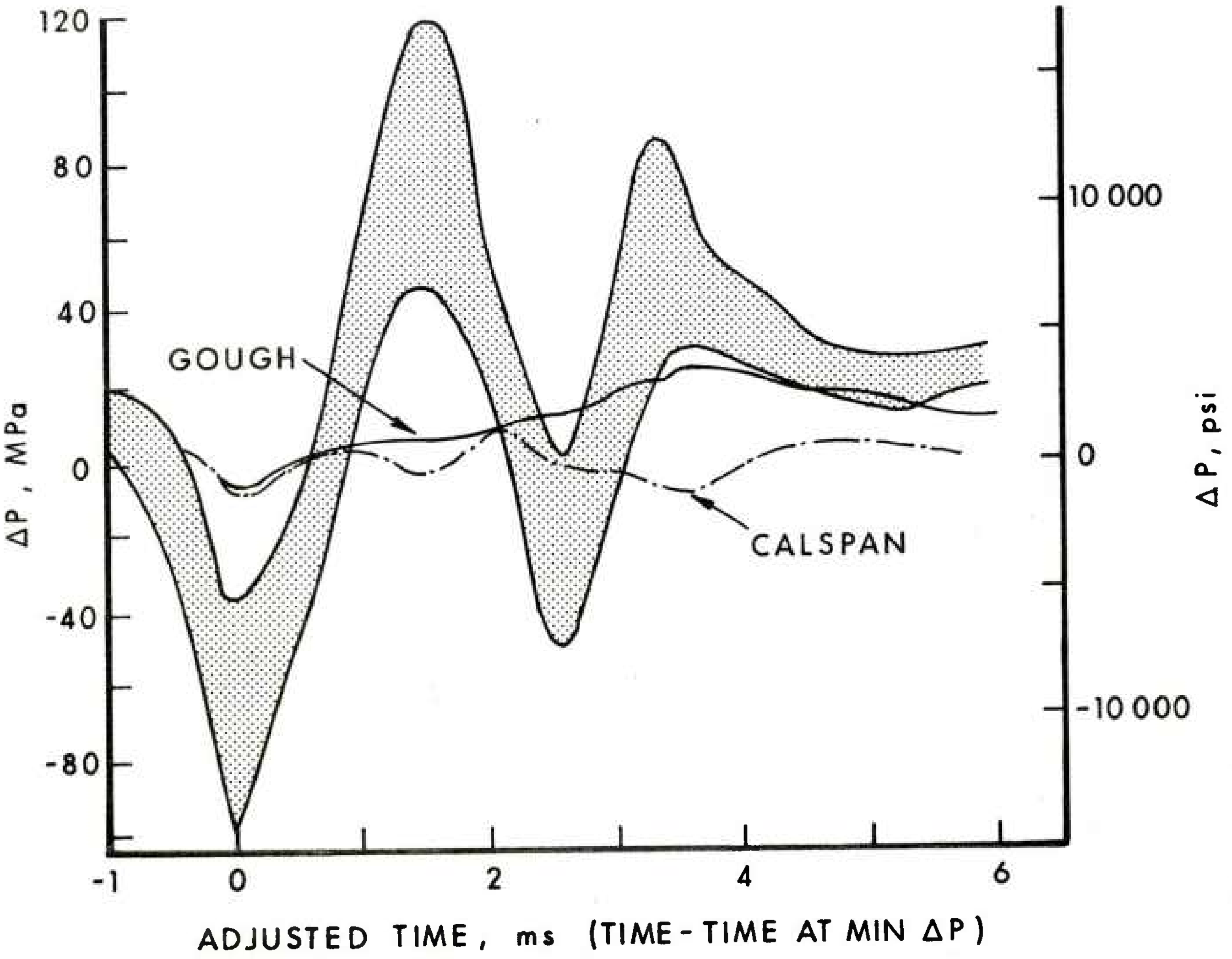

Figure 3. Pressure Differences, Base Pad Igniter Only

Such indifference to the presence of the center core raises a serious issue in predictive capability of the codes. If the igniter truly functions as described, the codes are somewhere missing an important piece of physics. If the codes are correctly formulated, the igniter must not be working as described. Only well controlled experiments in measurement and prediction will be able to resolve the difficulty.

It is beyond the scope of this report to examine each code's sensitivity to adjustments in input data in an attempt to match predictions with test results. The limited amount of such testing by this author and the codes' authors has shown that the drag coefficient and low pressure burning rate can be manipulated to obtain "correct" pressure waves and peak chamber pressures. Justification for such changes is a separate topic.

Predicted and measured breech pressure for the nominal igniter are shown in Figures 4 and 5.

For those who believe that a correct peak pressure and muzzle velocity is a necessary condition for acceptance of other code predictions, a higher resistance was hypothesized by assuming a weaker dependence of friction on projectile velocity. The wave dynamics were essentially unaffected.

Code efficiency can be measured by CPU time shown. To maintain stable calculations, the Illinois code restricts the time step severely during the first cycle of the pressure difference wave. Calspan's detailed igniter description causes long bed ignition delay time; and thus long times to problem completion. All times are for UNIVAC 1108.

The Calspan and Gough codes predict that the flame spreading speed increases from 0.2mm/μs to 0.5mm/μs as it traverses the bed. The Illinois code shows a smaller increase. Experimental values are not available for the true rate.

Anomalous Results

For those predictions which have not been verified by measurement, one must rely on intuition and analysis to decide whether to believe the predictions. Examination of the detailed results of these codes show anomalies that reveal errors in the models.

The Illinois code assumes that the bed is always fluidized. Experience says that at the charge loading porosity of about 0.45 there is particle interaction and increased resistance to particle motion within the bed. This fact is recognized in the Illinois code by arbitrarily establishing a lower limit on local porosity (here 0.25). An override operates whenever the solution of the equations says the porosity should be lower than this limit. Thus a continuous fluidization

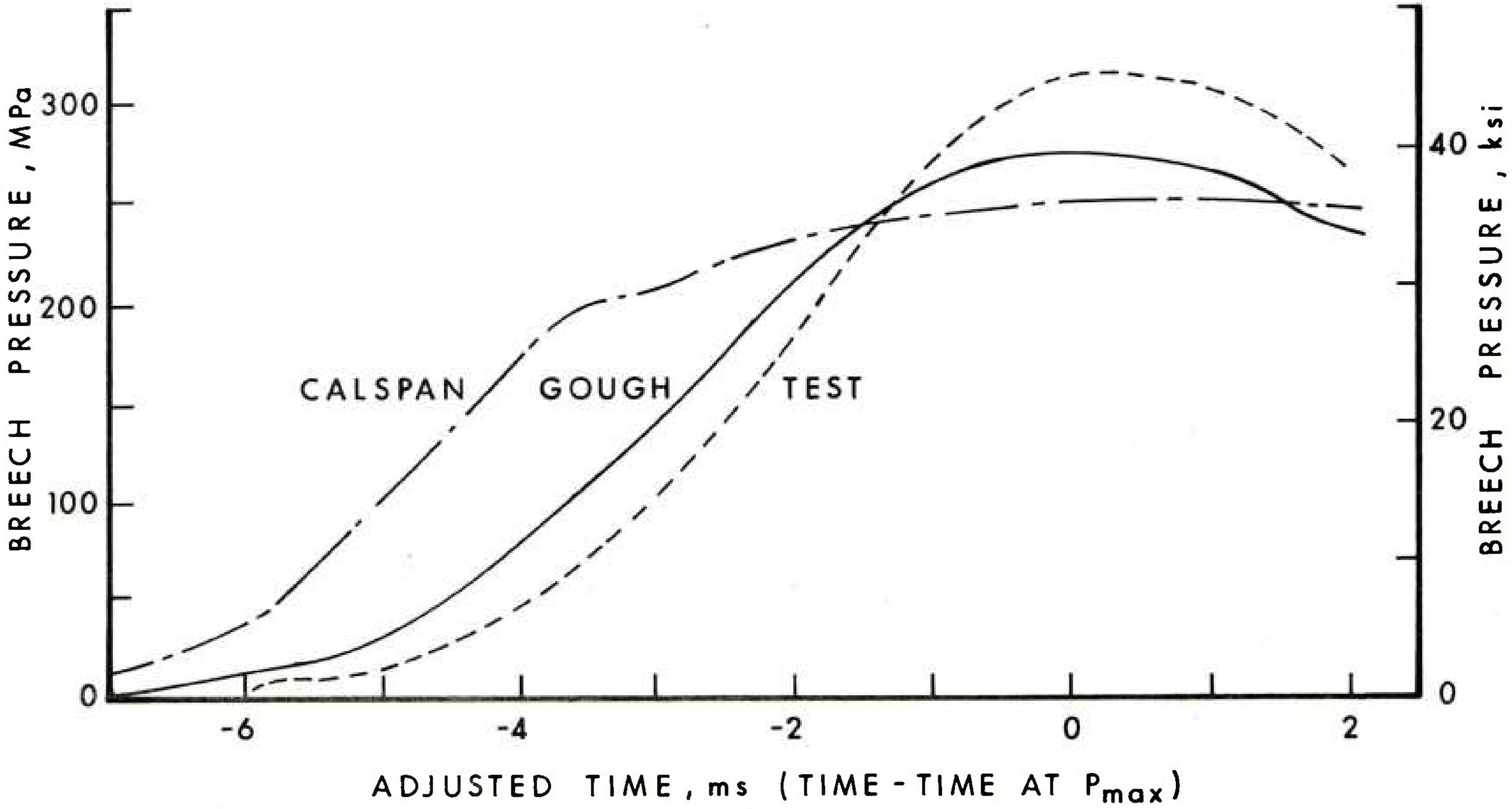

Figure 4. Breech Pressure, Nominal Input Data

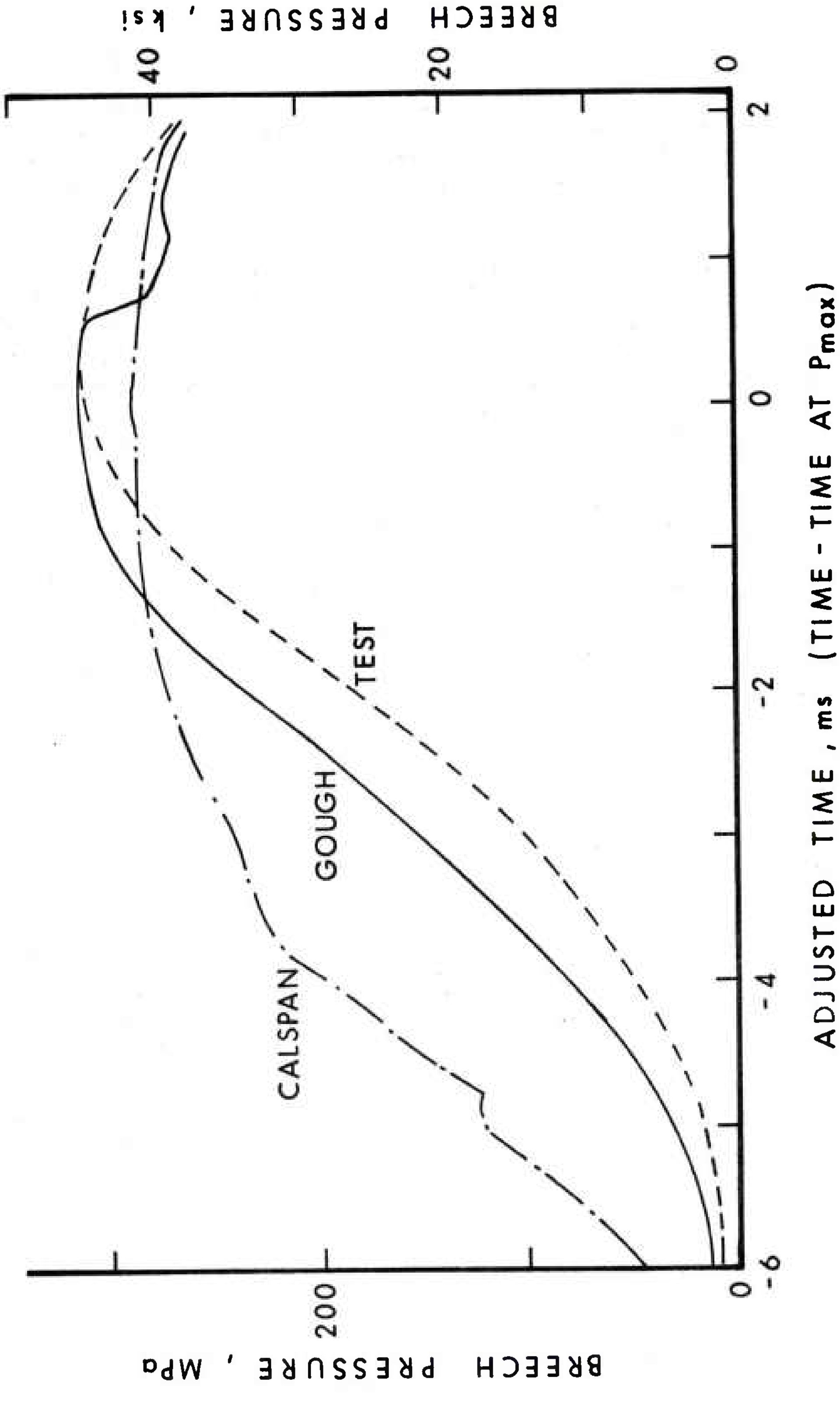

Figure 5. Breech Pressure, Higher Resistance

is assumed for all porosities above 0.25. Where the override is imposed, the solution is distorted by artificially changing the derivatives of porosity which appear in the governing equations. The degree of distortion cannot be estimated for the non-linear coupled equations. Whether the override offsets or aggravates the inaccuracies from ignoring compaction is not directly determinable. That the two may offset each other is not enough justification to believe the results.

Gas temperatures in the Illinois code indicate a deficiency in the energy equation. When the igniter functions at the breech end of the bed only, the gas temperatures in the forward portion of the bed drop below the initial temperature by as much as 50% while the solid phase temperature is rising with convective heat transfer between gas and particles as the only allowed mechanism, the second law of thermodynamics is being violated. Heat is free to flow in either direction between the phases before ignition.

The Calspan calculations show no compaction of propellant grains at the projectile base as the first pressurization wave reaches the forward end of the bed. Intuition and related experimental evidence say that drag carries propellant grains across the initial gap to stagnate at the projectile base. Numerical difficulties were observed in earlier versions of Gough's code in that event with an implicit representation of the internal boundaries. Whether the anomaly results from the governing equations or the numerics has yet to be determined.

IV. CONCLUSIONS

Three overall findings may be listed:

a. Each code predicts different pressure waves.

b. Pressure wave predictions are indifferent to the presence of the center core.

c. Nominal data are inadequate for quantitative predictions.

Although the debate on the implications of the differences in approach may have been assisted by this study, no judgments on general applicability or accuracy of any one code are justified on the basis of this one case. Each potential user must still make his own judgment of the merits of each code.

What is clear from the study is that the present combination of input data and governing equations must be improved considerably before *a priori* predictions can be made for Army type propelling charges. The state-of-the-art still requires some arbitrary assignment of parameters to force the desired agreement with test firings for a particular system. Sensitivity studies from that base can then be made but not without recognition of the limitations imposed by the assumptions.

Immediate Research Needs

Experimental measurements are needed to validate the formulations for bore resistance, drag and compaction, and igniter functioning. Bore resistance is important for calculating peak pressure and muzzle velocity. Drag and compaction laws and igniter functioning affect pressure wave behavior.

The present differences between the Calspan and Gough codes are not wide enough to justify detailed numerical studies. Physics, not numerics, seem dominant.

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