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ANALYSIS OF NITROGEN CONDENSATION IN AN EXPANDING NOZZLE FLOW

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16. ABSTRACT

Condensation of nitrogen flow in an expanding nozzle flow is analyzed using one-dimensional gas dynamic equations and the equations for nucleation and droplet growth. Effects of variations in the Tolman constant and the mass accommodation factor are discussed as well as the effect of foreign nuclei. Comparisons are made with experimental data obtained from a small, contoured nozzle.

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NOMENCLATURE

Symbol	Definition
A	nozzle cross-sectional area
C_p	specific heat at constant pressure
D	Tolman's Constant
g	mass fraction in condensed phase
J	nucleation rate per unit volume
k	Boltzmann's gas constant
L	latent heat of varpoization
M	local Mach number
$\dot{m}$	rate of mass flow
N	nucleation rate
N_A	Avogadro's number
$\dot{N}_d$	number flux of particles
p	static pressure
r	droplet radius
r_d	particle radius
$\dot{S}_d$	surface flux of particles
T	flow temperature
T_s	surface temperature of droplets
U	flow velocity

NOMENCLATURE (Concluded)

Symbol	Definition
X	distance along nozzle
α	mass accommodation factor
γ	ratio of specific heats
ϵ_p	fractional deviation of pressure from isentropic condition
ϵ_T	fractional deviation of temperature from isentropic condition
η	mass fraction of foreign particles
μ	molecular weight
ρ	density
ρ_d	density of particles
σ	surface tension

Superscripts and Subscripts

$(\ )^*$	droplets of critical size
$(\ )_L$	liquid phase
$(\ )_i$	incremental step in which droplets were formed originally
$(\ )_j$	incremental step being considered
$(\ )_\infty$	liquid phase of infinite radius

ANALYSIS OF NITROGEN CONDENSATION IN AN EXPANDING NOZZLE FLOW

INTRODUCTION

In a recent report [1], experimental results of vapor-liquid condensation in small, contoured nozzles were presented. In these experiments, condensation takes place very close to the saturation point, leaving almost no supersaturation in the flow. This is in contrast to most of the experimental data reported elsewhere [2-13]. To assess the factors which caused the discrepancies, a flow analysis based on the condensation model of Griffin and Sherman [14] has been performed. The discrepancies between analysis and experiment indicate that there are factors which are not considered in the analytical model.

The two factors known to have a major effect on the flow condensation are the rate of expansion and the degree of impurities. The former is a fluid dynamic factor and can be accounted for analytically using the equations of fluid flow. Using experimental data obtained primarily from supersonic and hypersonic wind tunnels, Daum and Gyarmathy [15] obtained a correlation between the onset of condensation and the rate of expansion of the nozzle. The expansion rate also affects the droplet growth once the onset of condensation has been reached. The second factor is a thermodynamic phenomenon and can be explained by the kinetic theory of liquids [16]. Experimental studies conducted by Arthur and Nagamatsu [5] indicate that the foreign particles act like additional nuclei which enhance condensation. For flows with large amounts of foreign particles, condensation may become so rapid that the flow follows the vapor pressure curve, leaving no supersaturation at all.

The present condensation model uses the theory of nucleation with the steady one-dimensional equations of motion for diabatic flows. Computer analyses for flows in one-dimensional nozzles using these equations can be found in other reports [17-19].

ANALYSIS

The analysis uses the equations of one-dimensional diabatic flow, the theory of nucleation, and the droplet growth rate equation. The basic assumptions used are as follows: (1) the flow is steady, one-dimensional, and the nozzle wall is frictionless and non-heat conducting; (2) the vapor is a perfect gas with known thermodynamic constants; (3) the flow is isentropic before the onset of condensation, and diabatic thereafter; (4) the condensed mass is liquid, and its interaction with the flow is negligible; (5) the volume of the condensed phase is negligible compared with the total volume. With these assumptions, the flow equations can be written as [17]:

$$\frac{d\rho}{\rho} + \frac{dU}{U} + \frac{dA}{A} = 0 \tag{1}$$

$$\frac{dp}{\rho} = -U\,dU \tag{2}$$

$$\frac{dp}{p} = \frac{d\rho}{\rho} + \frac{dT}{T} - \frac{dg}{1-g} \tag{3}$$

$$U dU + C_p dT - L dg = 0 \tag{4}$$

$$(\gamma-1) M^2 \left(\frac{dU}{U}\right) + \frac{dT}{T} - \left(\frac{L}{C_p T}\right) dg = 0 \tag{5}$$

where p, T, U, A, and ρ are flow quantities measured along the streamtube under consideration; L is the latent heat of evaporation; and g is the mass fraction in the condensed phase.

Equations (1) through (5) serve as the isentropic condition when g and dg are zero, and the diabatic condition when the condensed phase is present ($g \neq 0$). Replacing the differentials in these equations by differences and rearranging, the following equations for the step change of pressure and temperature can be obtained:

$$\frac{\Delta p}{p} = -\left[\frac{\gamma M^2}{M^2 - 1}\right] \frac{\Delta A}{A} \left(1 - \epsilon_p\right) \tag{6}$$

and

$$\frac{\Delta T}{T} = -\left[\frac{(\gamma-1) M^2}{M^2 - 1}\right] \frac{\Delta A}{A} \left(1 - \epsilon_T\right) \tag{7}$$

where

$$\epsilon_p = \frac{A}{\Delta A} \left[\frac{L}{C_p T} - 1\right] \Delta g \tag{8}$$

and

$$\epsilon_T = \frac{A}{\Delta A} \left\{ \left[\frac{\gamma - \left(\frac{1}{M^2}\right)}{\gamma - 1}\right] \frac{L}{C_p T} - 1 \right\} \Delta g \tag{9}$$

are the fractional deviation of pressure and temperature from their corresponding isentropic conditions. From the measured flow quantities along the nozzle, equations (6) through (8) give the values of ϵ_T and ϵ_p. From equations (8) and (9) it is obvious that $\epsilon_T > \epsilon_p$ for $M > 1$ and $\epsilon_T < \epsilon_p$ for $M < 1$. Hence, in a supersonic flow the temperature measurements will give better indications of onset of condensation.

To calculate the increment Δg, the equations for the rate of nucleation and the droplet growth rate are used. From the kinetic theory description of Volmer [20], a condensation nucleus is formed spontaneously upon collisions between clusters of vapor molecules. When the nucleus, so formed, reaches a critical radius, it will continue to grow upon further collisions with vapor molecules; otherwise, it will evaporate and diminish eventually. Assuming that (1) the collision probability on a unit surface is given by an equilibrium particle distribution, (2) the saturation vapor pressure equals that of a droplet of infinite radius, and (3) the radius of the droplet is smaller than the mean free path of the vapor, the following equations can be obtained [17]:

$$J_i = \left(\frac{p}{kT}\right)^2 \frac{1}{\rho_L} \left(\frac{2\sigma\mu}{\pi N_A}\right)^{1/2} \exp\left(-\frac{4\pi\sigma r^{*2}}{3kT}\right) \tag{10}$$

$$r_i^* = \left(\frac{2\sigma\mu}{\rho_L}\right) RT \ln\left(\frac{p}{p_\infty}\right) \quad , \tag{11}$$

where J_i is the number of critical drops formed per unit volume per unit time, k the Boltzmann constant, N_A the Avadro's number, μ the molecular weight of the vapor, σ the surface tension of the liquid, and r_i^* is the critical drop radius.

The number of droplets formed in a step increment of Δx_i is then given by

$$N_i = J_i A_i \Delta x_i \quad . \tag{12}$$

By a consideration of heat transfer in a rarefied gas, the growth rate of a droplet can be found as

$$\Delta r_j = \frac{\alpha}{L} \frac{p}{\rho_L} \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{kN_A}{\mu T}\right)^{1/2} (T_s - T) \frac{\Delta x_i}{U} \tag{13}$$

where α is an accommodation factor and T_s is the temperature of the liquid.

By summing up the growth in the step increment Δx_j of droplets formed in all the previous steps, the net mass fraction condensed in this step increment can be obtained as

$$\Delta g_j = \frac{4\pi\rho_L}{\dot{m}} \left[\sum_{i=1}^{j-1} N_i r_{ij}^2 \Delta r_j + \frac{1}{3} N_j r_j^{*3} \right] \quad . \tag{14}$$

The surface tension, σ, used in equations (10) and (11) is a function of the droplet radius. A relation given by Tolman [20] is used here:

$$\sigma = \frac{\sigma_\infty}{1 + \frac{D}{r}} \tag{15}$$

where σ_∞ is the surface tension when the drop radius approaches infinity. The parameter D is the Tolman constant which is closely related to the intermolecular distance in the liquid drop. The value of the order of 10^{-8} cm has been suggested in References 21 and 22. However, the calculations used are not sufficiently reliable to give an exact value. Variations in the value of Tolman's constant are thus included in this analysis.

To start the calculation, the rate of expansion (distribution of area A) of an equivalent nozzle is obtained from the Mach number distribution of the actual nozzle flow. Using this area distribution as an input, and with a given chamber condition, isentropic relations can be used until saturation condition is reached. The nucleation relations, equations (10) and (11), are then used to calculate the initial condensation at each increment of x thereafter. By comparing the droplet size with a given critical drop size, the point of onset of condensation can also be defined. The droplet growth equations (12) and (13) are then included in the calculation providing complete flow parameters at each step Δx.

The effect of foreign nuclei on the onset of condensation can be included by assuming that all the nuclei are of the same size, and an equivalent radius r_d for the nuclei can be defined. With a given density ρ_d and mass fraction η for the foreign nuclei in a flow of mass flux $\dot{m}$, this equivalent radius can be related to the number flux $\dot{N}_d$ and surface flux $\dot{S}_d$ of the nuclei by the following equations:

$$\dot{N}_d = \frac{3\dot{m}}{4\pi\rho_d} \frac{\eta}{r_d^3} \tag{16}$$

and

$$\dot{S}_d = \frac{3\dot{m}}{\rho_d} \frac{\eta}{r_d} \quad . \tag{17}$$

Note that the factor $\dot{m}\eta/\rho_d$ gives the volume flux of the foreign nuclei.

By neglecting the interaction between the foreign nuclei and the vapor flow, the only effect caused by the presence of the foreign nuclei is to provide additional surfaces on which the vapor can condense. Under this circumstance, the vapor starts to condense on the foreign nuclei immediately upon reaching the saturation condition. Homogeneous condensation may still occur later and the same procedure mentioned in the previous paragraph will follow.

RESULTS AND DISCUSSIONS

Analysis of nitrogen flow in the contoured nozzle used in Reference 1 has been performed for two sets of chamber conditions: (1) $P_c = 681.9\ N/cm^2$ (989 psia), $T_c = 280$ K (504°R), and (2) $P_c = 548.1\ N/cm^2$ (795 psia), $T_c = 278.3$ K (501°R). These conditions correspond to Test Runs 9 and 10 in Reference 1 (Table 1). Results of parametric studies for various values of the mass accommodation factor, α, and the Tolman's constant, D, are also presented.

The distribution of temperature, percentage condensed, and the rate of nucleation for chamber condition (1) are given in Figures 1, 2, and 3. It is evident from these figures that the onset of condensation moves upstream as the value of Tolman's constant increases. An upper bound of approximately $D = 4.0 \times 10^{-7}$ cm, however, does exist, beyond which the numerical scheme breaks down. This may be due to the large amount of condensation which occurs in a single stepsize that stops the calculation.

The effect on the onset of condensation due to changes in the accommodation factor is rather small. Its main effect, rather, shows in the rate of nucleation. From Figure 3 it can be shown that for large accommodation factors the nucleation occurs at high rates over a very narrow region, giving a sudden and drastic change in the thermodynamic states of the fluid. At very low values, e.g., $\alpha = 0.01$, the rate of nucleation becomes so small that its effect on the flow is compensated by the rate of expansion in the flow. Continuous nucleation at moderate rates extends all the way toward the exit of the nozzle. This phenomenon can also be shown clearly in the pressure-temperature distribution given in Figure 4 where all the curves approach a parallel to the saturation curve. The transition from the isentrope to the parallel is where the thermodynamic non-equilibrium occurs. The diminishing of this transition region for small α's indicates a state of thermodynamic quasi-equilibrium with supersaturation kept at a constant level.

The results presented in Figures 1 through 4 for the chamber condition (1) are typical of all chamber conditions. Similar results have been obtained for chamber condition (2), but are not presented in this paper.

Analysis of heterogeneous condensation with foreign nuclei are performed under six different conditions. These conditions, given in Table 2, cover a wide range of number density of particles and of particle size distribution. The resulting static pressure distribution for chamber condition (2) with α = 0.75 and D = 4.0×10^{-7} is given in Figure 7. It is obvious that under such a chamber condition, the condensation is affected very little by the variations in the foreign particles.

Experimental measurements of the static pressure distribution from Reference 1 are presented in Figures 5, 6, and 7 and compared with analytical results. Results indicate that the flow condensation occurs sooner than predicted by the analysis. This difference cannot be accounted for even if foreign particles were introduced in the analysis (Fig. 7). It is thus concluded that certain phenomena other than the spontaneous condensation of nitrogen exist in these flows.

The tests conducted in Reference 1 have chamber conditions which lead to high saturation temperatures and pressures. A quick calculation for an adiabatic expansion from chamber condition (1) yields a saturation Mach number of 3.8 and Reynolds number per unit length of 3×10^{-6} cm^{-1}. For a nozzle with a length scale of 1 cm as the one used in Reference 1, such a combination requires the flow to be treated as a continuum [23]. This indicates that the free molecular assumptions used in the analytical model are no longer valid under this circumstance. The addition of viscous effect and molecular interaction are thus needed to better describe the flow. This observation is by no means an isolated one, as similar deviation from analysis (Fig. 8) is also found in the data of Goglia and Van Wylen [7]. Although the deviation was explained in Reference 15 as due to the possible presence of foreign particles, it could well be the result of neglecting the effect of viscosity and molecular interaction.

TABLE 1. EXPERIMENTAL CONDITIONS [1]

Run No.	Vapor	P_c N/cm^2 (psia)	T_c K (° R)
9/1(1)	N_2	681.9 (989)	280.0 (504)
10/0(8)	N_2	548.1 (795)	278.3 (501)
14/0(10)	N_2	475.7 (690)	281.7 (507)
11/0(8)	N_2	413.7 (600)	280.0 (504)
13/0(10)	N_2	344.7 (500)	280.0 (504)
12/0(5)	N_2	275.8 (400)	279.4 (503)

TABLE 2. FOREIGN NUCLEI CONDITIONS

Case	η (%)	r_d (cm)	$\dot{N}_d$ $\frac{\text{drops}}{\text{s}}$	$\dot{S}_d$ $\frac{\text{cm}^2}{\text{s}}$
1	0	—	—	—
2	0.01	5×10^{-7}	9.2×10^{17}	2.89×10^{6}
3	0.01	5×10^{-8}	9.2×10^{20}	2.89×10^{7}
4	1	5×10^{-6}	9.2×10^{16}	2.89×10^{7}
5	1	5×10^{-7}	9.2×10^{19}	2.89×10^{8}
6	1	5×10^{-8}	9.2×10^{22}	2.89×10^{9}

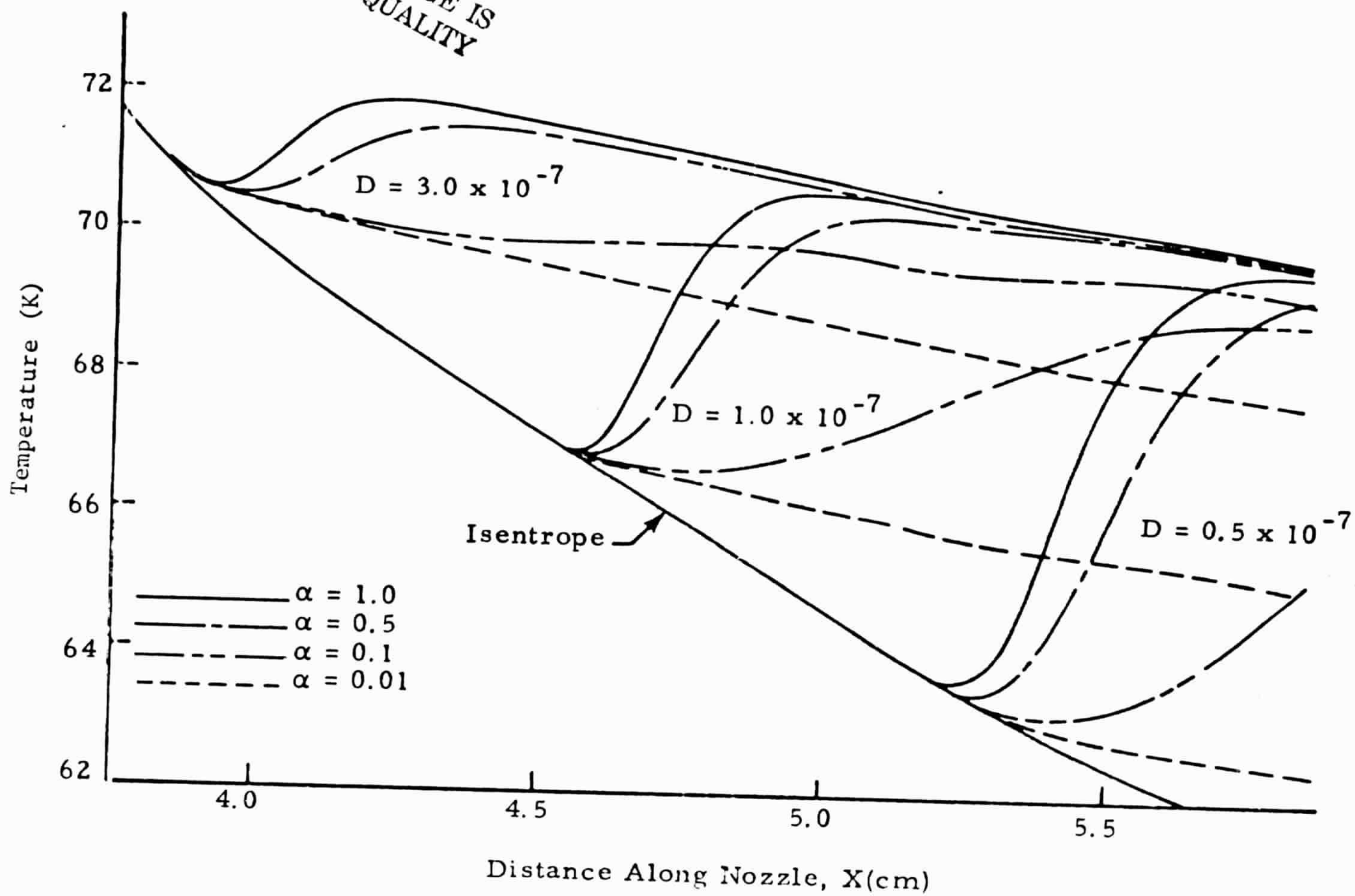

Figure 1. Variation of temperature distribution with accommodation factor and Tolman's constant (run 9).

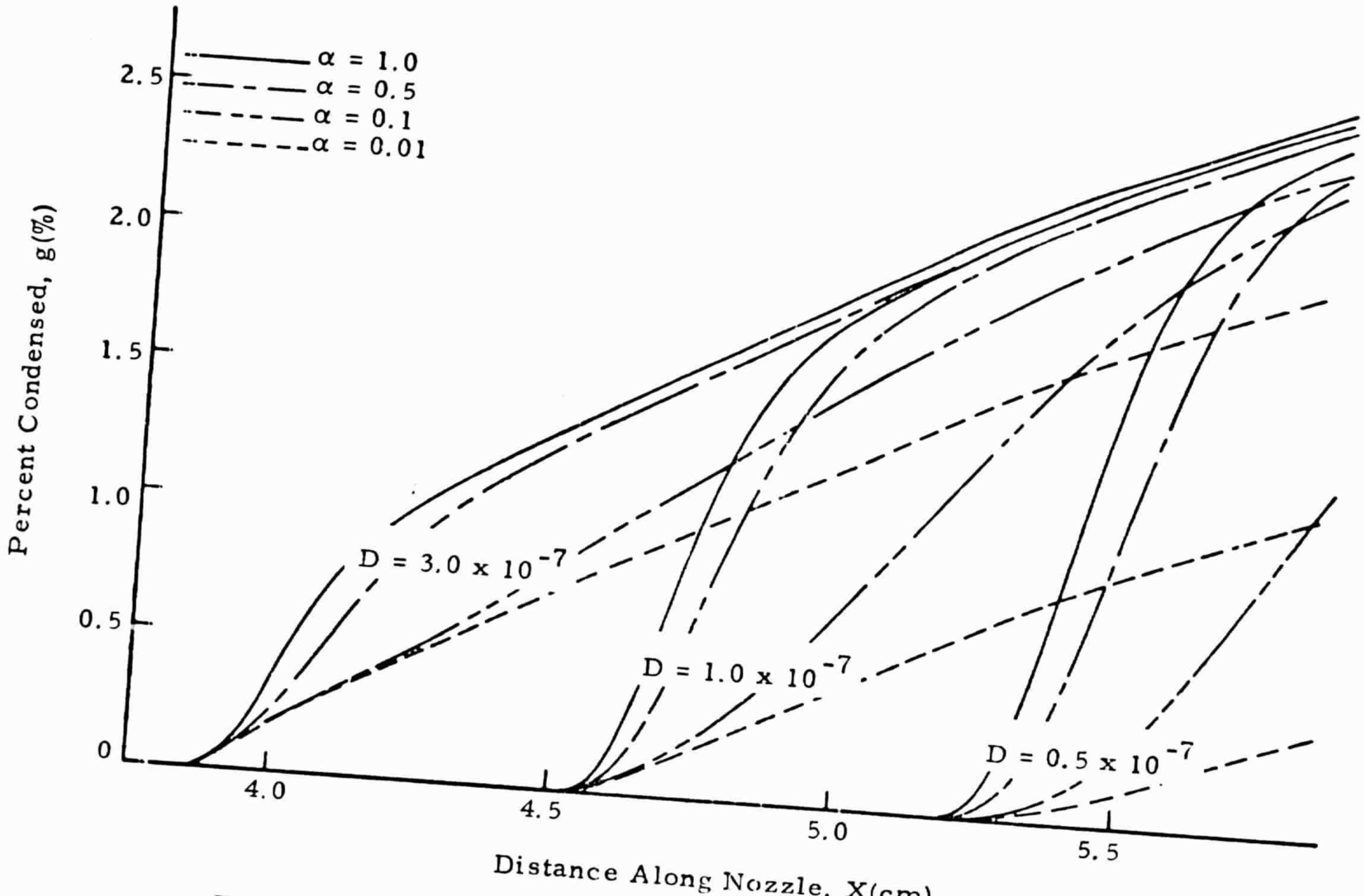

Figure 2. Variation of percentage of condensed phase distribution with accommodation factor and Tolman's constant (run 9).

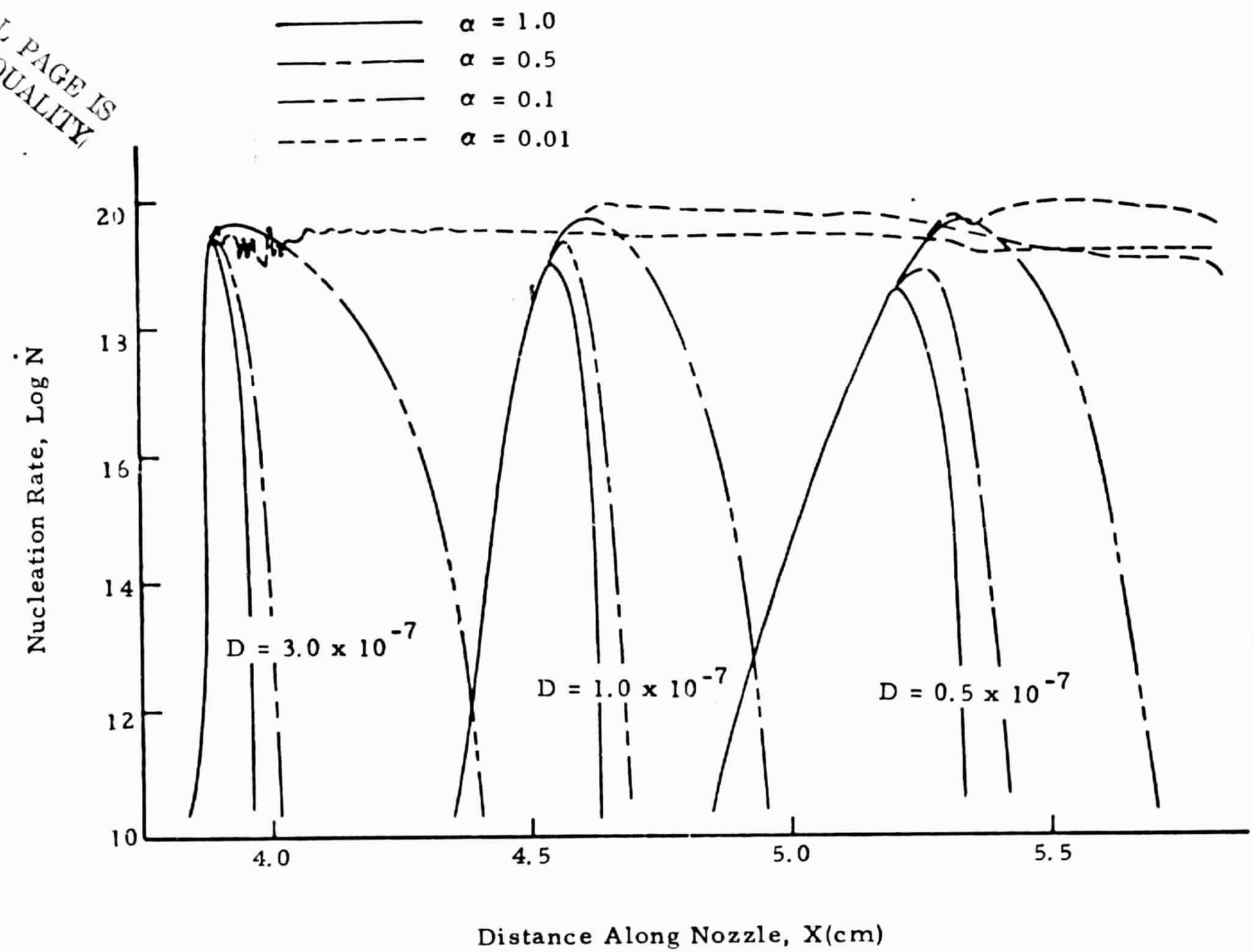

Figure 3. Variation of rate of nucleation distribution with accommodation factor and Tolman's constant (run 9).

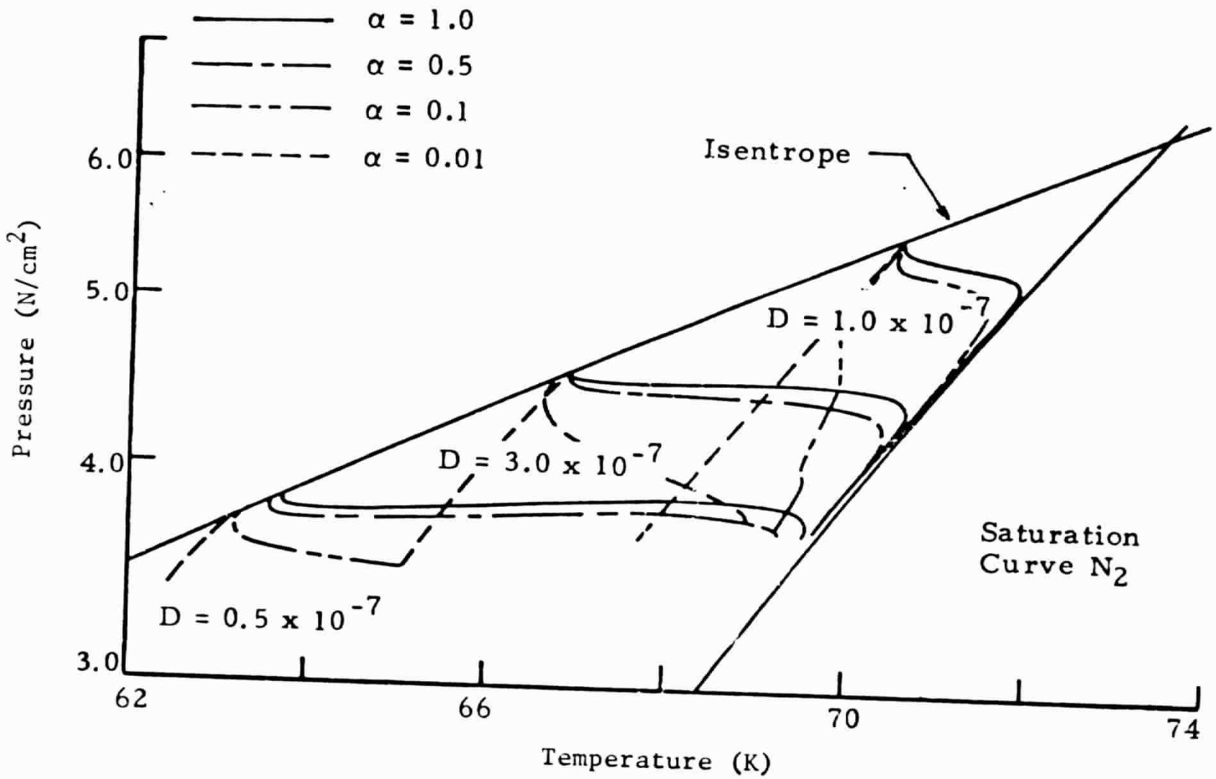

Figure 4. Variation of pressure-temperature diagram (run 9).

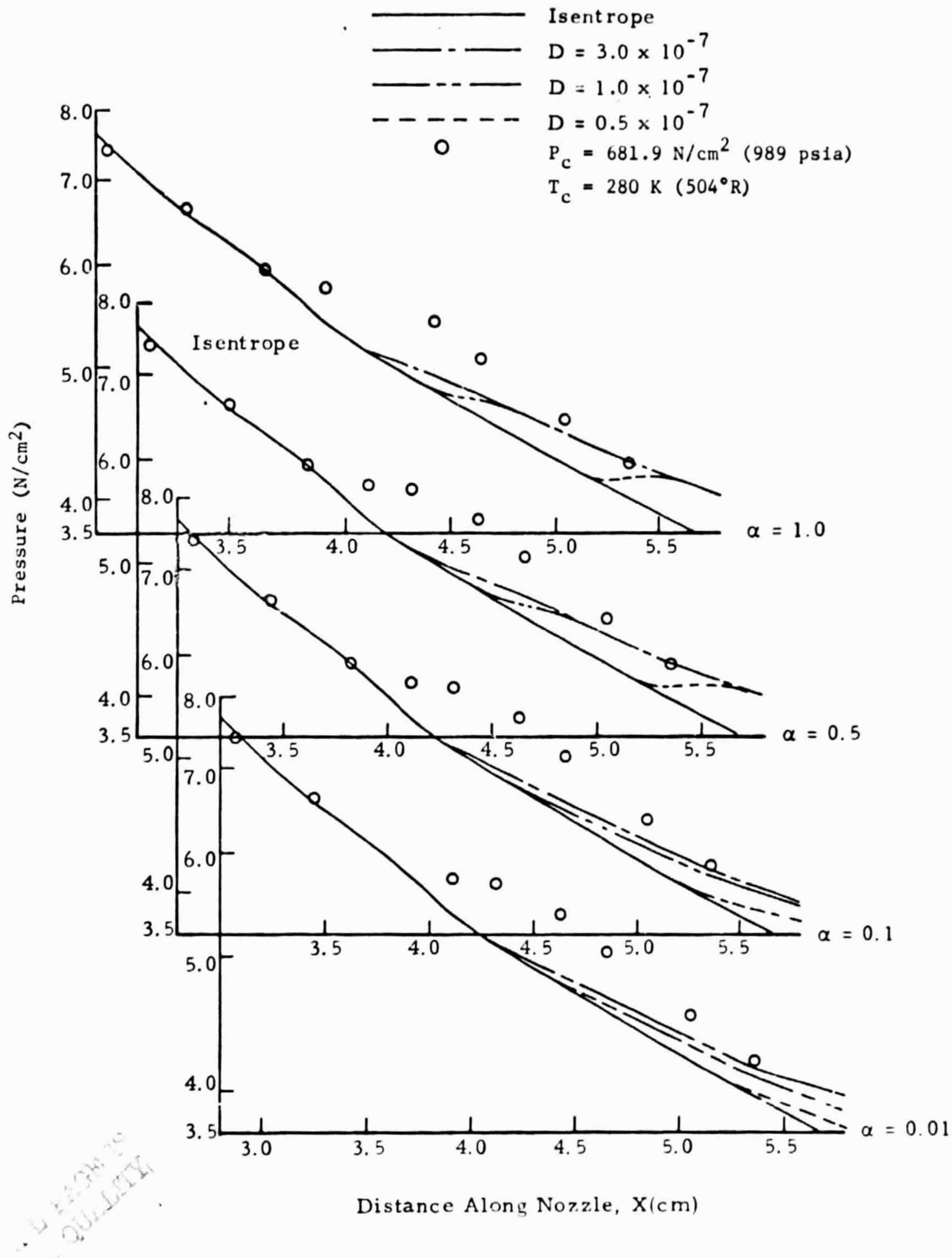

Figure 5. Variation of static pressure distribution with accommodation factor and Tolman's constant (run 9).

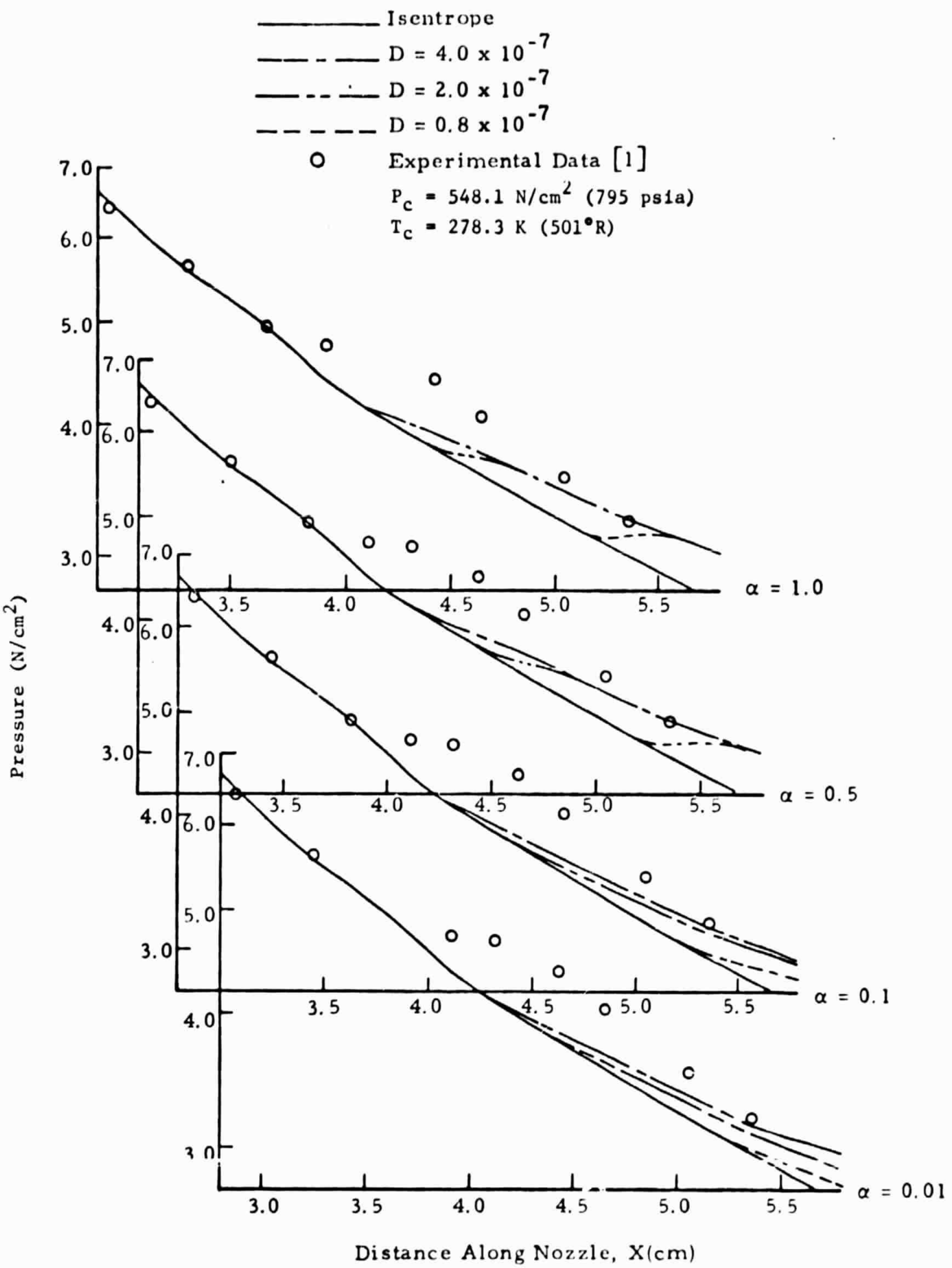

Figure 6. Variation of static pressure distribution with accommodation factor and Tolman's constant (run 10).

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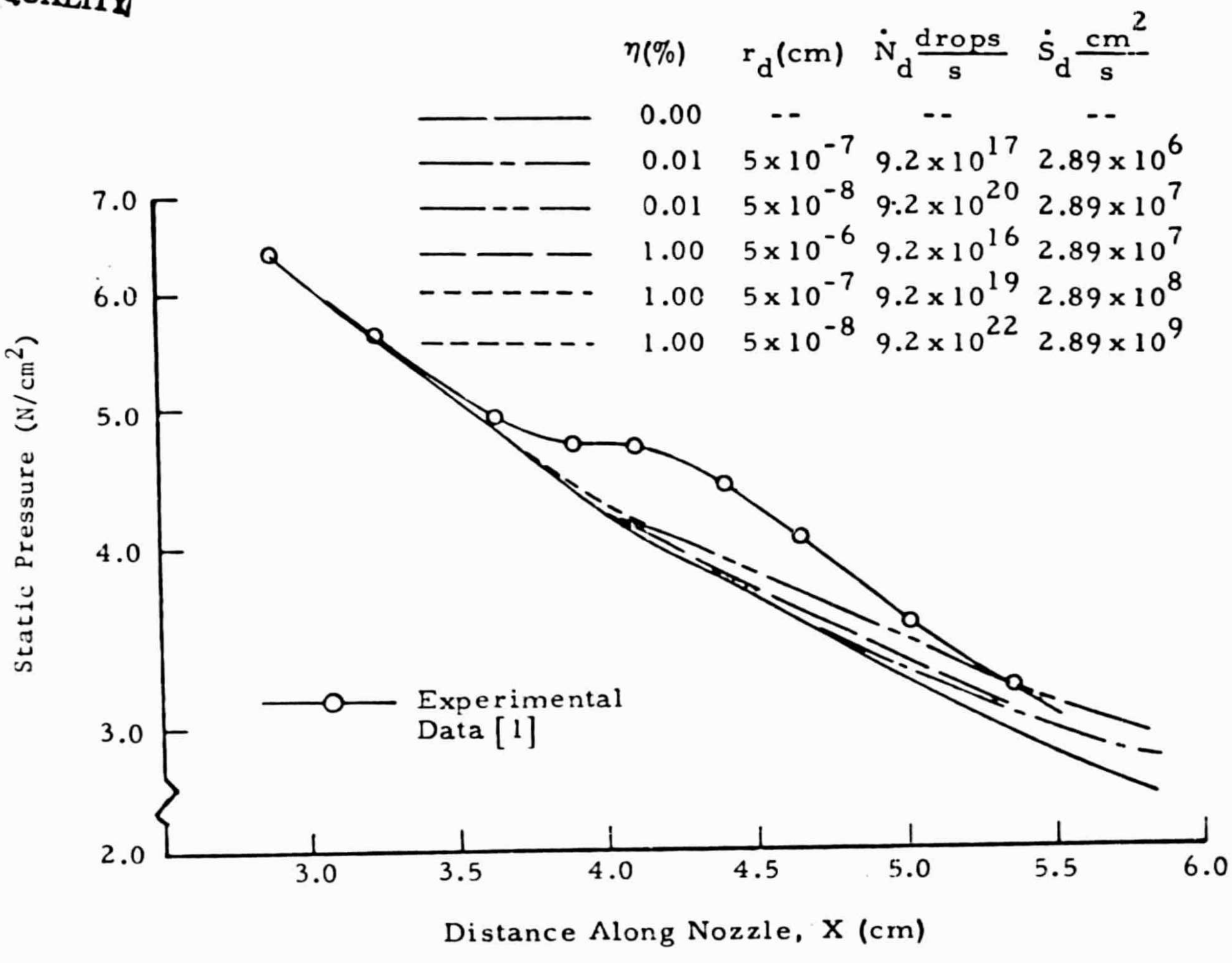

Figure 7. Variation of static pressure distribution with foreign particles (run 10).

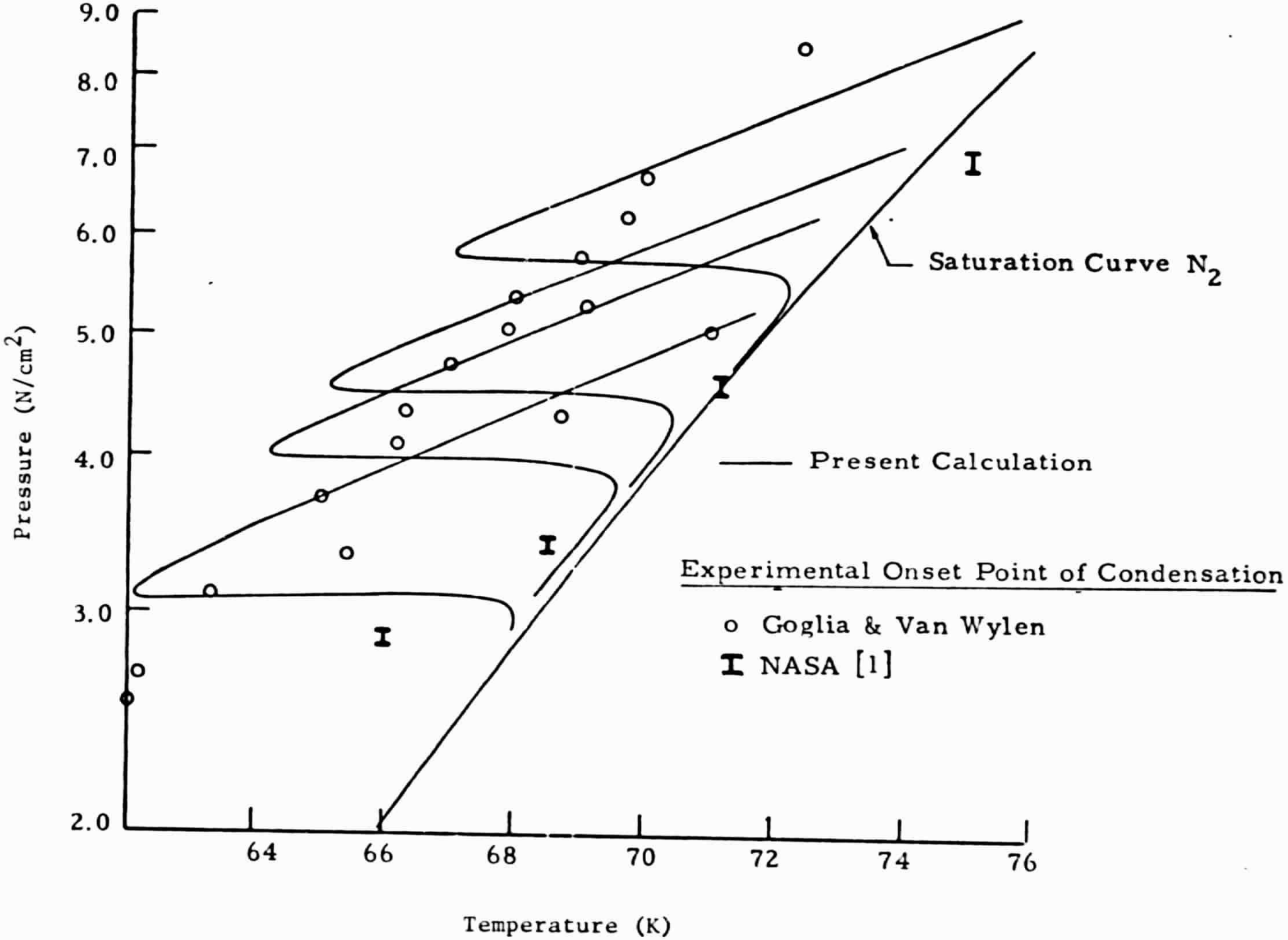

Figure 8. Comparison of nitrogen condensation onset behavior above the triple point.

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APPROVAL

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The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

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