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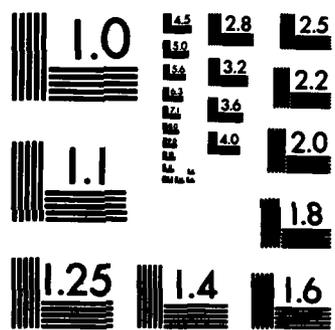
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ON THE NUMERICAL ACCURACY OF
HOMOGENEOUS SOLID PROPELLANT
COMBUSTION MODELS

Martin S. Miller
Terence P. Coffee

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Most theoretical treatments of solid propellant combustion assume a highly idealized mechanism: an exothermic surface decomposition reaction followed by a single exothermic gas-phase reaction. Despite its conceptual simplicity this mechanism does not permit an exact solution to the conservation equations. Published combustion models addressing the stated idealization rely on various approximation schemes which have never been tested for accuracy. This report examines the numerical reliability of a number

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Abstract (Cont'd):

20. of these schemes by direct comparison of model results with accurate numerical integrations of the conservation equations. Four propellant data sets which span a wide range of kinetics parameters were utilized. None of the approximations proved accurate for all the data sets but some models are quite accurate in certain limiting cases. The calculations provide a benchmark against which future models might be tested.

TABLE OF CONTENTS

3

LIST OF ILLUSTRATIONS

I. INTRODUCTION

The mechanism of solid propellant combustion is commonly idealized as a single exothermic pyrolysis reaction occurring at the surface followed by a single exothermic chemical reaction in the gas phase. Additional assumptions, such as constant thermal conductivity, and unit Lewis number, are also usual. The appropriate equations and boundary conditions are derived elsewhere.[1] A comparison of the solution to these equations with experimentally measured burning rates should provide information as to the correctness of the assumed mechanism. In practice one of the difficulties with this line of reasoning (others are discussed in Ref. 2) is that these equations do not have analytic solutions and indeed can sometimes be difficult to solve numerically. Generally this problem has been dealt with by making further simplifications in the equations to obtain a convenient computational algorithm. The object of this paper is to test the accuracy of these algorithms by direct comparison with numerical solutions.

It has previously been shown[1] that most models addressing the stated mechanism can be catalogued by the assumed manner of heat release in the gas-phase. These methods of specifying the heat release are generally appropriate to complementary ranges in the kinetics parameters. Since no general agreement exists on the values of these parameters for any propellant, we have developed several data sets which cover a sufficient range of variation to probe the strengths and weaknesses of all the model algorithms. The reasoning behind these data sets is given in a companion paper[2] but the values are summarized here in Table 1 for convenience.

II. DESCRIPTION OF PROBLEM AND NUMERICAL SOLUTION

A. Basic Idealization.

The mechanism used in this study is common to more models than probably any other. Along with the attendant conservation equations, it is thoroughly discussed in Reference 1. In brief, it is assumed that propellant molecules "A" pyrolyze at the solid surface into gaseous products "B" and "C" at the mass burning rate M ($gm/cm^2 s$) which depends on the surface temperature T_s according to

$$M = M_o \exp(-E_s/RT_s) . \tag{1}$$

(Symbols are identified in the List of Symbols and in Reference 1). This surface reaction is exothermic by an amount Q_s(cal/gm). The pyrolysis product B is the reactant for the gas-phase reaction of order ν. B is converted by this reaction into non-reactive products C with the release of Q_G calories per gram of B.

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[1] Miller, M.S., "In Search of an Idealized Model of Homogeneous Solid Propellant Combustion," *Combustion and Flame*, Vol. 46, pp. 51-73, 1982.

[2] Miller, M.S. and Coffee, T.P., "A Fresh Look at the Classical Approach to Solid Propellant Combustion Modeling," to be published in *Combustion and Flame*.

TABLE I.

	RDX1	NC1	NC2	NC3	T1
M_o (gm/cm^2 sec)	1.035E12	8.0E10	3456	460	1.0E12
E_s (kcal/mole)	47.8	42	10	8	45.0
Q_s (cal/gm)	160	75	53	75	75
A_G	2.5E16 (sec^{-1})	2.5E9 (cc/gm sec)	1.44E12 (sec^{-1})	1.2E5 (sec^{-1})	100T (sec^{-1})
E_G (kcal/mole)	46.2	15	54	5	0
Q_G (cal/gm)	460	400	422	350	500
W_B (gm/mole)	222	40	40	40	50
ν	1	2	1	1	1
m_B^{-0}	.48	1	1	1	1
N_2	6	1.33	1.33	1.33	1
ρ_s (gm/cm^3)	1.6	1.6	1.55	1.6	1.6

$\lambda = 2.0E - 4$ cal/cm sec°K $\qquad C_p = .35$ cal/gm°K

3

In the pyrolysis reaction for every unit mass of A the fraction m_B^{-o} is converted to B and $(1-m_B^{-o})$ is converted directly to C. At some temperature T, in the gas, the rate at which B is converted to C is given by

$$R = (m_B \rho)^\nu A_G \exp(-E_G/RT) \qquad (2)$$

where m_B is the local mass fraction of B and ρ is the local mass density of the gas. For every mole of B which reacts N_2 moles of C are produced.

B. Numerical Solution.

The linear burning rate r is to be calculated for a semi-infinite block of propellant whose surface is situated normal to the x axis. Because the propellant is homogeneous, the burning is one-dimensional. Two levels of approximation to the conservation equations are discussed in Reference 1. The more general of the two is discussed here (termed Level I in Ref. 1).

The method used to obtain a burning rate in this paper has been discussed schematically in Reference 1. First the conductive heat feedback, ϕ_G, from the gas phase to the surface of the solid is computed numerically for many values of T_s at a given pressure. A value for T_s is then sought for which ϕ_G is equal to the heat flux, ϕ_s, required by the solid to maintain a mass regression rate M when the inital temperature is T_o, i.e.,

$$\phi_s = MC_p(T_s-T_o-Q_s/C_p). \qquad (3)$$

By using this method the numerical functions $\phi_G(T_s,P)$ do not depend on either Q_s or T_o.

The gas-phase equations are solved by a computer code designed to handle premixed, laminar, one-dimensional flames involving elementary chemistry.[3,4] This code is based on the package PDECOL developed by Madsen and Sincovec[5] to solve sets of second order partial differential equations using finite element techniques.

Although the equation governing m_B can be eliminated using the unit Lewis number assumption, both the m_B and the T equations are integrated by the code. The self-consistency of the two solutions can then be checked, as will be explained (Eq. 4).

[3] Coffee, T.P. and Heimerl, J.M., "A Method for Computing the Flame Speed for a Laminar, Premixed, One Dimensional Flame," Ballistic Research Laboratory Technical Report ARBRL-TR-02212, January 1980. (AD A082803)

[4] Coffee, T.P., "A Computer Code for the Solution of the Equations Governing a Laminar, Premixed, One Dimensional Flame," Ballistic Research Laboratory Memorandum Report No. ARBRL-MR-03165, April 1982. (AD A114041)

[5] Madsen, N.K. and Sincovec, R.F., "PDECOL, General Collocation Software for Partial Differential Equations," ACM TOMS, Vol. 5, pp. 326-351, 1979.

The basic numerical procedure is to work with the time dependent equations using arbitrary starting profiles for m_B and T. The cold boundary condition is just $T = T_s$. For the mass fraction equation it is[1]

$$m_B^{+o} - \frac{\rho D}{M}\left(\frac{\partial m_B}{\partial x}\right)_{+o} = m_B^{-o} \quad ,$$

which expresses the required continuity of B mass flux across the boundary. The first derivatives of m_B and T are taken to be zero at the hot boundary. Numerically the hot boundary was chosen sufficiently distant from the surface that the m_B and T profiles were essentially unaffected by its location. These boundary conditions were previously used to model burner stabilized flames.[4]

The equations are integrated in time until the steady state solution is reached. Since a finite element code is used, the solution profiles are represented by piecewise polynomials and the temperature gradient at the surface is available. As a check the heat feedback is also calculated by the formula

$$\phi_G = Q_G M(m_B^{-o} - m_B^{+o}) \tag{4}$$

which follows from the unit Lewis number assumption.

The steady state solution is usually quickly reached, taking on the order of a second on a CDC 7600. The exception is when M becomes so large (due to high T_s) that the flame is blown far from the surface. This strong convective flow allows little heat to be conducted back to the solid. As a result the flame is barely stabilized and tends to oscillate before finally approaching the steady state.

As a partial check on the code, it was run on a test data set (T1) for which an exact analytic solution exists (Eq. 31 of Ref. 1). The numerical solution proved accurate to within a small fraction of a percent except when T_s became large enough so that the heat feedback was negligibly small. Even there the numerical solution was good to a few percent (and could be improved by using a finer grid). In the subsequent figures the numerical computations will be denoted by N.

C. Analytic Models Used for Comparison .

Most of the models which deal with our assumed mechanism have been recently reviewed and classified into one of three idealizations of the gas-phase heat release.[1] The constant temperature reaction rate (CTRR) approach should apply in the limit of very low E_G. The quasi-constant heat release (QCHR) model[1] might pertain to moderate values of E_G whereas the delta function heat release (DFHR) models would be appropriate to very high E_G. We shall in this paper compare our numerical calculations to the following specific models in each of these classes.

A solution to ϕ_G under the CTRR assumption is not available for $\nu=2$ in a Level I (diffusion not neglected) treatment[1]; therefore, Equation (33) of Reference 1 is used to compute ϕ_G for the NC1 data set. (Eq. 31 of Ref. 1 is used for the $\nu=1$ cases). A comparison of the solutions with and without

diffusion for the $\nu=1$ cases shows that the burning rate is not greatly affected by this assumption so long as the solution value of T_s lies to he right of the peak in the $\phi_G(T_s)$ curve. For example, Fig. 5 suggests that the use of the no-diffusion ϕ_G is probably justified for T_o greater than about $300°K$.

It became apparent during the course of this work that, while the QCHR model ϕ_G gives good results for ϕ_G at high T_s for some cases, at sufficiently low T_s the model σ_G exceeds the maximum possible heat feedback ($Q_G M m_B^{-o}$). This occurs because at low T_s the characteristic transport distance ($\lambda/M C_p$) becomes so large (as M diminishes) that the integrated heat release exceeds $Q_G m_B^{-o}$. This problem is easily corrected by assuming a constant heat release, q_o, only for $x < x_1$ where x_1 is chosen by the energy conservation requirement

$$Q_G \; M m_B^{-o} = \int_o^{x_1} q_o \; dx \quad .$$

Thus we have the "constant heat release" (CHR) model given by

$$\phi_G = \frac{\lambda q_o}{M C_p} [1 - \exp(-M C_p x_1/\lambda)] \tag{5}$$

which will be used in the present paper (cf. Eq. (46) of Reference 1). At high T_s the QCHR and CHR results for ϕ_G merge. The unknown value of m_B^{+o} in q_o is found by requiring self-consistency between Equations (4) and (5).

In Reference 1 it was argued that the BDP monopropellant model[6], although a delta function model, is likely to overestimate ϕ_G in the limit of high E_G because of an improper choice for the flame standoff distance.[7] This assessment is borne out in the calculations to follow. Fortunately there does exist an accurate high E_G theory which was advanced by Williams[8] and elaborated by Buckmaster, et al.[9] The theory is based on the asymptotic analysis of Bush and Fendell[10] for laminar gas flames. In our notation the burning rate[9] for general reaction orders is given by

$$M^2 = \frac{2\nu! \lambda P^\nu A_G R^{\nu+1} C_p^\nu T_f^{2(\nu+1)}}{(E_G Q_G m_B^{-o})^{\nu+1}} \; (\frac{\bar{W}}{RT_f})^\nu \; \exp(-E_G/RT_f). \tag{6}$$

In this paper we shall designate the theory by A.

[6] Beckstead, M.W., Derr, R.L., and Price, C.E., "The Combustion of Solid Monopropellants and Composite Propellants," Thirteenth Symposium (International) on Combustion, The Combustion Institute, pp. 1047-1056, 1971.

[7] Hermance, C.E., "A Model of Composite Propellant Combustion Including Surface Heterogeneity and Heat Generation," AIAA Journal, Vol. 4, pp. 1629-1637, 1966.

[8] Williams, F.A., "Quasi-Steady Gas-Flame Theory in Unsteady Burning of a Homogeneous Solid Propellant," AIAA Journal, Vol. 11, pp. 1328-1330, 1973.

[9] Buckmaster, J.D., Kapila, A.K., and Ludford, G.S.S., "Linear Condensate Deflagration for Large Activation Energy," Acta Astronautica, Vol. 3, pp. 593-614, 1976.

[10] Bush, W.B. and Fendell, F.E., "Asymptotic Analysis of Laminar Flame Propagation for General Lewis Numbers," Comb. Sci. Tech., Vol. 1, pp. 421-428, 1970.

III. RESULTS

In this section we shall first show how the model heat release and temperature profiles compare with the numerical ones. The comparison is then extended to the heat feedback functions $\phi_G(T_s,P)$, the burning rates $M(P)$, and finally the temperature sensitivities $\sigma_p(T_o)$.

A. Flame Structure

Sample comparisons are made in Figs. 1-4 for a high E_G data set (RDX1) and one with low E_G (NC3). In both cases the conditions of pressure and initial temperature are 1000atm and 300°K. It is clear that all of the models give very simplistic representations of the heat release ($q(x)$) profiles (Figs. 1 and 3). In Fig. 1 the tendency of the BDP model to underestimate the flame standoff distance[1] for high activation energy is evident. The high activation energy case (Fig. 2) causes the greatest divergence in predicted temperature profiles. The asymptotic theory does quite well, however, at points near the surface. As expected the CHR and CTRR models give significantly better temperature profiles than the flame sheet models for the low activation energy case (Fig. 4).

B. Heat Feedback vs. Surface Temperature

Figures 5-11 display the numerical and model values of heat feedback (i.e., $\lambda \frac{dT}{dx}\big|_{x=+o}$) as a function of surface temperature for the model propellants. At sufficiently low T_s all of the models predict ϕ_G to approach the maximum value, i.e., $Q_G M m_B^{-o}$. In this limit the bulk of the energy release takes place close (compared with λ/MC_p) to the surface. Increasing T_s promotes two competing effects. The gas reaction is accelerated tending to increase ϕ_G, but M also increases by the pyrolysis law tending to blow the "flame" further away from the surface and reducing the effectiveness of energy release at any given distance from the surface (see the discussion of Eq. (6) in Ref. 1). Eventually the latter processes dominate and ϕ_G decreases with T_s.

Also shown in these figures is $\phi_s(T_s)$ computed by Eq. (3) for $T_o=300°K$. The intersection of $\phi_s(T_s,T_o)$ and $\phi_G(T_s,P)$ occurs at the value of T_s pertinent to the conditions (T_o,P). With this solution value of T_s one can compute the burning rate via Eq.(1).

An important feature to notice in these figures is that the CHR model gives the correct value of ϕ_G in the high T_s limit. (The CHR and QCHR models are identical in this limit). Although the solution to $\phi_s=\phi_G$ can always be forced to occur in this region by considering a sufficiently high value of T_o, the fractional heat feedback ($\frac{\phi_G}{Q_G M m_B^{-o}}$) may be so small there that the gas phase processes no longer affect the burning rate.

Another interesting feature is the way that the BDP model exhibits similarities to both the asymptotic (A) and CTRR solutions. This results from the BDP model using the delta function (high E_G) formalism but with a flame standoff which is appropriate to the low E_G limit. (See discussion in Section IIIB of Ref. 1).

12
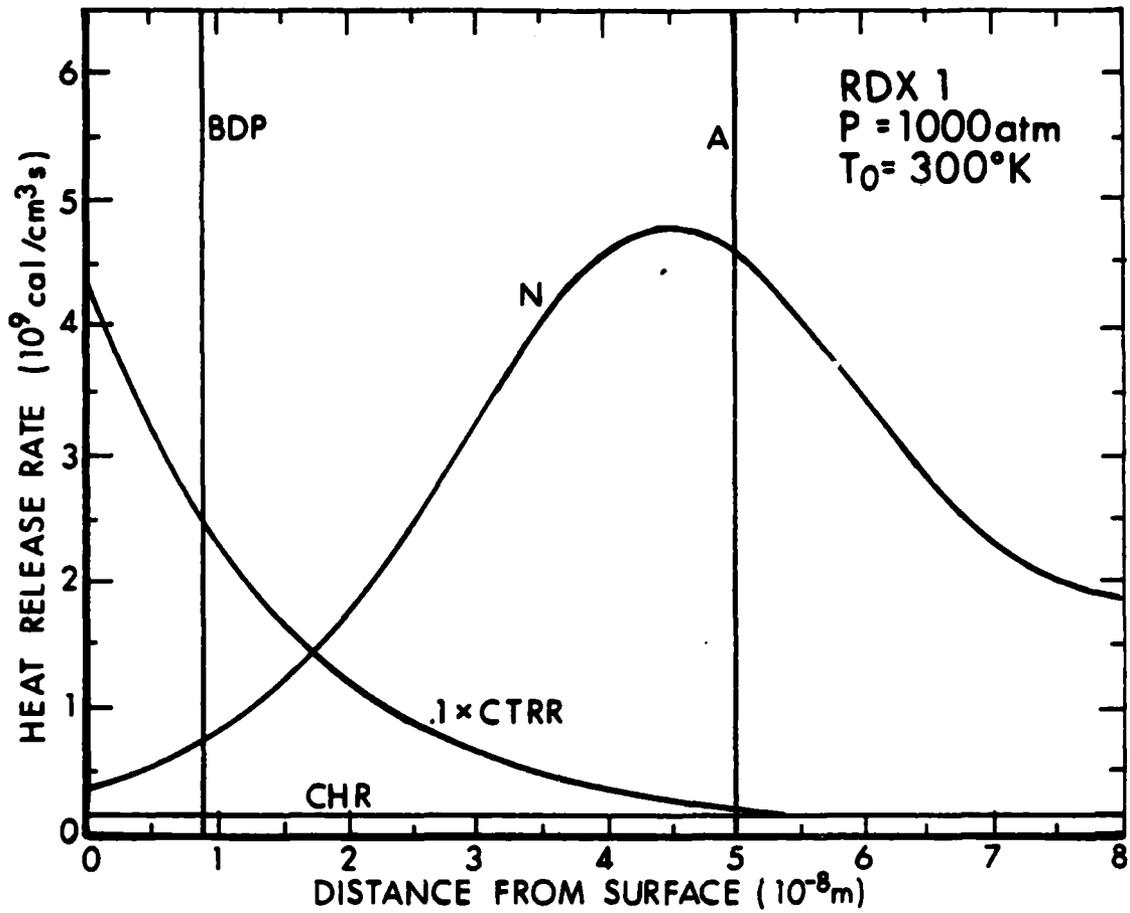
Fig. 1.   Comparison of numerical (N) and model heat
   release profiles for the RDX1 data set.
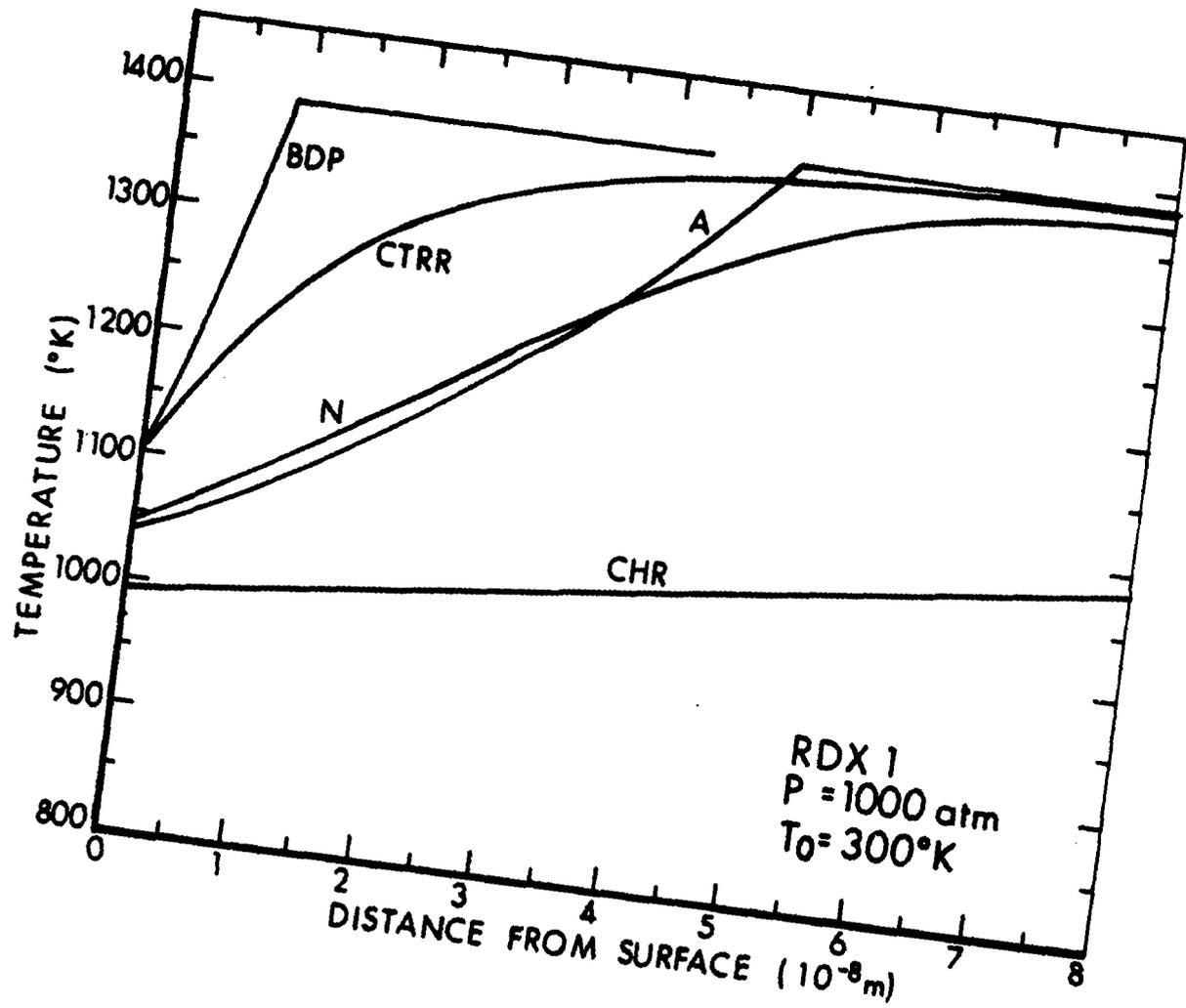
Fig. 2. Comparison of numerical (N) and model temperature profiles for the RDX1 data set.

14
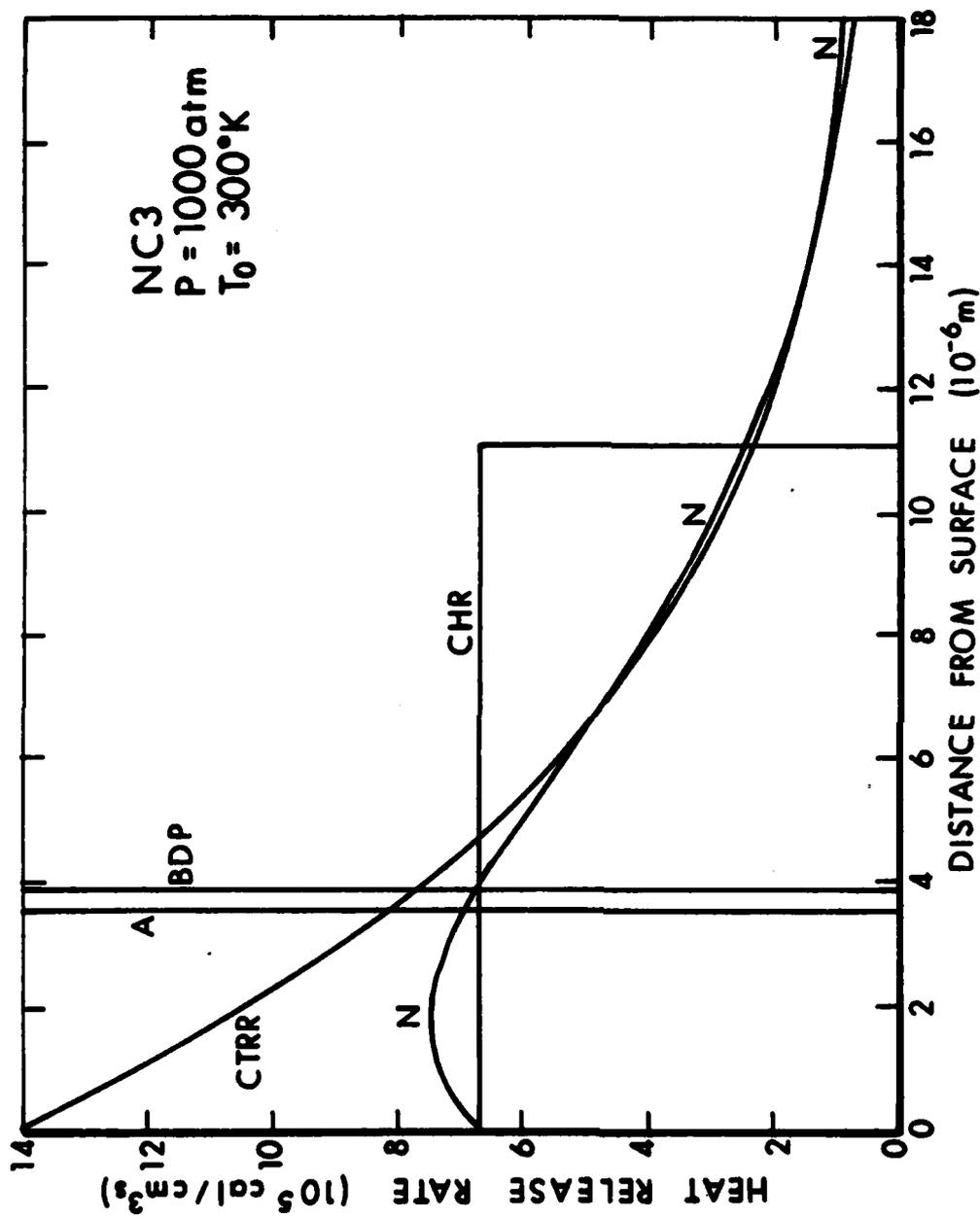
Fig. 3. Comparison of numerical (N) and model heat release profiles for the NC3 data set.

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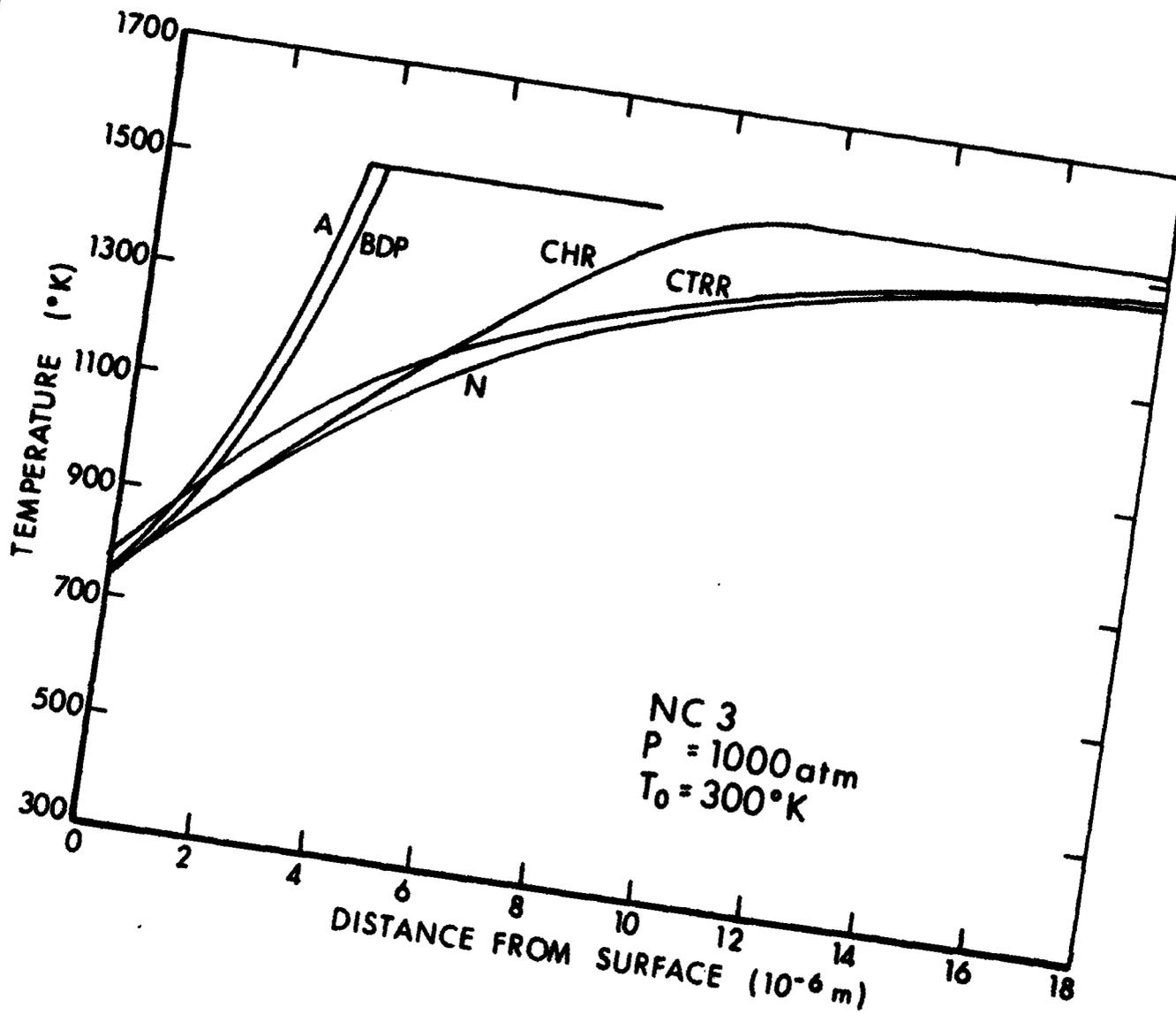
Fig. 4. Comparison of numerical (N) and model temperature profiles for the NC3 data set.
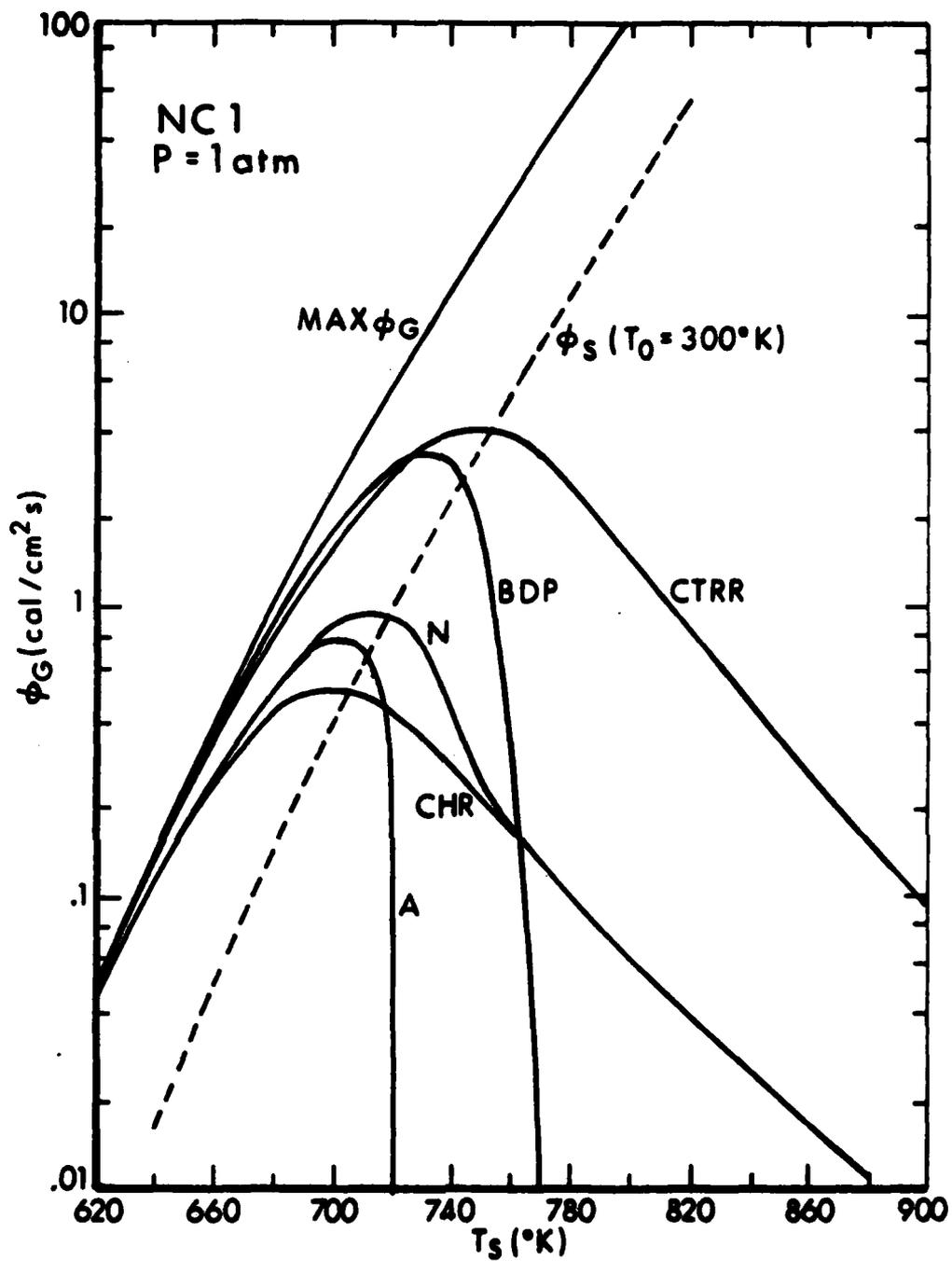
Fig. 5. Heat feedback vs. surface temperature for NC1
at 1 atm.

17
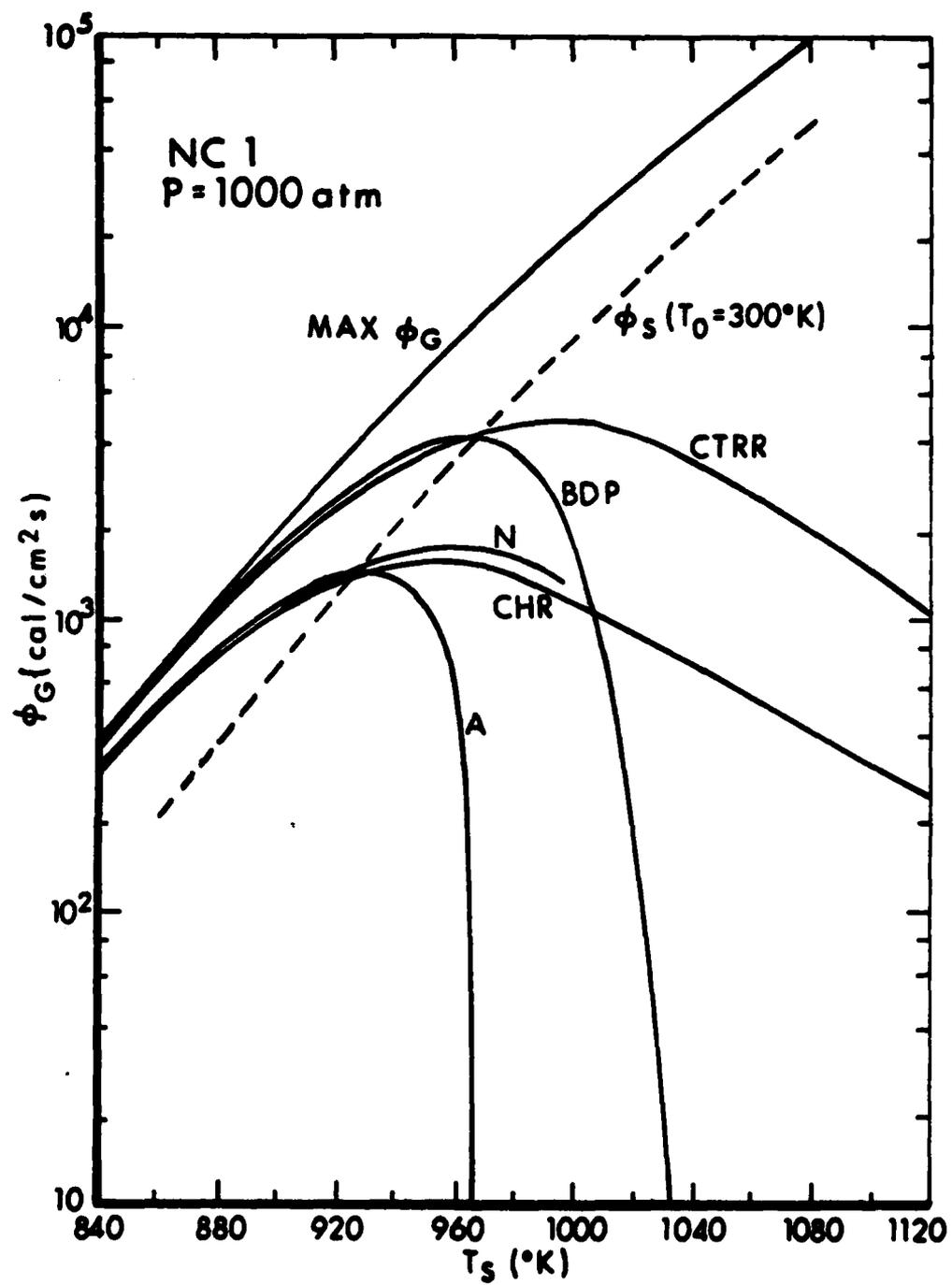
Fig. 6. Heat feedback vs. surface temperature for NC1 at 1000 atm.
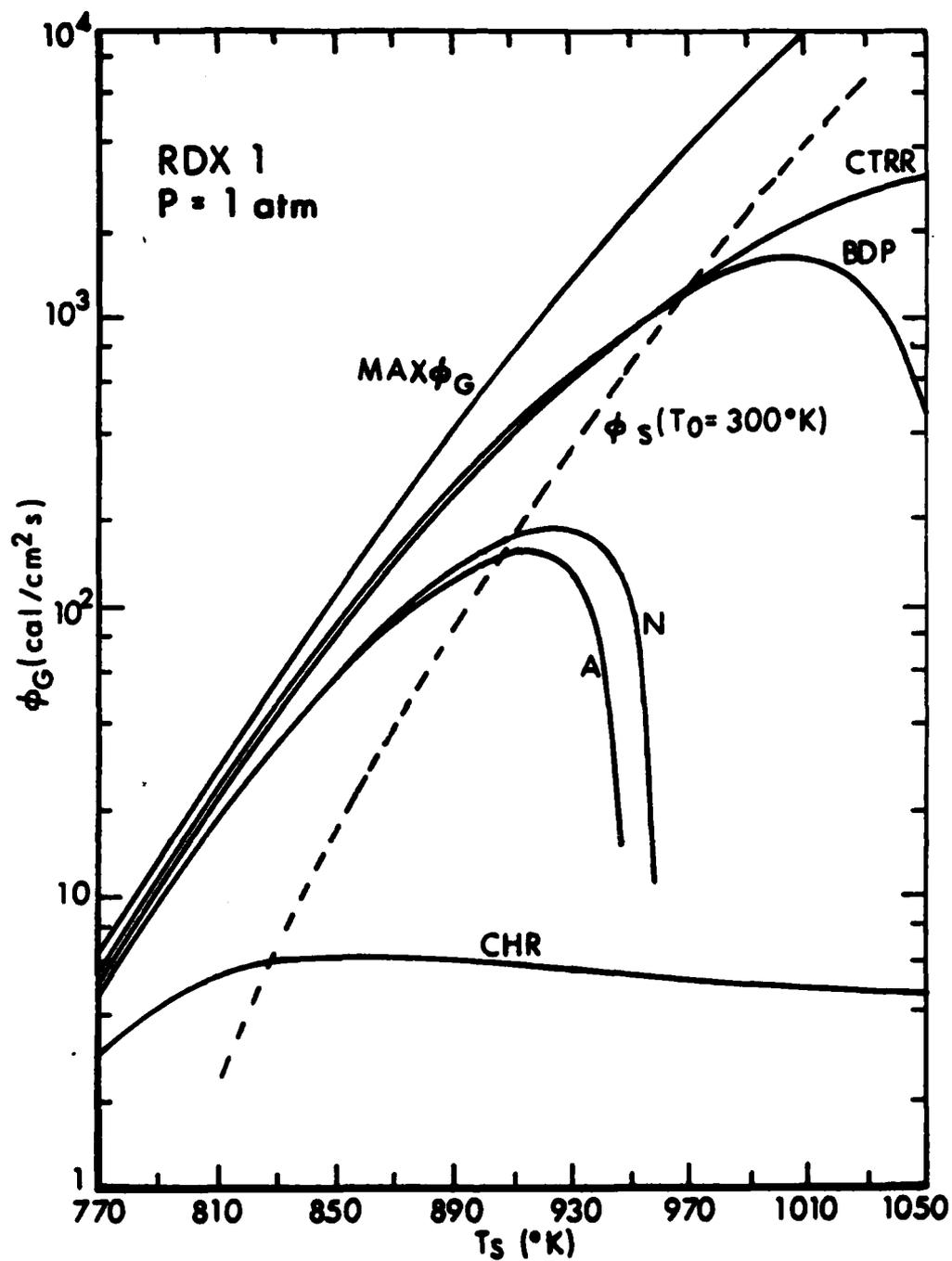
Fig. 7. Heat feedback vs. surface temperature for RDX1
at 1 atm.
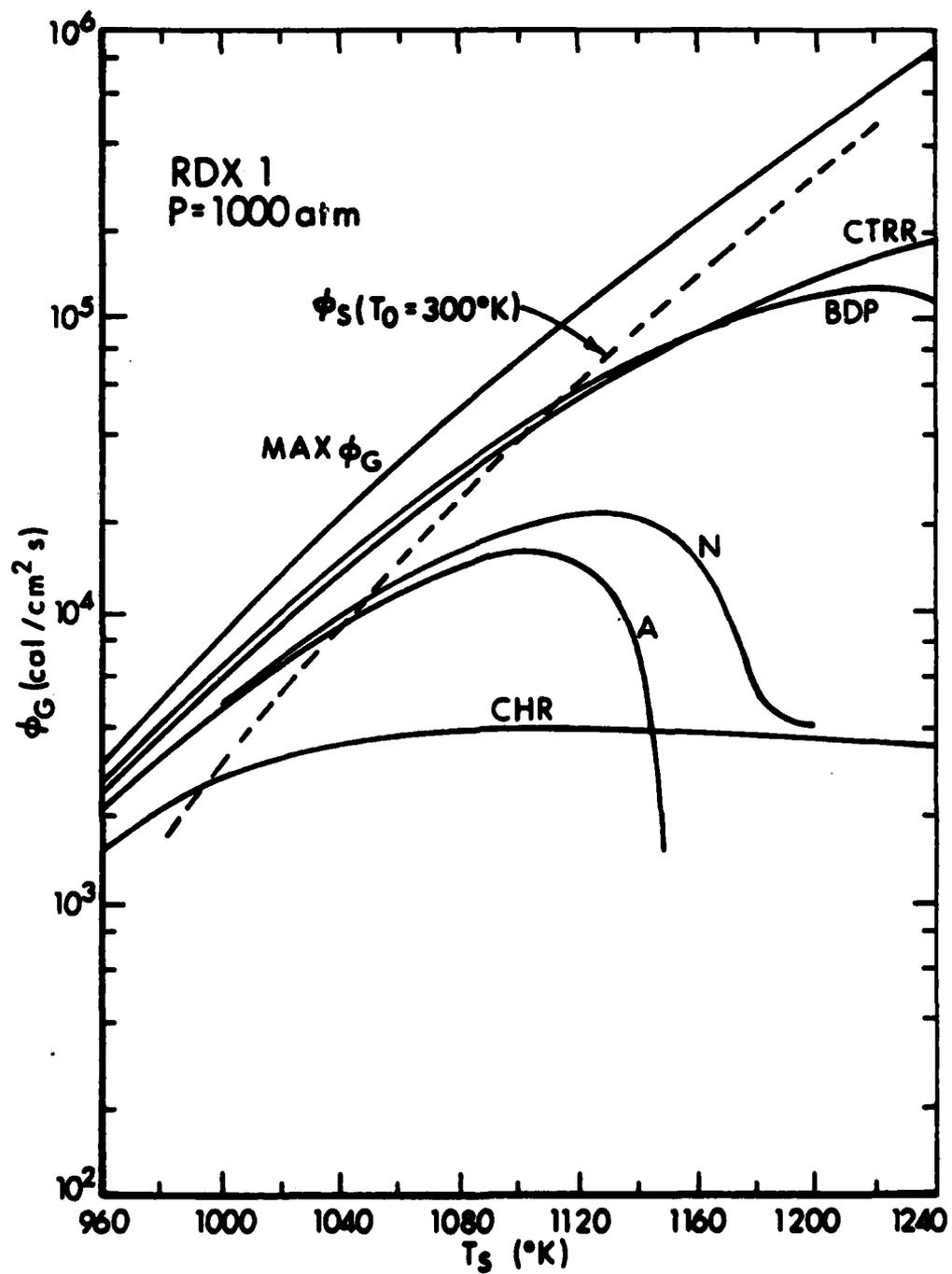
Fig. 8. Heat feedback vs. surface temperature for RDX1 at
1000 atm.
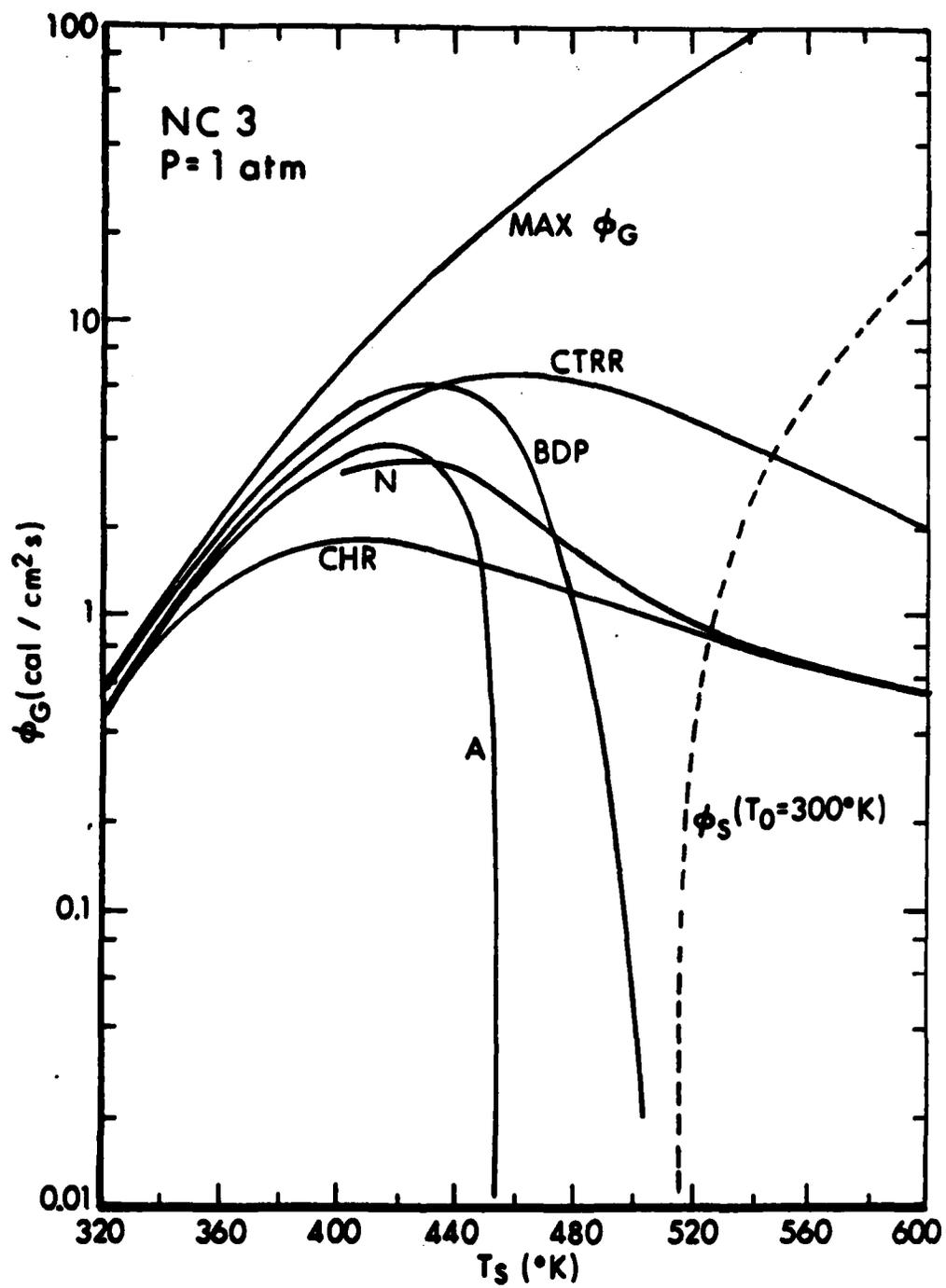
Fig. 9. Heat feedback vs. surface temperature for NC3
   at 1 atm.
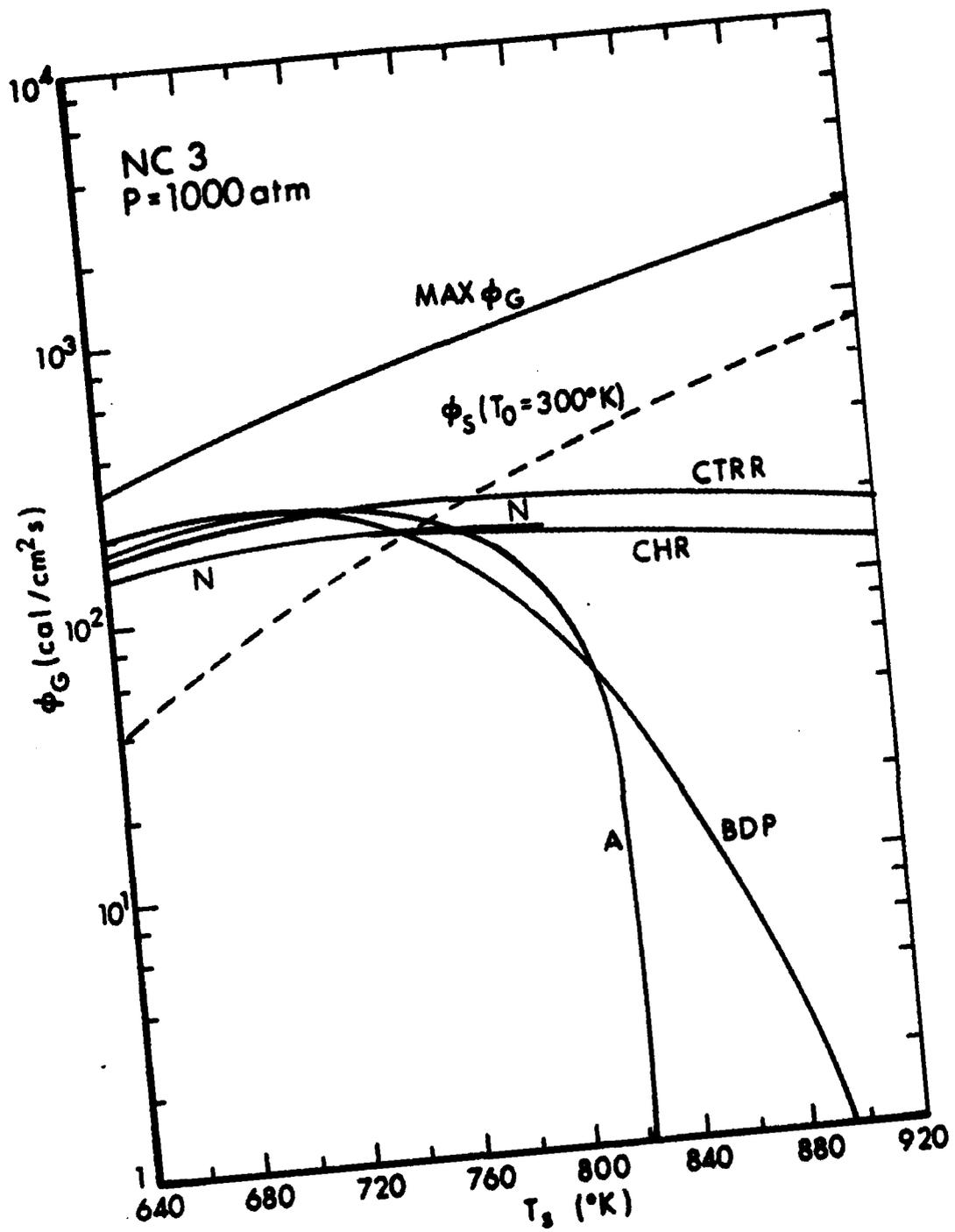
Fig. 10. Heat feedback vs. surface temperature for NC3 at 1000 atm.
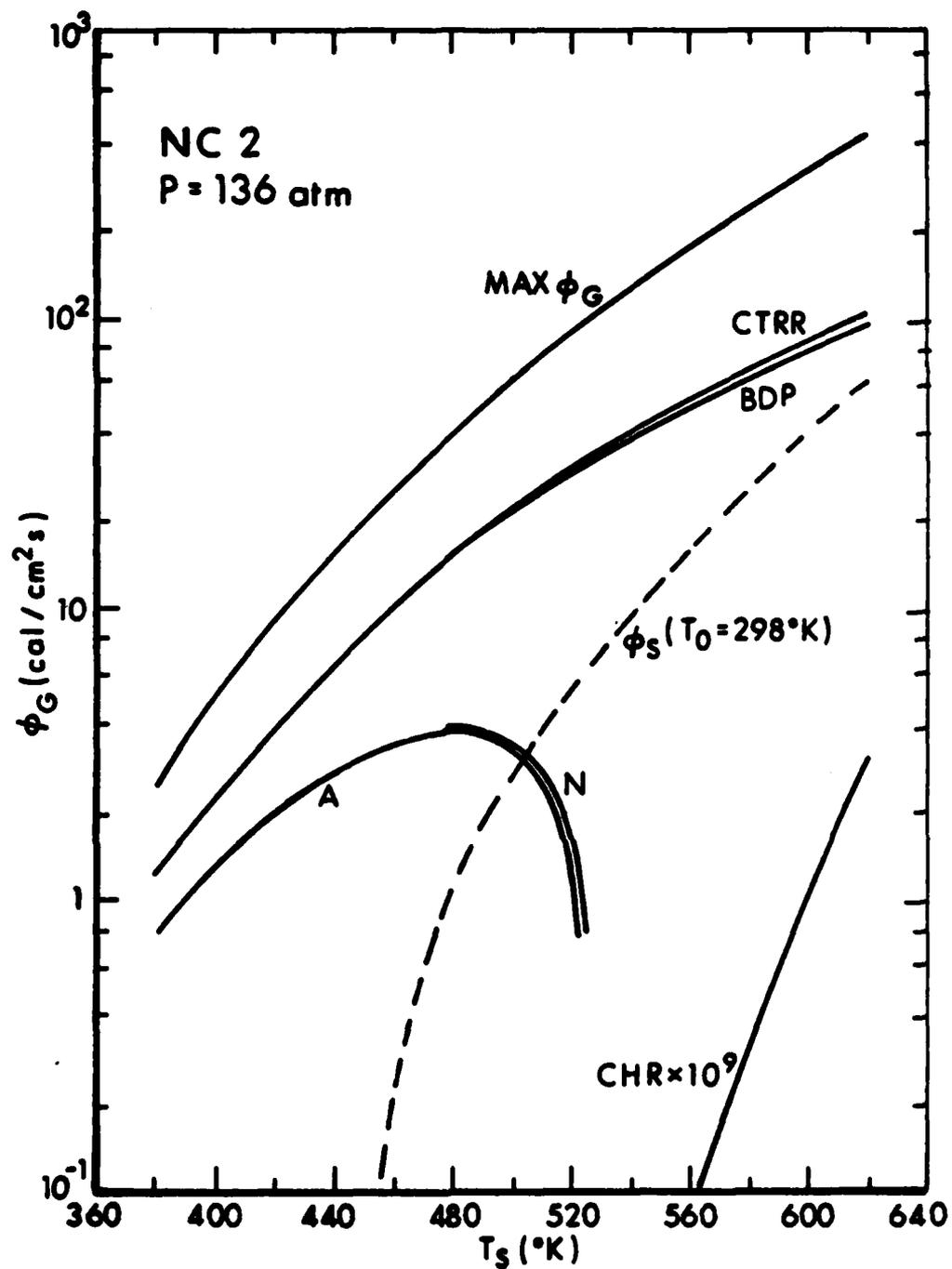
Fig. 11. Heat feedback vs. surface temperature for
NC2 at 136 atm.

23

In general the CTRR approximation is the poorest and is most notably so in the high T_s region. In this portion of the curve the neglect of diffusion has almost no effect on the numerical value of ϕ_G since $\dfrac{P_o}{M^2}$ is small there. (See Section IIIA of Ref. 1).

Finally, Fig. 11 gives good evidence that the asymptotic theory is numerically accurate in the high E_G limit. The approach to this limit is also evident in Figs. 7 and 8. The asymptotic theory, in fact, does quite well generally although Fig. 9 and high T_o cases in Figs. 5-8 are exceptions.

In short it is clear that no single combustion model that we have considered can be relied upon for even approximate results under all conditions of T_o and P for any set of propellant data.

C. Burning Rate

The burning rate as a function of initial temperature for the NC2 data set is shown in Fig. 12 at a pressure of 136 atm. The NC2 data set is obtained[2] by a fit of the BDP model to double-base propellant burning rates. However it is clear that the BDP model is particularly inaccurate for the parameters obtained by this fit, overestimating the numerical rate by an order of magnitude. Note that only the asymptotic theory gives good accuracy for this flame-sheet case.

Figures 13, 14, and 15 indicate that, for the most part, the pressure index (exponent) is slightly less than $\nu/2$ and that the model algorithms approximate this value fairly well. Eq. (61) of Reference 1, which connects the pressure index with E_s and E_G, is found to be inaccurate for values other than $\nu/2$. The absolute accuracy of M depends rather strongly on the parameters of the data set. In general the asymptotic theory does best at the highest E_G (RDX1) and the CHR model does best at the lowest E_G(NC3). As expected from the discussion of Figures 5-11, the BDP model leads to an overestimate of the burning rate for high E_G. All of the burning rates in Figs. 8-10 are computed for an initial propellant temperature of 300°K. We note also that the burning rates are computed only at 1,10,100,1000 atm. For clarity, straight lines are used to connect these points.

D. Temperature Sensitivity vs. Initial Temperature

The temperature sensitivity at constant pressure, σ_p, is defined by

$$\sigma_p \equiv \left(\frac{d\ln M}{dT_o}\right)_p . \tag{7}$$

Like the pressure sensitivity $\left(\equiv \dfrac{d \ln M}{d\ln P}\right)$ its usefulness lies in the fact that it is nearly constant over variable ranges of practical concern. Though nearly constant, σ_p has nonetheless been observed[2] to increase generally with increases
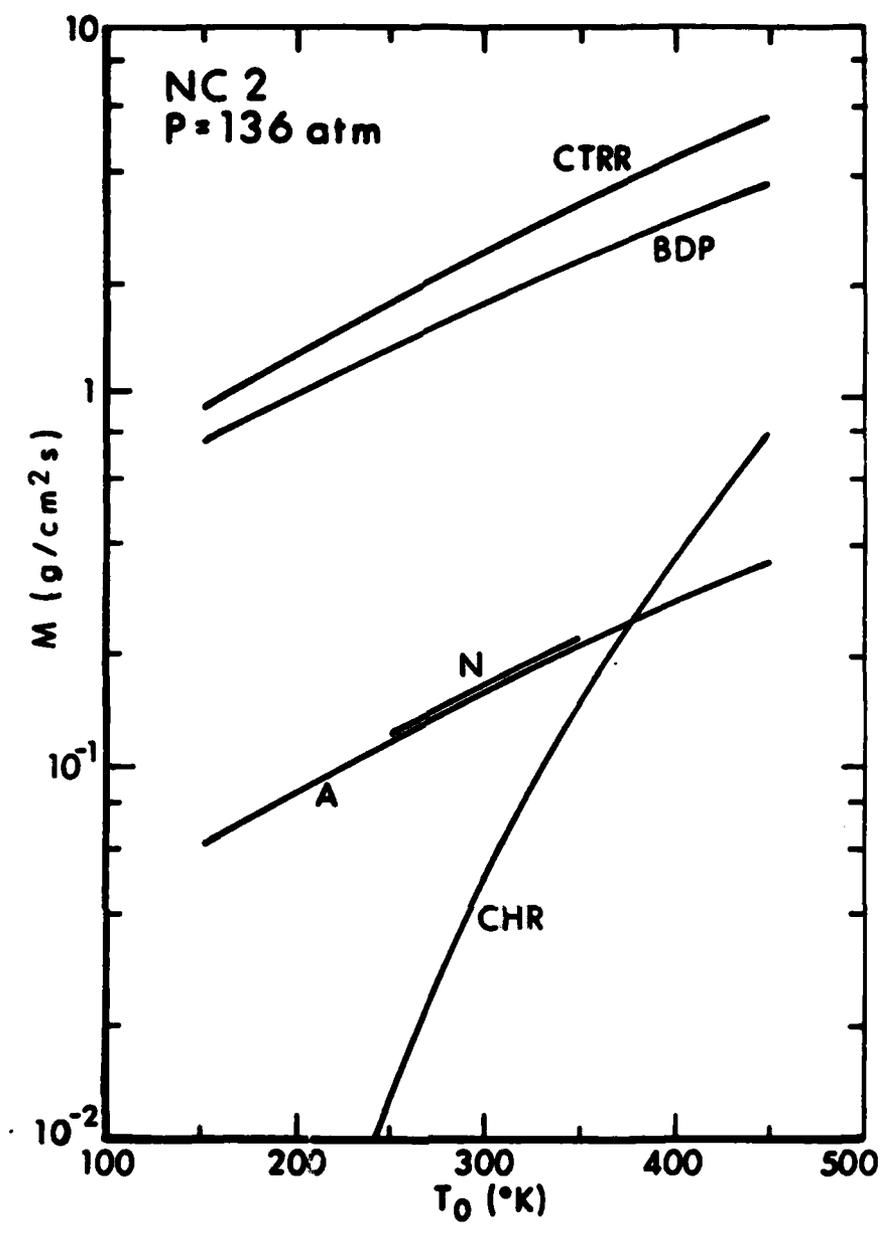
Fig. 12.   Mass burning rate vs. initial temperature for
   NC2 at 136 atm.
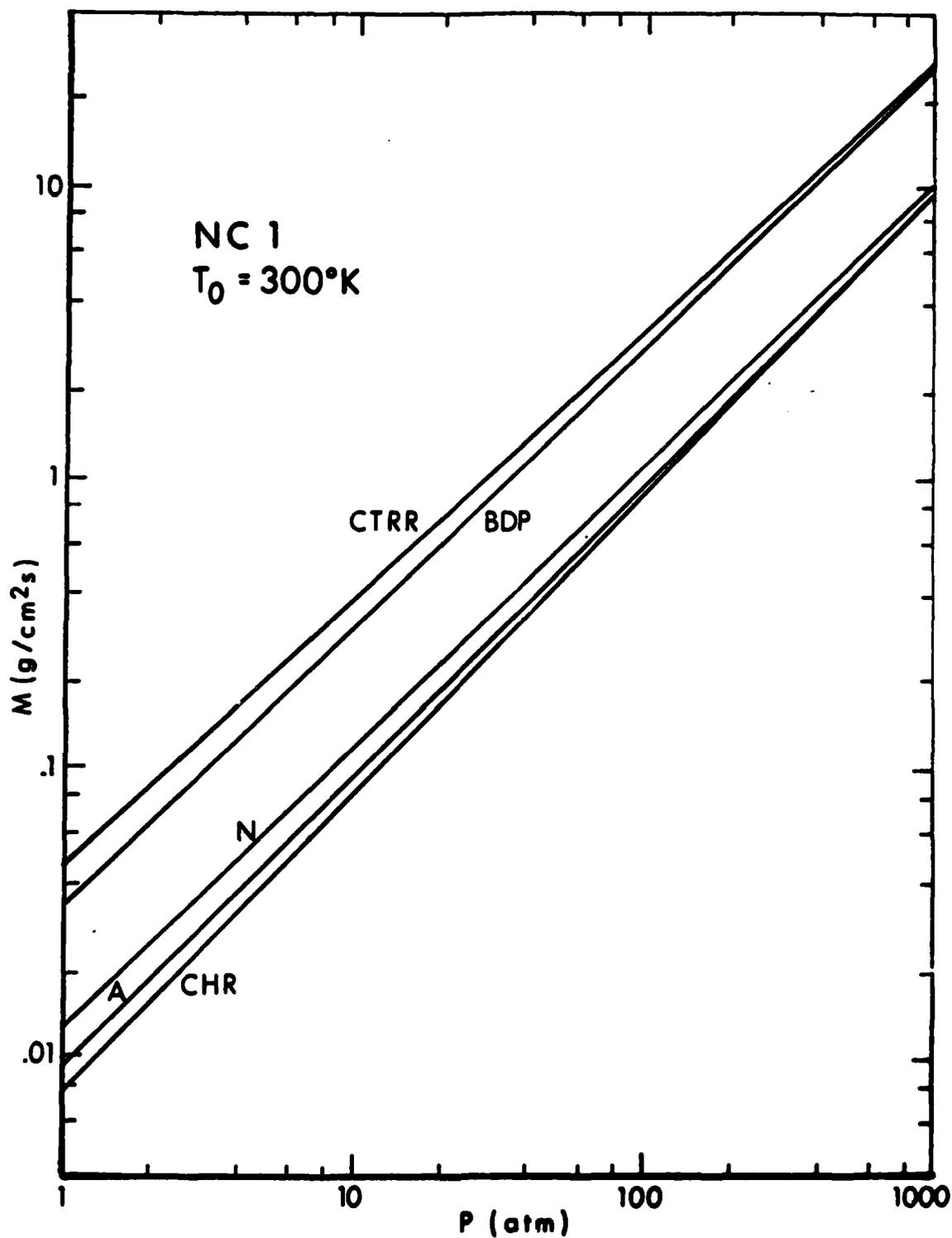
Fig. 13. Mass burning rate vs. pressure for NC1
initially at 300°K.

26
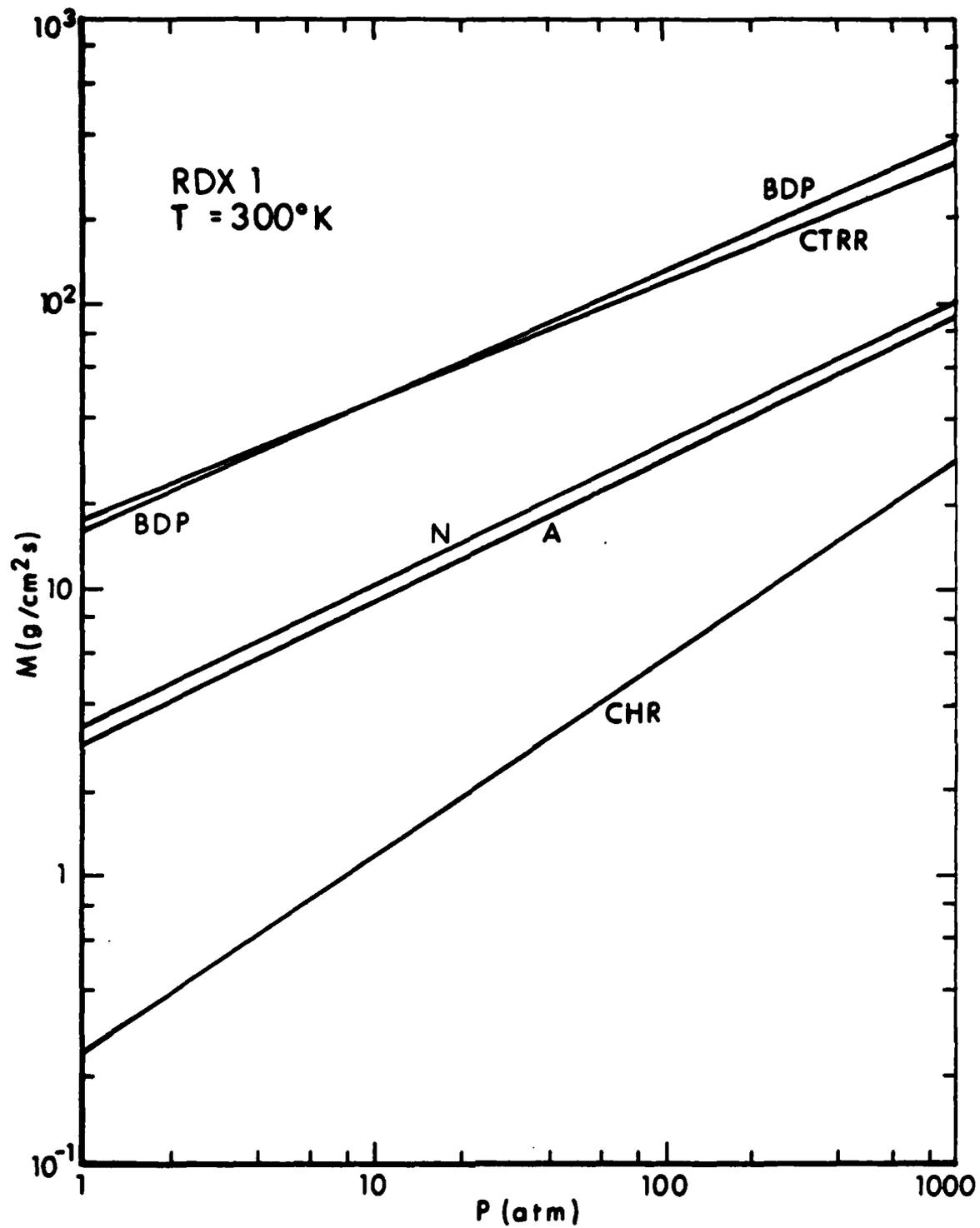
Fig. 14. Mass burning rate vs pressure for RDX1
initially at 300°K.
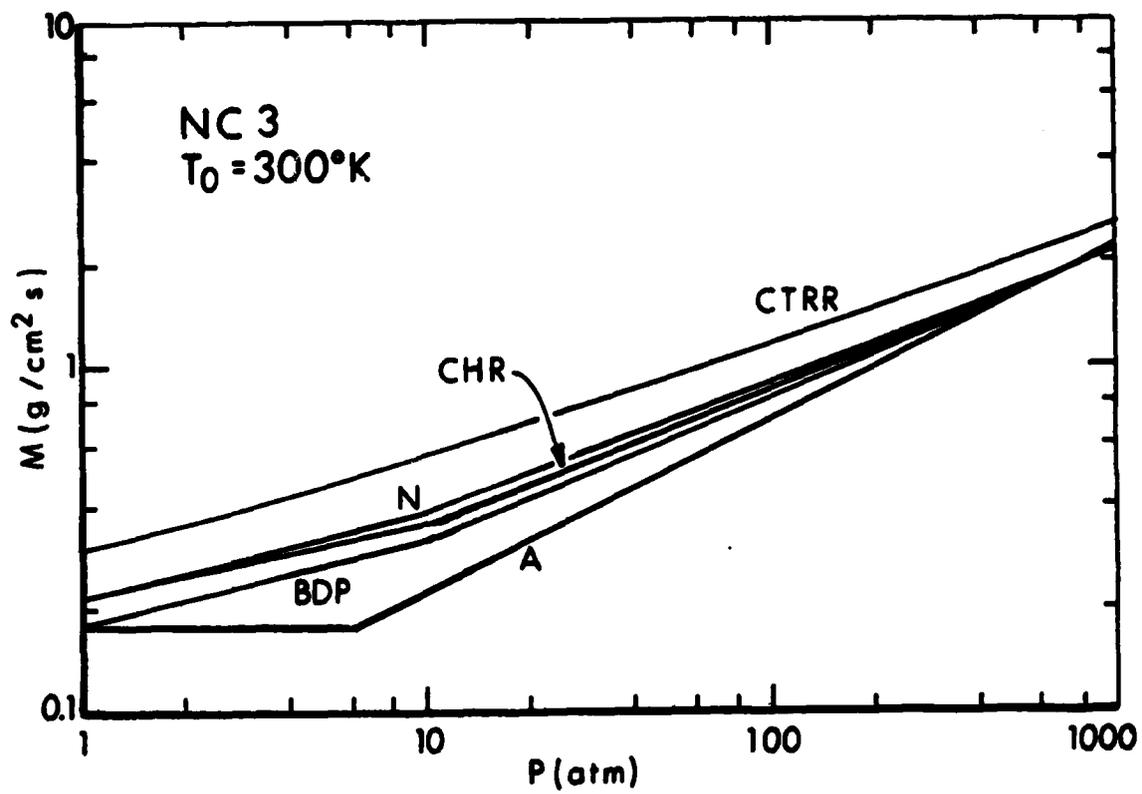
Fig. 15. Mass burning rate vs. pressure for NC3 initially at 300°K.

in T_o. Applying Eq. (7) to the asymptotic theory (Eq. (6)) one obtains (cf. Coates[11] Eq. 23)

$$\sigma_p = (1 + \frac{\nu}{2} + \frac{E_G}{2RT_f}) / T_f , \qquad (8)$$

which predicts σ_p to be a monotonic decreasing function of T_o (since $T_f = T_o +$ Q_T/C_p). The QCHR model[1], on the other hand, predicts σ_p to increase monotonically with T_o. Figures 16-21 show the resolution of this conflict. In all of the figures the abrupt transition of the asymptotic theory curve (A) to the solid-phase control limit (given by $\dfrac{E_s}{R(T_o + Q_s/C_p)^2}$) does not derive from Eq. (8), but rather from the condition that the surface temperature cannot drop below $T_s' =$ $T_o + Q_s/C_p$. It can also be seen that in the CHR model σ_p does decrease with increasing T_o at sufficiently low T_o. This behavior contradicts the QCHR formula derived in Ref. 1 even though most of the conditions for the derivation are satisfied. The discrepancy can be traced to the fact that the QCHR formula was based on a neglect of diffusion.

Figures 18 and 19 for RDX1 show a slight hump in the numerical $\sigma_p(T_o)$ curves just to the left of the minimum. The numerical integrations were recomputed in this region with increased accuracy for the 1 atm case. The hump remained, indicating that it is apparently not an artifact of the numerical method.

Although the abscissa in Figs. 12-17 is given as T_o, it could also be $(T_o + Q_s/C_p)$ with equal validity since Q_s is fixed for each of the data sets. However if one assumes T_o to be fixed and increases in the abscissa to be due to higher Q_s, one sees that the consequences for σ_p depend on the data set. For example increasing Q_s by 50 cal/gm would decrease σ_p over the practical range for the RDX1 data set but increase σ_p for the NC3 case (at 1000 atm). Thus it would seem that if combustion models were looked to for guidance in making formulation changes to affect σ_p, a determination of the effective kinetic parameters for the unmodified propellant is first required.

IV. CONCLUSIONS

The objective of this study was to assess the numerical accuracy of the computational algorithms employed by several combustion models by direct comparision with accurate numerical solutions of the conservation equations. This comparison was made for a number of data sets with widely varying kinetics parameters. None of the algorithms were found to give reliable numerical accuracy for all data sets and conditions of pressure and temperature. Such inaccuracies can confuse efforts to associate idealized combustion mechanisms with real propellants and give erroneous guidance for performance tailoring attempts.

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[11] Coates, R.L., "An Analysis of a Simplified Laminar Flame Theory for Solid Propellant Combustion," Comb. Sci. Tech., Vol. 4, pp. 1-8, 1971.
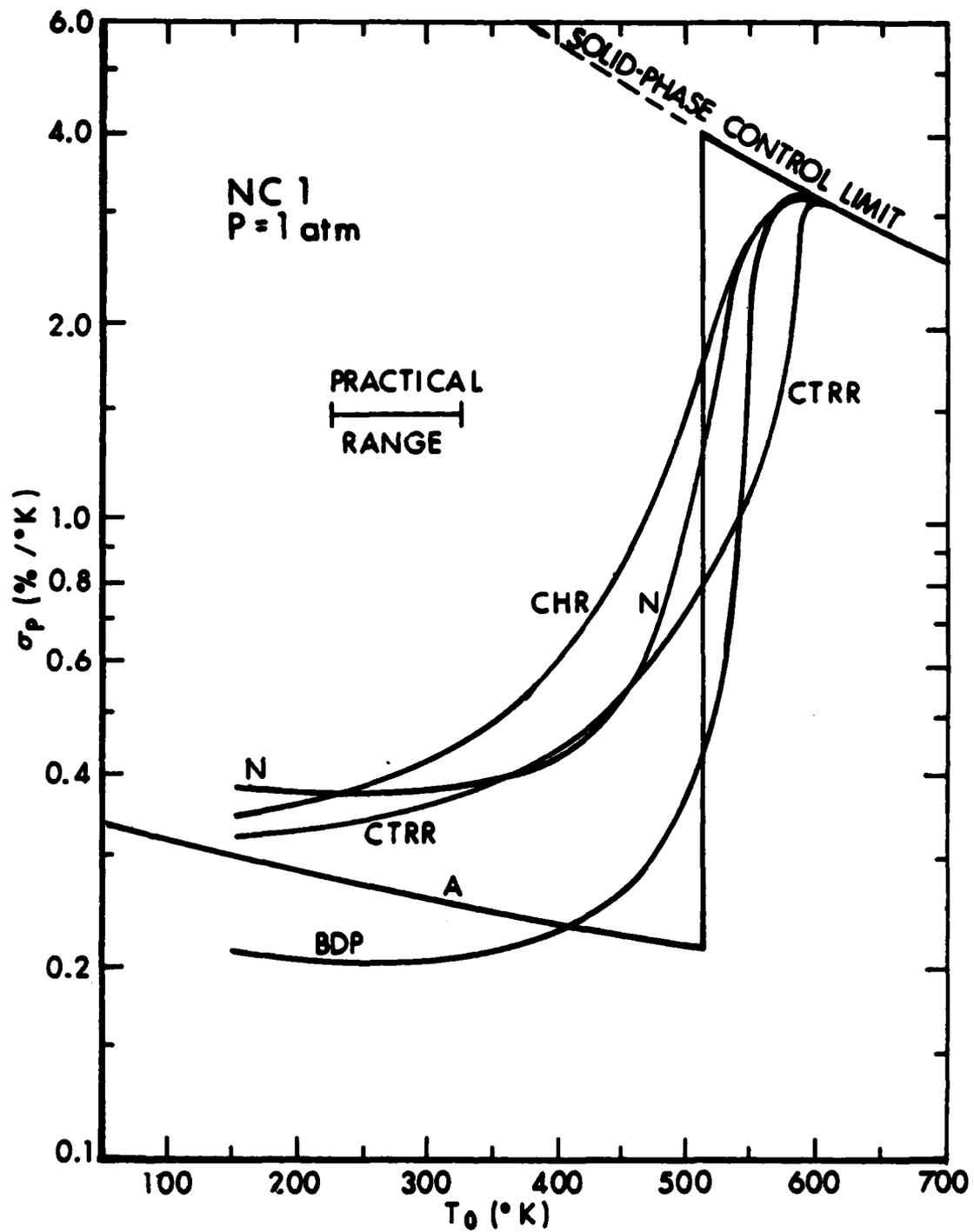
Fig. 16. Temperature sensitivity vs. initial temperature for NCl at 1 atm.
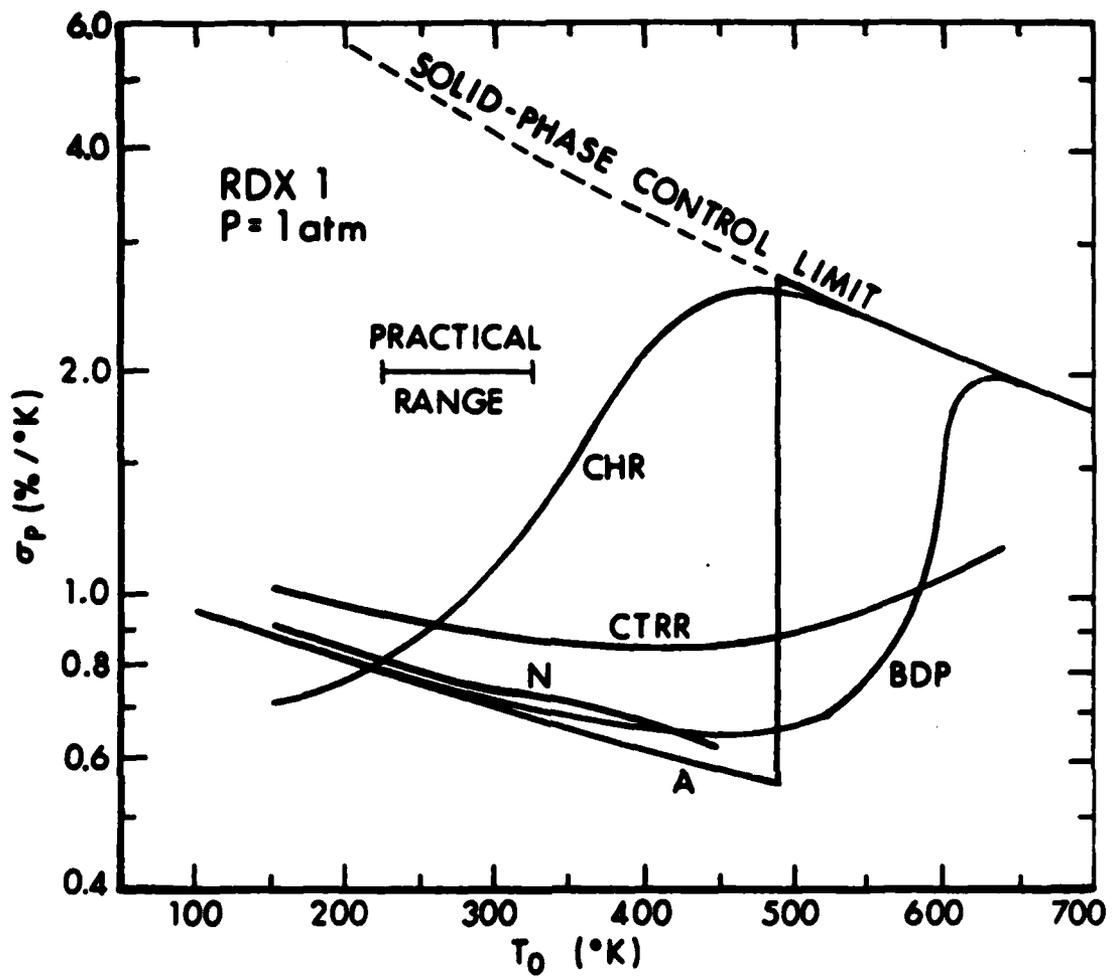
Fig. 18. Temperature sensitivity vs. initial temperature
for RDX1 at 1 atm.
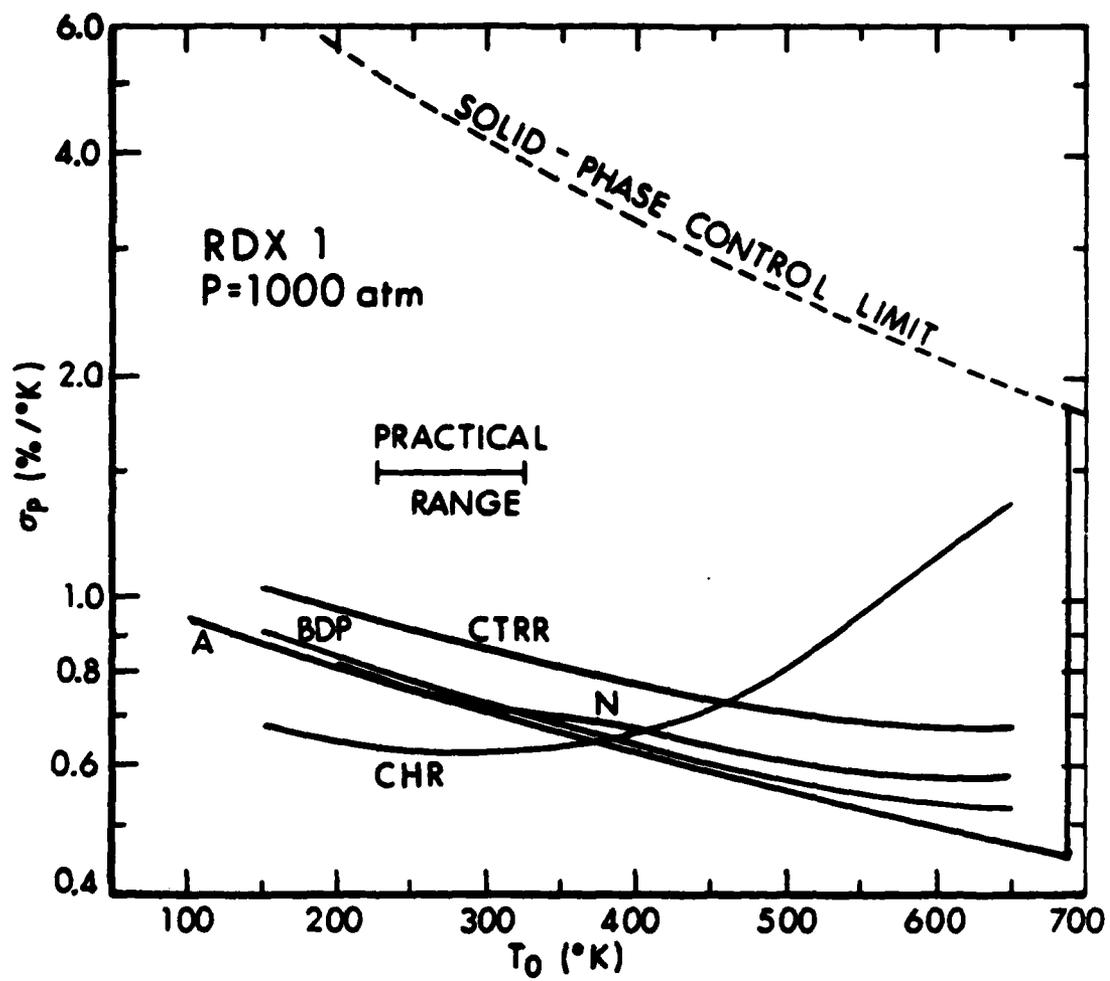
Fig. 19. Temperature sensitivity vs. initial temperature
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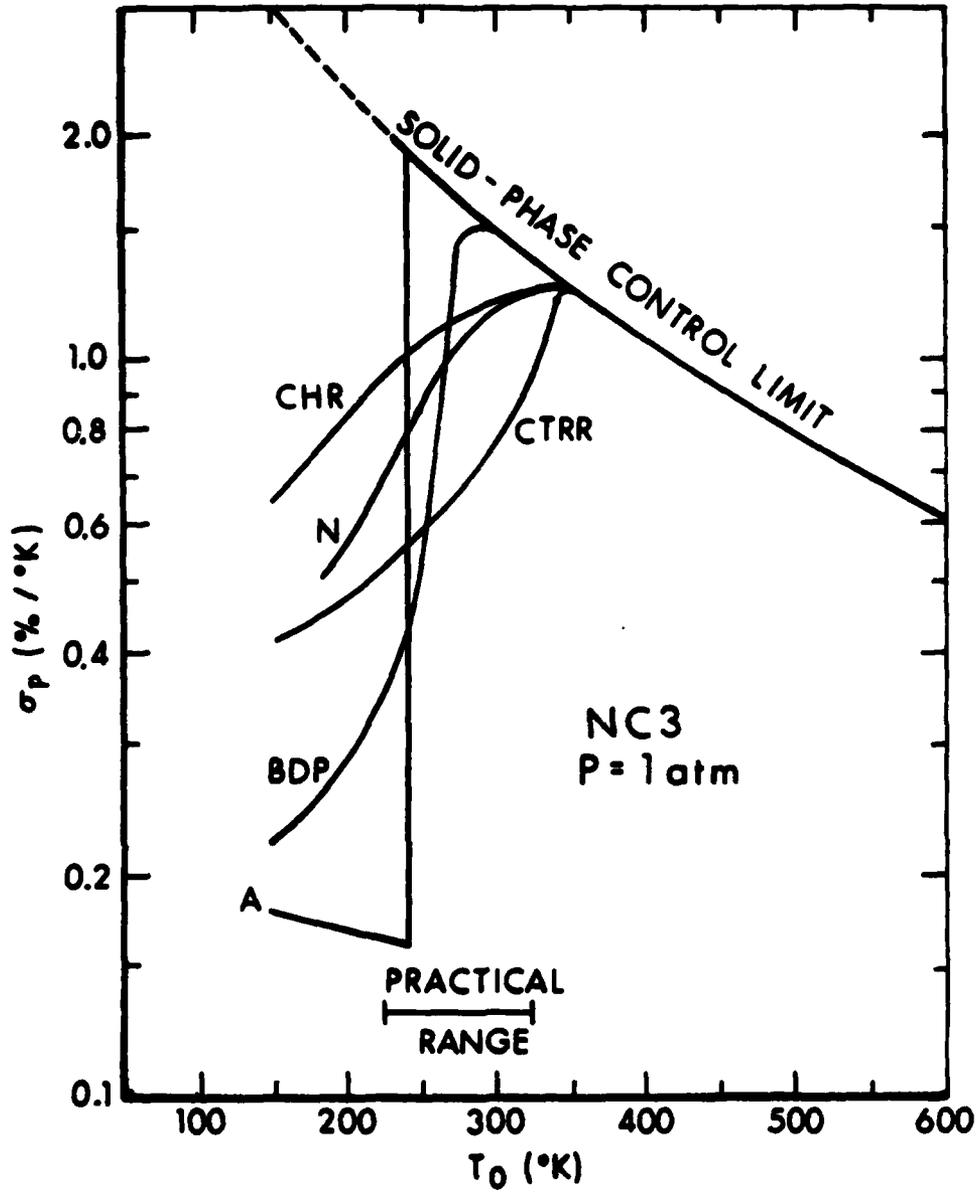
Fig. 20.   Temperature sensitivity vs. initial temperature
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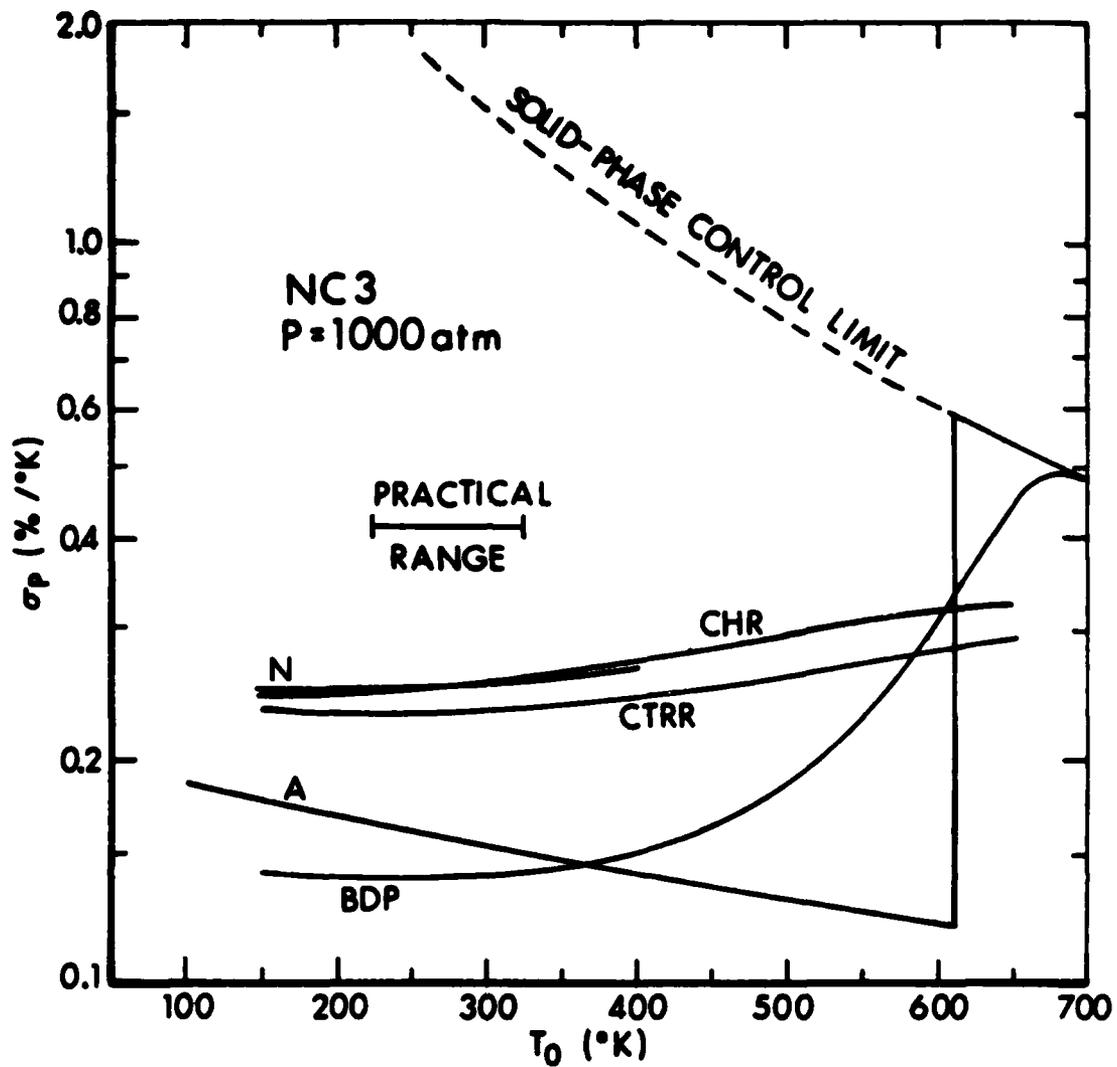
Fig. 21. Temperature sensitivity vs. initial temperature
for NC3 at 1000 atm.

In spite of the poor reliability of these algorithms in general, some of the models were shown to give accurate results under certain limiting conditions. However, quantitative criteria for identifying these limits may be difficult to establish for a priori use.

Finally, we have reported numerical calculations of gas-phase heat feedback for a wide range of kinetics parameters. It is hoped that future algorithm developers will find in them a ready means for validating their efforts.

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LIST OF SYMBOLS

A - propellant molecule label

A_G - gas-phase reaction frequency factor

B - gas-phase reactant label

C - gas-phase product label

C_p - specific heat for solid and gas phases

D - diffusion coefficient

E_G - activation energy for gas-phase reaction

E_s - activation energy for solid-phase reaction

M - mass regression rate (mass flux)

M_o - constant in pyrolysis surface decomposition mechanism

m_B^{-o}, m_B^{+o} - mass fraction of B evaluated at negative and positive sides of the solid/gas interface, respectively.

N_2 - number of moles of C produced per mole of B which reacts

P - total pressure

Q_s - heat of reaction per unit mass for solid reaction (positive for exothermic)

Q_G - exothermic gas-phase reaction heat per unit mass of B

Q_T - total exothermic reaction heat (solid + gas) per unit mass of A

$q(x)$ - gas-phase heat release per unit volume per unit time at x

q_o - value of the heat release function at the surface

R - universal gas constant

$R(x)$ - mass of B reacting per unit volume per unit time at x

R_o - constant mass reaction rate in Constant Temperature Reaction Rate model

r - linear regression rate of propellant surface

$T, T(x)$ - temperature at x

T_o, T_s, T_f - initial, surface, and flame temperatures, respectively

$\bar{W}$ - average molecular weight of mixture in gas-phase

x - spatial variable

LIST OF SYMBOLS (Cont'd)

λ - heat conductivity in gas-phase

ν - gas-phase reaction order

ρ - local mass density in gas-phase

σ_p - temperature sensitivity at constant pressure

ϕ_G - heat flux from gas phase to surface supplied by gas-phase heat release

ϕ_s - heat flux from gas phase required by solid to maintain steady-state regression

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