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CALCULATIONS FOR AIR FLOWS IN DISSOCIATION EQUILIBRIUM

by

Nathan Gerber
Joan M. Bartos

November 1965

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BALLISTIC RESEARCH LABORATORIES
ABERDEEN PROVING GROUND, MARYLAND

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Nathan Gerber
Joan M. Bartos

Exterior Ballistics Laboratory

RDT & E Project No. 1A222901A201

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NGerber and JMBartos
Aberdeen Proving Ground, Md.
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CALCULATIONS FOR AIR FLOWS IN DISSOCIATION EQUILIBRIUM

ABSTRACT

Results of calculations carried out for a model of air in dissociation equilibrium are presented in graphical form. The quantities computed are i) flow variables (including species concentrations) behind normal and oblique shock waves, ii) flow variables in axisymmetric conical flow fields, iii) stagnation point values of flow variables on the 'stagnation' streamline behind two-dimensional and axisymmetric detached shock waves, and iv) flow variable gradients at the shock wave on stagnation streamlines. Computations are given for free stream temperatures of 273.16°K and 300°K, free stream pressures of 1.0, .1, .01, .001, and .0001 atmospheres, and a range of initial Mach numbers and cone angles to provide flow field temperatures in the range 3000°K - 10,000°K. Brief derivations of the equations employed are given.

The present calculations are oriented toward application in experiments in hypersonic flow with ground facilities such as shock tubes and ballistic ranges. In addition, they furnish important supplementary information to theoretical studies of nonequilibrium flows.

TABLE OF CONTENTS

SYMBOLS

$A_{k\ell}$	Functions occuring in Eqs (2.6) and (2.9)
c_i	Concentration of ith species [k mol/kg of mixture]
c_p	Specific heat of air at constant pressure [Dyn m/kg deg K] (1 Dyn = 1 Newton = 10^5 dynes)
c_{p_i}	$= dh_i/dt$ (see Table II) [Dyn m/k mol deg K]
c_v	Specific heat of air at constant volume [Dyn m/kg deg K]
h	Specific enthalpy [Dyn m/kg] $= \sum c_i h_i$
h_i	Molar specific enthalpy of ith species (see Table II)
k_{f_j}, k_{b_j}	Reaction rate constants for jth reaction, forward and backward, respectively (see Table I)
K_j	($\equiv k_{f_j} / k_{b_j}$). Equilibrium constant for jth reaction (see Table I)
K_w	Shock wave curvature
M_∞	Free stream Mach number
n	Arc length along curve normal to streamlines [m, mm]
p	Pressure $\left[\text{Dyn/m}^2\right]$
q	Flow velocity [m/sec]
R	Universal gas constant = 8312.4 [Dyn m/k mol deg K]
R_w	Shock wave radius of curvature ($= 1/K_w$)
r	Radial polar coordinate $\left(= \left[x^2 + y^2\right]^{1/2}\right)$
s	Arc length along streamline [m, mm]
T	Temperature [deg K]
U	Velocity component in r direction ($= q \cos [\theta - \varphi]$)
V	Velocity component in φ direction ($= q \sin [\theta - \varphi]$)
W_i	Molecular weight of ith species [kg/k mol]
W_∞	Molecular weight of air (= 28.8587 gm/mol)
θ	Angle between shock wave and x-axis [radians, deg]
γ	Ratio of specific heats of air (c_p/c_v)

ϵ	= 0 for two-dimensional flow; = 1 for axisymmetric flow
θ	Angle between streamline and x-axis [radians, deg]
ρ	Density $\left[kg/m^3\right]$
σ	Arc length along shock wave
φ	Angular polar coordinate (φ = arctan y/x)

Subscripts

b	Body surface
i	i^{th} species
j	j^{th} reaction
t	Stagnation point
w	Shock wave
∞	Free stream

1. INTRODUCTION

Current experimental research in hypersonic flow over two-dimensional and axisymmetric bodies makes it desirable to have available calculations for air in chemical (dissociation) equilibrium. Primarily these are values of the flow variables (including concentrations of chemical species) behind shock waves and in conical flow fields. Furthermore, it is desired to have these data for ranges of free stream conditions applicable to experiments with ground facilities, such as shock tubes and ballistic ranges. To this end extensive calculations of shock wave quantities and conical flows have been carried out on the BRL high-speed computers for a model of air (see Section 2) in chemical equilibrium, and results are presented graphically here in Figs. I.1 through II.9.* Brief derivations of the equations are given in Sections 3 and 4. Although computations of the above have already been carried out by other authors (e.g., Refs. 1 through 4 and the references contained in them), the present paper furnishes information hitherto not available, to the authors' knowledge, in a form convenient for work in hypersonic ground facilities.

The present calculations also supply important supplementary information for the determination of nonequilibrium dissociating airflow over wedges and cones.[5]** Certain features of these nonequilibrium flows (e.g., entropy layers, oblique shock equilibrium regions) require knowledge of equilibrium values.

Studies being conducted at BRL on the subsonic region in front of a supersonic blunt body by analysis of interferometric data suggest that theoretically determined information on the stagnation streamline would be useful. Therefore, extensive calculations were performed to obtain stagnation values of the flow variables, and, in addition, gradients of the flow variables along the stagnation streamline at the shock wave. These results are presented graphically in Figs. III.1 through IV.8; derivations are given in Sections 5 and 6.

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*The computer program is available for cases not explicitly graphed in this report should exact values be required.

** Superscript numbers denote references which may be found on page 56.

2. AIR MODEL

The air is considered to be a mixture of neutral species consisting of O and N atoms, and N_2, O_2, and NO molecules. This mixture of particles is assumed to be in translational, rotational, and vibrational equilibrium at all times. Effects of electronic excitation and vibration-dissociation coupling are neglected. The chemical reactions are listed in Table I.

Let c_i denote the concentration of the i^{th} species M_i (moles of M_i per unit mass of air) and K_j the equilibrium constant of the j^{th} reaction. K_j can be determined quite accurately from quantum statistical calculations, and the results are often fitted to an equation of the form

$$K_j = A_j T^{n_j} \exp(-E_j/T) \ ,$$

where T is temperature, and A_j, n_j, and E_j are constants. The values listed for equilibrium constants in Table I are based on data given in Refs. 6 and 7.

The law of mass action for equilibrium flow leads to the relations

$$c_{O_2} = \frac{\rho c_O^2}{K_1} \ , \ c_{N_2} = \frac{\rho c_N^2}{K_2} \ , \ c_{NO} = \frac{\rho c_N c_O}{K_5} \ , \qquad (2.1)$$

(where ρ is the density of the air) plus the following restrictions:

$$L_1(T) \equiv \frac{K_6 K_7}{K_{10}} = 1, \qquad L_2(T) \equiv \frac{K_2 K_7}{K_1 K_6} = 1, \qquad L_3(T) \equiv \frac{K_5 K_7}{K_1} = 1 \ .$$

Calculation shows that L_1, L_2, and $L_3 = 1 \pm .10$ for a limited temperature range, the results being valid only within this range ($\sim 4000^\circ$ -- $8000^\circ K$).

The flows studied here are produced by objects moving at constant supersonic speed in stationary air, taken to be a mixture of two ideal gases O_2 and N_2 having concentrations

$$c_{O_{2_\infty}} = \frac{.21153}{W_\infty} \ \frac{\text{mole}}{\text{gm air}} \ , \ c_{N_{2_\infty}} = \frac{.78847}{W_\infty} \ \frac{\text{mole}}{\text{gm air}}$$

where the subscript ∞ denotes free stream conditions, and W_∞ is the molecular weight of air (= 28.85870).

The conservation of chemical elements leads to the following relations:

$$\begin{aligned} c_{O_{2_\infty}} &= c_{O_2} + (1/2)\, c_O + (1/2)\, c_{NO} \\ c_{N_{2_\infty}} &= c_{N_2} + (1/2)\, c_N + (1/2)\, c_{NO} \;. \end{aligned} \tag{2.2}$$

Substitution of Eq. (2.1) into Eq. (2.2) gives

$$\begin{aligned} c_{O_{2_\infty}} &= \frac{\rho c_O^2}{K_1} + (1/2)\, c_O + (1/2)\, \frac{\rho c_N c_O}{K_5} \\ c_{N_{2_\infty}} &= \frac{\rho c_N^2}{K_2} + (1/2)\, c_N + (1/2)\, \frac{\rho c_N c_O}{K_5} \;. \end{aligned} \tag{2.3}$$

Considering each component as an ideal gas, the equation of state for the i^{th} species is (p, ρ, and T being pressure, density, and temperature, respectively)

$$p_i = R\rho_i T/W_i$$

and for the mixture (where $p = \sum_i p_i$, $\rho = \sum_i \rho_i$)

$$p = R\rho T \sum_i c_i \qquad (\text{with } c_i = (\rho_i/\rho)/W_i) \;. \tag{2.4}$$

R is the universal gas constant, W_i the molecular weight of the i^{th} species, c_i the concentration. By Eq. (2.2)

$$\sum_i c_i = (1/W_\infty) + (1/2)(c_O + c_N) \cdot \qquad (2.5)$$

The differentiated versions of Eqs. (2.4) and (2.3) give the following useful set of linear equations for $d\rho$, dc_O, dc_N, and dT:

$$A_{11}d\rho + A_{12}dc_O + A_{13}dc_N + A_{14}dT = (2/p)\ dp \qquad (2.6a)$$

$$A_{21}d\rho + A_{22}dc_O + A_{23}dc_N + A_{24}dT = 0 \qquad (2.6b)$$

$$A_{31}d\rho + A_{32}dc_O + A_{33}dc_N + A_{34}dT = 0 \cdot \qquad (2.6c)$$

Expressions for the coefficients $A_{k\ell}$ are presented in the Appendix.

A fourth relation, valid along streamlines, is obtained from the energy equation

$$dh = (1/\rho)dp \qquad (2.7)$$

where h is enthalpy per unit mass. The total enthalpy is the sum of the enthalpies of the components:

$$h = \sum_i c_i h_i \cdot \qquad (2.8)$$

Expressions for h_i (enthalpy per mole) and dh_i/dT ($\equiv c_{p_i}$) are given in Table II for all the species. Eq. (2.7) becomes

$$A_{41}d\rho + A_{42}dc_O + A_{43}dc_N + A_{44}dT = (1/\rho)\ dp\ , \qquad (2.9)$$

the coefficients appearing in the Appendix.

Eqs. (2.1) are differentiated to give

$$dc_{O_2} = (c_O/K_1)\left[c_O d\rho + 2\rho dc_O - (\rho c_O/K_1)(dK_1/dT)dT\right]$$

$$dc_{N_2} = (c_N/K_2)\left[c_N d\rho + 2\rho dc_N - (\rho c_N/K_2)(dK_2/dT)dT\right] \qquad (2.10)$$

$$dc_{N_O} = \frac{1}{K_5}\left[c_O c_N\ d\rho + \rho(c_N dc_O + c_O dc_N) - \frac{\rho c_O c_N}{K_5}\ \frac{dK_5}{dT}\ dT\right] .$$

3. SHOCK WAVE CALCULATIONS

The conditions immediately behind a shock (denoted by the subscript w) are given by the following relations obtained from the conservation laws* (referring to Fig. 3.1):

$$\rho_w \tan(\beta - \theta_w) = \rho_\infty \tan\beta \qquad (3.1)$$

$$q_w \cos(\beta - \theta_w) = q_\infty \cos\beta \qquad (3.2)$$

$$p_w = p_\infty + \rho_\infty q_\infty{}^2 (1 - \rho_\infty/\rho_w)\sin^2\beta \qquad (3.3)$$

$$h_w = h_\infty + (1/2)q_\infty^2\ [1 - (\rho_\infty/\rho_w)^2]\sin^2\beta \qquad (3.4)$$

where β is the angle of inclination of the shock wave, q the flow speed, and θ the angle of inclination of the flow. In the free stream

$$h_\infty = (7/2)RT_\infty/W_\infty\ , \qquad p_\infty = R\rho_\infty T_\infty/W_\infty \qquad (3.5)$$

$$\rho_\infty q_\infty{}^2/p_\infty = \gamma_\infty M_\infty{}^2\ ,$$

where M_∞ is the Mach number and γ_∞ is the ratio of specific heats, having the value 1.4.

The flow variables behind the shock wave are determined by solving Eqs. (3.1), ..., (3.4), together with the equation of state Eq. (2.4), plus Eqs. (2.1) and (2.3). These form a set of ten functional equations for the ten variables p_w, θ_w, q_w, T_w, ρ_w, $(c_{O_2})_w$, $(c_{N_2})_w$, $(c_O)_w$, $(c_N)_w$, and $(c_{NO})_w$, when the parameters M_∞, T_∞, ρ_∞, (or p_∞) and β are given. The system of

---

*The basic jump conditions for a steady oblique shock wave requiring conservation of mass, momentum, and energy can be found in many places; e.g., p. 8 of Ref. 8.

equations is solved on the BRL high speed computers by successive application of the method of "regula falsi," or "false position." Frequently θ_w is given, and β is the unknown quantity; an additional iterative procedure (e.g., regula falsi) can then find the β corresponding to a given θ_w.

Figs. I.1 through I.11 contain curves of flow variables behind normal and oblique shock waves. Pressure, temperature, density, and species concentrations are conveniently expressible as functions of the parameter $M_\infty \sin \beta$ for given free stream temperature and pressure. For the flow deflection θ, another parameter, M_∞, is required.

4. CONICAL FLOW

In axisymmetric conical flow a straight cone of half angle θ_b gives rise to a straight attached shock wave inclined at angle β. It is convenient here to introduce polar coordinates r, φ (as in Fig. 3.1.b) and to employ U and V, the components of velocity in the r and φ directions, respectively. The values of φ at the shock and body are, respectively

$$\varphi_w = \beta \ , \qquad \theta_b = \varphi_b \tag{4.1}$$

With the condition that the flow variables be independent of radius ($\partial/\partial r = 0$), the mass and momentum conservation relations reduce to

$$dU/d\varphi = V \tag{4.2.a}$$

$$dV/d\varphi = -(V/\rho)d\rho/d\varphi - [2U + V \cot \varphi] \tag{4.2.b}$$

$$dp/d\varphi = V^2 \, d\rho/d\varphi + \rho V[U + V \cot \varphi] \tag{4.2.c}$$

On substituting $dp/d\varphi$ from Eq. (4.2.c) into the right hand sides of Eqs. (2.6) and (2.9) one obtains four linear algebraic equations for $d\rho/d\varphi$, $dc_O/d\varphi$, $dc_N/d\varphi$, and $dT/d\varphi$, which are solved to give differential equations

$$d\rho/d\varphi = F_1, \ dc_O/d\varphi = F_2, \ dc_N/d\varphi = F_3, \ dT/d\varphi = F_4 \tag{4.3}$$

where F_1, F_2, F_3, and F_4 are functions of φ, U, V, ρ, p, T, c_O, and c_N. Eqs. (4.2), (4.3), and (2.10) form a set of ten first order differential equations for U, V, p, ρ, T, c_{O_2}, c_{N_2}, c_O, c_N, and c_{NO}, which can be integrated numerically by the Runge-Kutta method[9] on the high speed computers.

The initial conditions are taken at the shock wave; for a given atmosphere, speed, and shock inclination, all quantities are known here. The terminal condition is $V_b = 0$. This condition makes it convenient to use V as the independent variable instead of φ.

Figs. II.1 through II.9 contain data for conical flow, for which many properties of interest can be accurately represented as functions of the parameter $M_\infty \sin \theta_b$, given the free stream conditions. Pressure, temperature, density, and species concentrations on the body surface are plotted against $M_\infty \sin \theta_b$, the shock wave angle is also presented in this form.

5. STAGNATION VALUES BEHIND NORMAL SHOCKS

Calculations are made of the flow variables when the fluid is brought to rest behind a normal shock wave, as for instance, at the intersection of the axial streamline with the surface of a symmetric blunt body (point O in Fig. 3.1.a). The independent variable in eqs. (2.6), (2.9), and (2.10) is taken to be the velocity q. These equations plus the momentum relation

$$dp/dq = - \rho q$$

form a set of differential equations which are integrated numerically from $q = q_w$ to $q = 0$, the terminal values of the variables giving the stagnation conditions.

Figs. III.1 through III.9 present the thermodynamic variables and species concentrations for stagnation flow behind normal shock waves as functions of M_∞. This information is useful in studying the subsonic region between the surface of a two-dimensional or axisymmetric blunt body and the detached shock wave ahead of it.

6. GRADIENTS AT SHOCK ON STAGNATION STREAMLINE

The flow variable gradients along the central streamline behind a curved shock (point P in Fig. 3.1.a) can be calculated if the curvature of the shock K_w is known. If σ is arc length along the shock wave, it is seen from the relation

$$\frac{d}{d\sigma} = K_w \frac{d}{d\beta} = [\cos(\beta - \theta)] \frac{\partial}{\partial s} + [\sin(\beta - \theta)] \frac{\partial}{\partial n}$$

(where s and n are arc lengths along streamlines and their orthogonal trajectory, respectively) that

$$(\partial/\partial n)_{x\text{-axis}} = K_w \, (d/d\beta)_{\beta = 90^\circ} \; . \qquad (6.1)$$

The momentum conservation equation*

$$\rho q^2 \, \partial\theta/\partial s = - \, \partial p/\partial n \qquad (6.2)$$

shows that $(dp/d\beta)_{\beta = 90^\circ} = 0$. Then, by Eq. (2.6) and Eq. (3.4) differentiated with respect to β, $d\rho/d\beta = dT/d\beta = dc_O/d\beta = dc_N/d\beta = 0$ at the x-axis. By the differentiated Eq. (3.1) and Eq. (6.1)

$$(\partial\theta/\partial n)_{\beta = 90^\circ} = [1 - \rho/\rho_\infty]K_w \; . \qquad (6.3)$$

Expanding $[(\sin \theta)/y]$ near the x-axis, noting that $dy_w = d\sigma \sin \beta$,

$$(\sin \theta)/y_w = [d\theta/dy)_{y_w = 0} \, y_w + \cdots]/y_w = (d\theta/d\sigma)_{y_w = 0} + \cdots \, .$$

Therefore

$$(\sin \theta)/y_w \cong K_w(d\theta/d\beta)_{\beta = 90^\circ} = [1 - (\rho/\rho_\infty)]K_w \; . \qquad (6.4)$$

Substituting Eqs. (6.3) and (6.4) into the flow equation

$$\frac{1}{\rho}\frac{\partial \rho}{\partial s} - \frac{1}{\rho q^2}\frac{\partial p}{\partial s} + \frac{\partial \theta}{\partial n} + \epsilon \frac{\sin \theta}{y} = 0 \qquad (6.5)$$

where $\epsilon = 0$ and 1 for two-dimensional and axisymmetric flow, respectively, one obtains

$$dp/ds = q^2 \, d\rho/ds - (1 + \epsilon)K_w \rho q^2 \, [(\rho/\rho_\infty - 1)] \; . \qquad (6.6)$$

On substituting dp/ds from Eq. (6.6) into Eq. (2.6) the gradients of the flow variables are determined. It is seen that the gradients are all proportional to K_w, and that for a given M_∞ the axisymmetric gradients are

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*Eqs. (6.2) and (6.5) expressing conservation of mass and momentum are found, e.g., in Section 3 of Ref. 5.

twice those for two-dimensional flow.

Gradients along the stagnation streamline at the shock wave are shown in Figs. IV.1 through IV.8 for the thermodynamic variables and the species concentrations. Arc length is given in terms of the radius of curvature of the shock wave, R_w, at the x-axis.

7. COMPUTATIONAL RESULTS

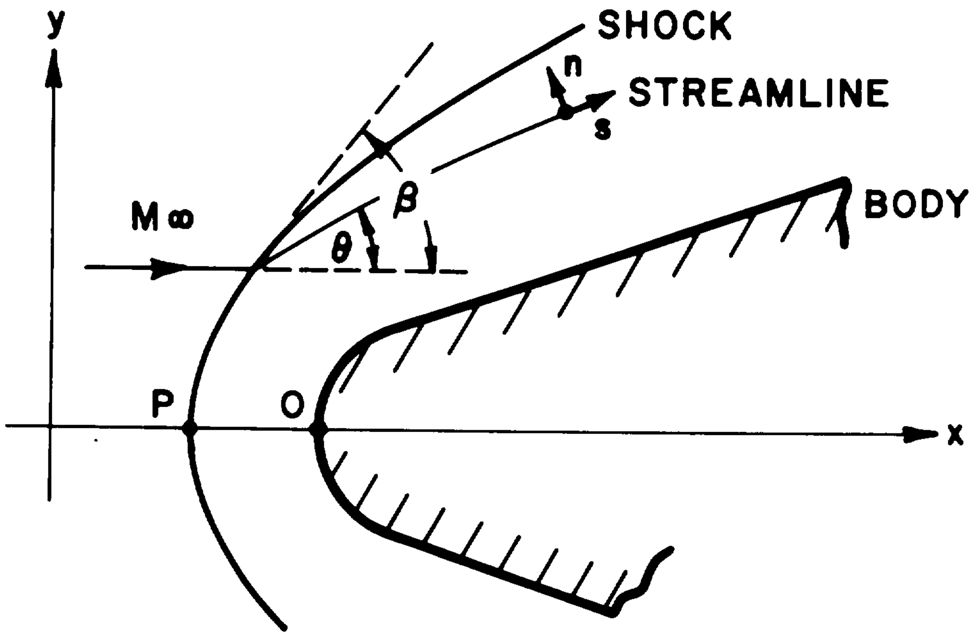
Computational results are presented in the diagrams which follow. Graphs of desired quantities are plotted for free stream temperatures of 273.16°K and 300°K, and free stream pressures of 1.0, .1, .01, .001, and .0001 atmospheres; the choice of Mach numbers, cone angles and shock wave angles makes possible a temperature range coverage of 3,000°K to 10,000°K. A complete survey for air in dissociation equilibrium is not feasible because of the multitude of combinations of parameters. It is felt, nevertheless, that the following set of diagrams can be used to obtain approximate information adequate for planning experiments, predicting and checking experimental results over a wide range of conditions attainable in the laboratory.

Comparisons were made of the present results with previously published results in which more accurate models of high temperature air were assumed. For example, conical flow parameters (Fig. II.1 - - II.4) practically coincide with those of Romig (Ref. 4). A comparison of shock and stagnation pressure calculations with those of Feldman (Ref. 1) is shown in Fig. 7.1; the largest discrepancy of all the parameters is found in the stagnation pressure.

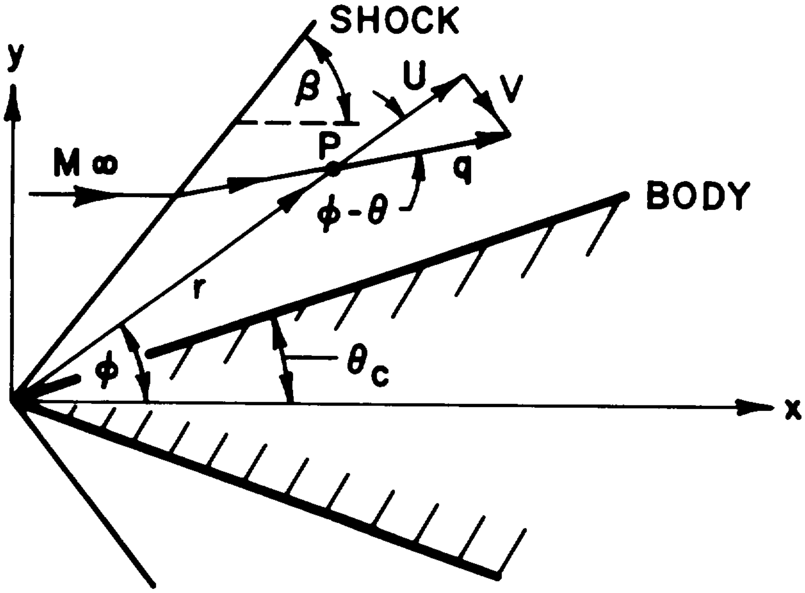
ACKNOWLEDGEMENTS

The authors wish to express their appreciation to the following persons: Barbara Bilsborough, for programming the calculations of shock wave quantities and conical flows; Donald Taylor, for assistance on computational problems; Joseph Spurk, for assistance on questions concerning aerodynamical theory; William Hammond and Vernon Mackey, for preparing the diagrams in this report.

NATHAN GERBER JOAN M. BARTOS



a. DETACHED SHOCK



b. ATTACHED SHOCK

FIG. 3.1. CROSS-SECTION DIAGRAM OF FLOW FIELD

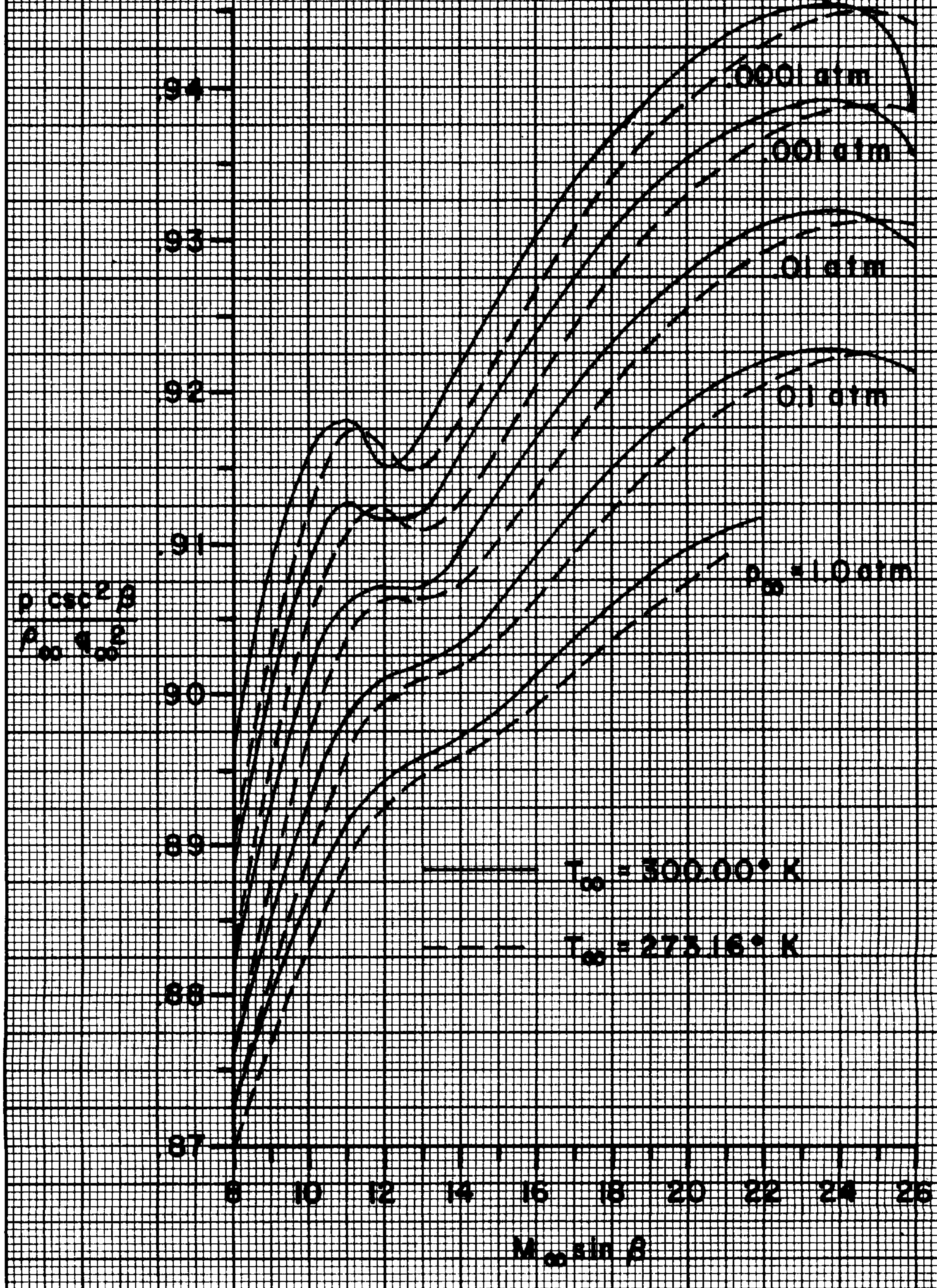


FIG. I.1. VARIATION OF PRESSURE ACROSS SHOCK WAVES

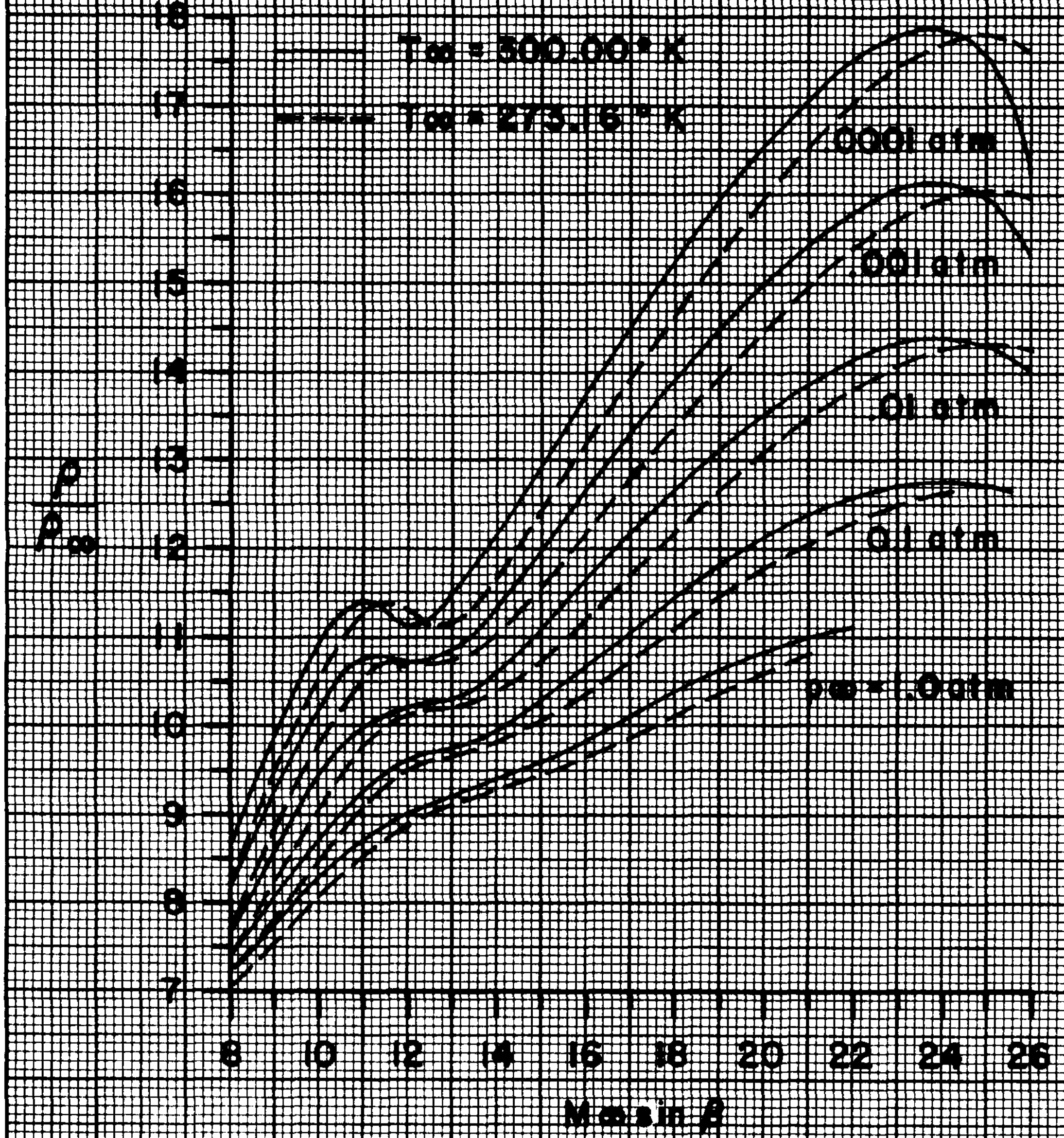


FIG. I.2. VARIATION OF DENSITY ACROSS SHOCK WAVES

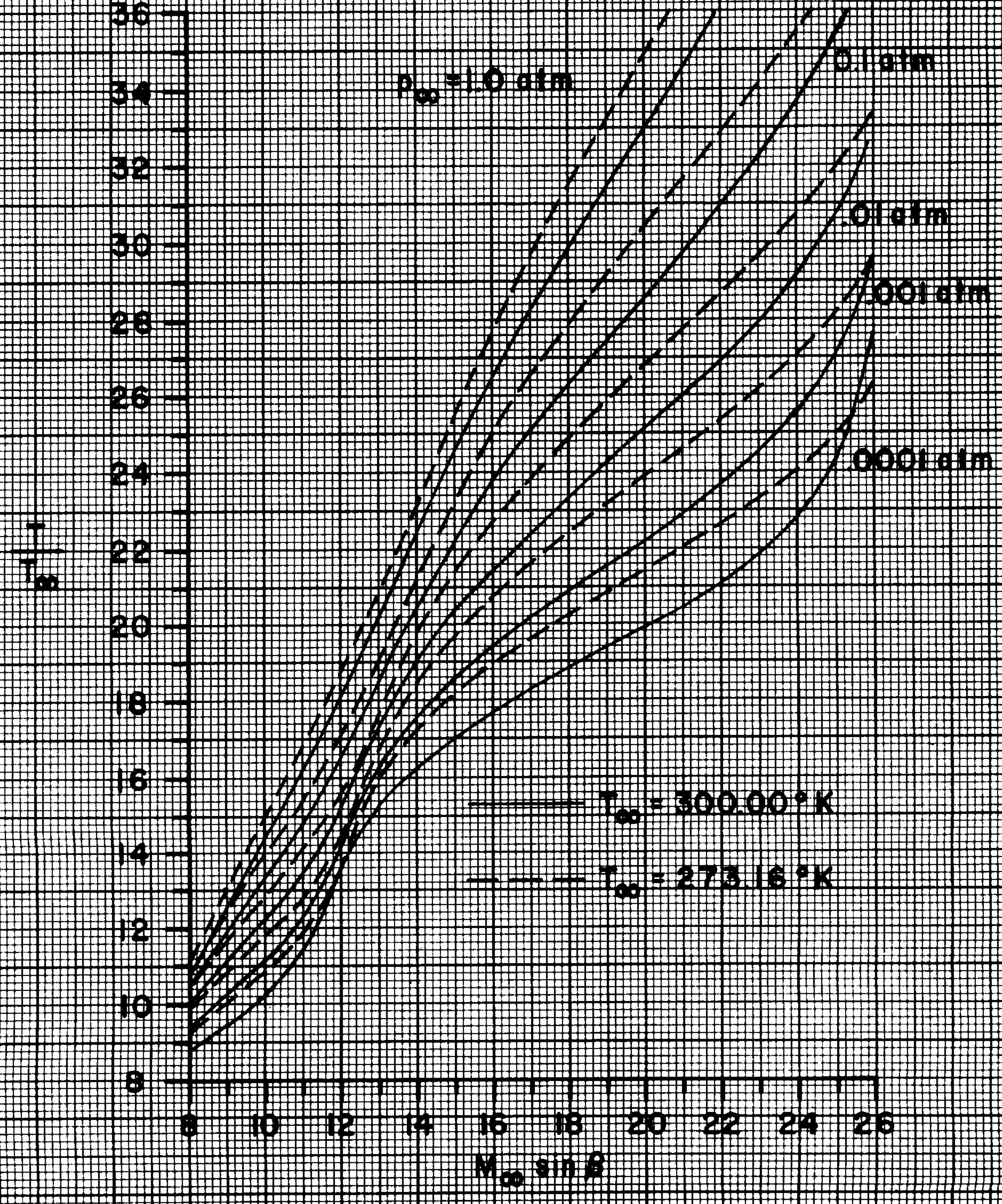


FIG. I.3. VARIATION OF TEMPERATURE ACROSS SHOCK WAVES

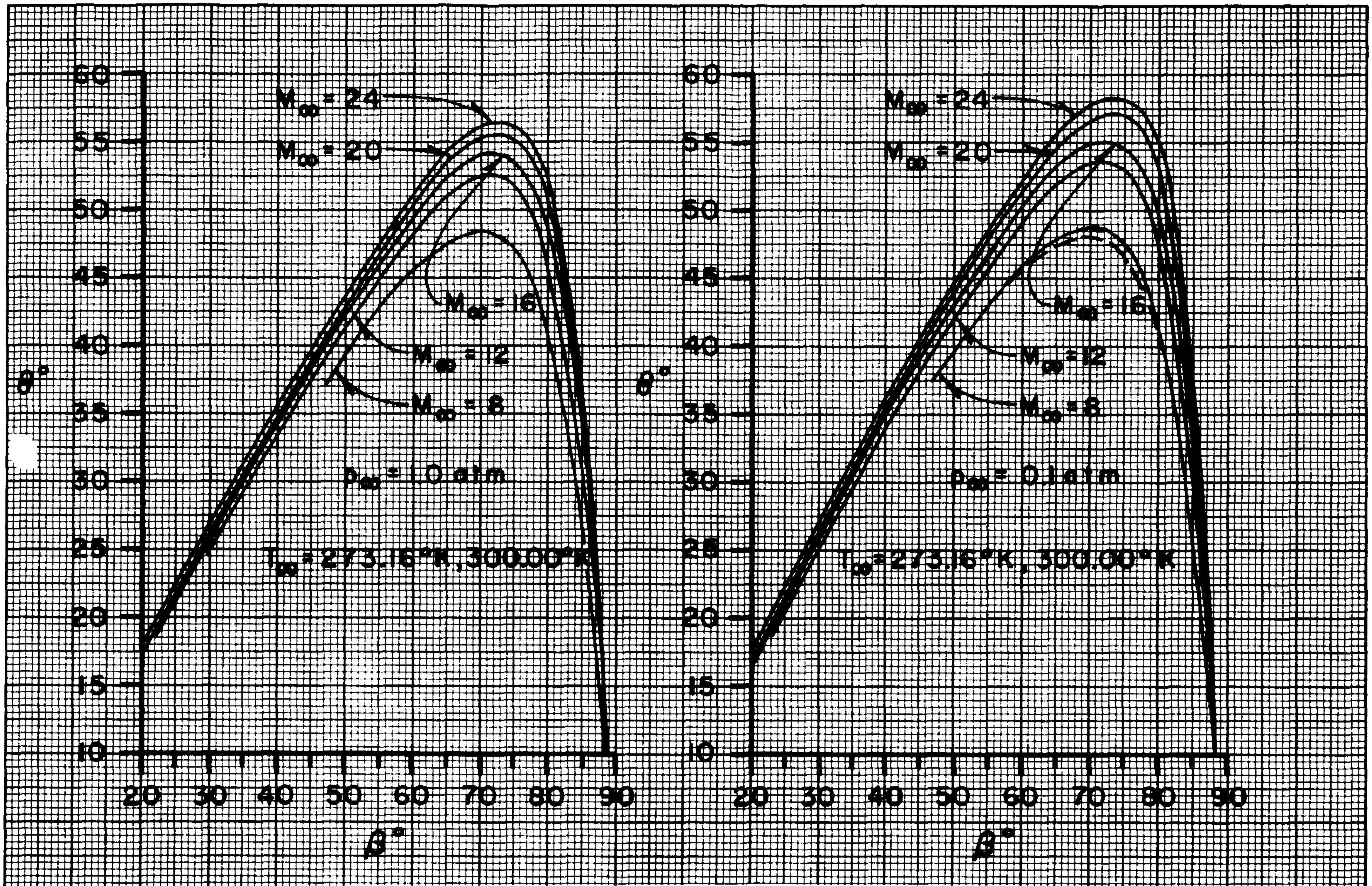


FIG. I.4. VARIATION OF ANGLE OF FLOW - DEFLECTION ACROSS SHOCK WAVES (P_∞ = 1.0 ATM., 0.1 ATM.)

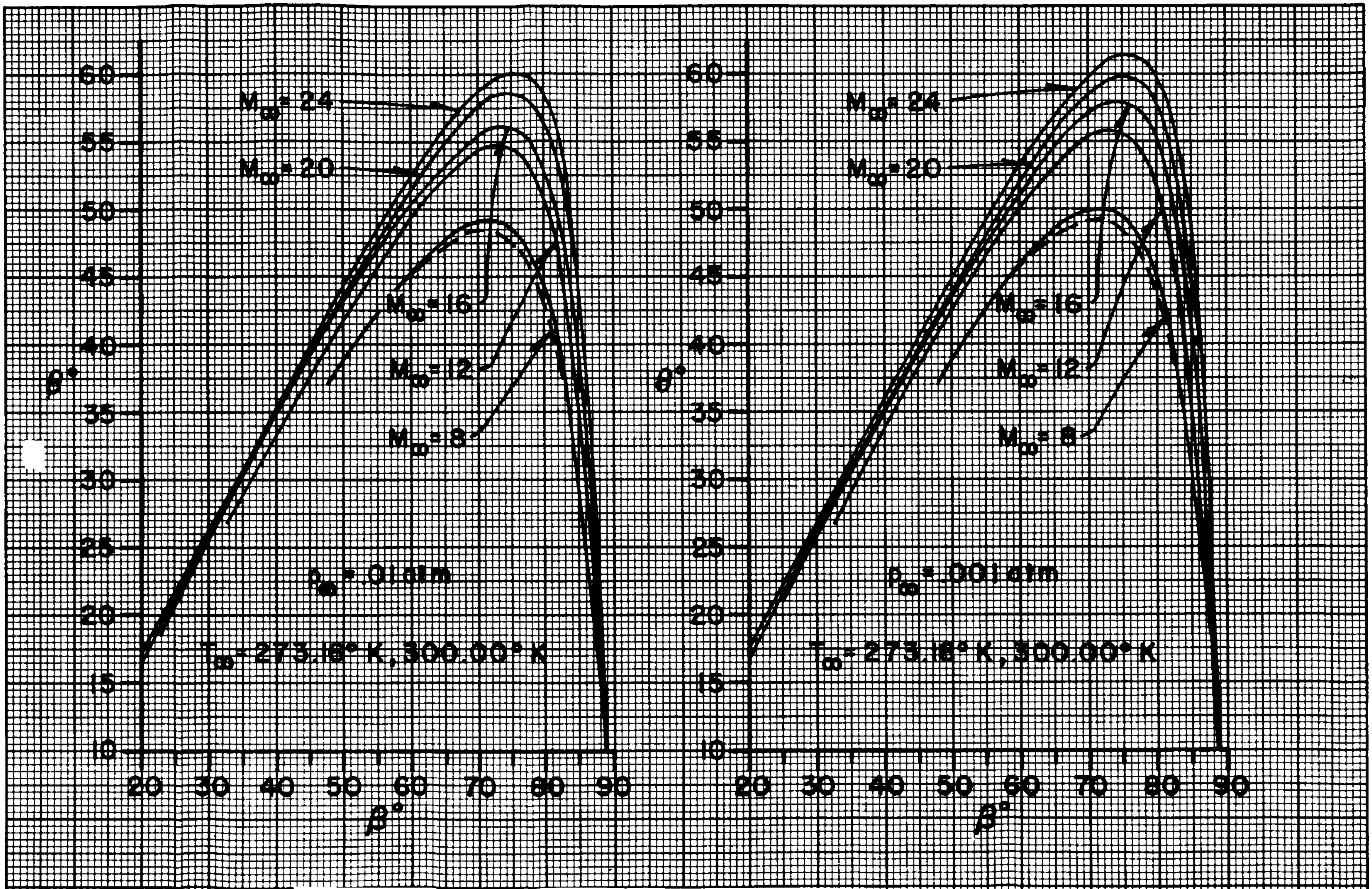


FIG. I.5. VARIATION OF ANGLE OF FLOW - DEFLECTION ACROSS SHOCK WAVES (p_∞ =.01 ATM., .001 ATM.)

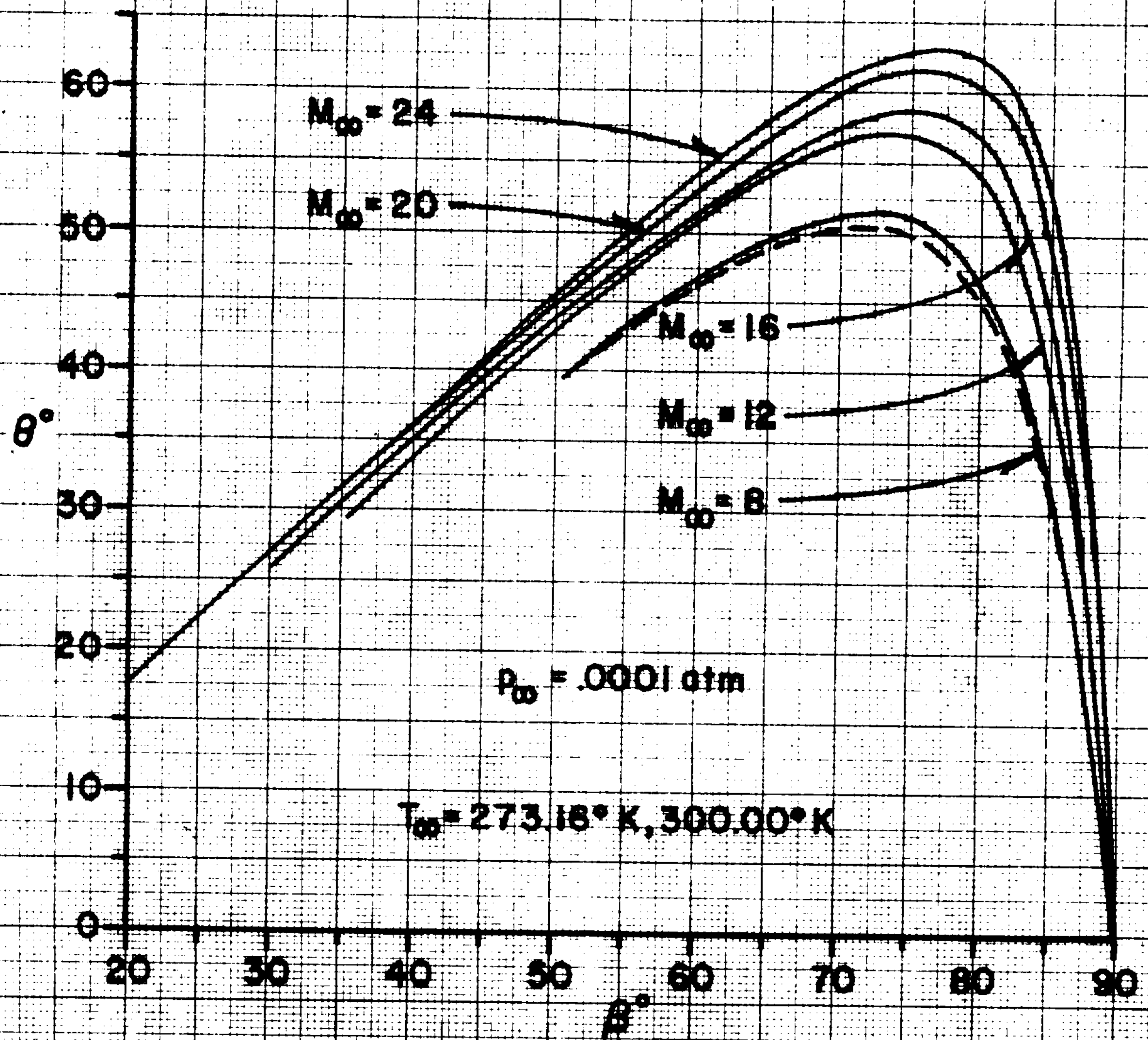


FIG. I.6. VARIATION OF ANGLE OF FLOW - DEFLECTION ACROSS SHOCK WAVES (p_∞ = .0001 ATM.)

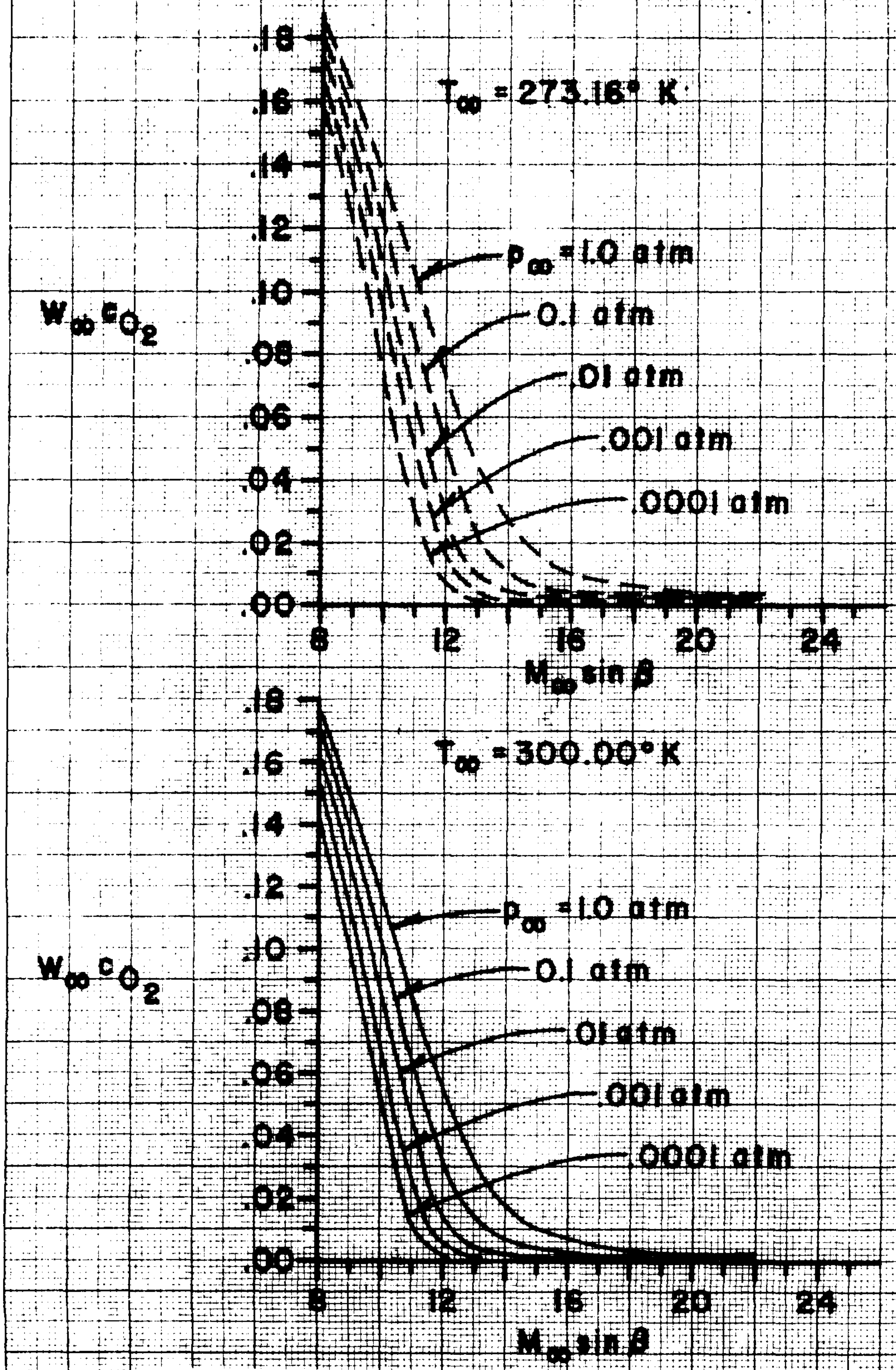


FIG. I.7. VARIATION OF O_2 CONCENTRATION ACROSS SHOCK WAVES (W_∞ = 28.86 GM/MOLE)

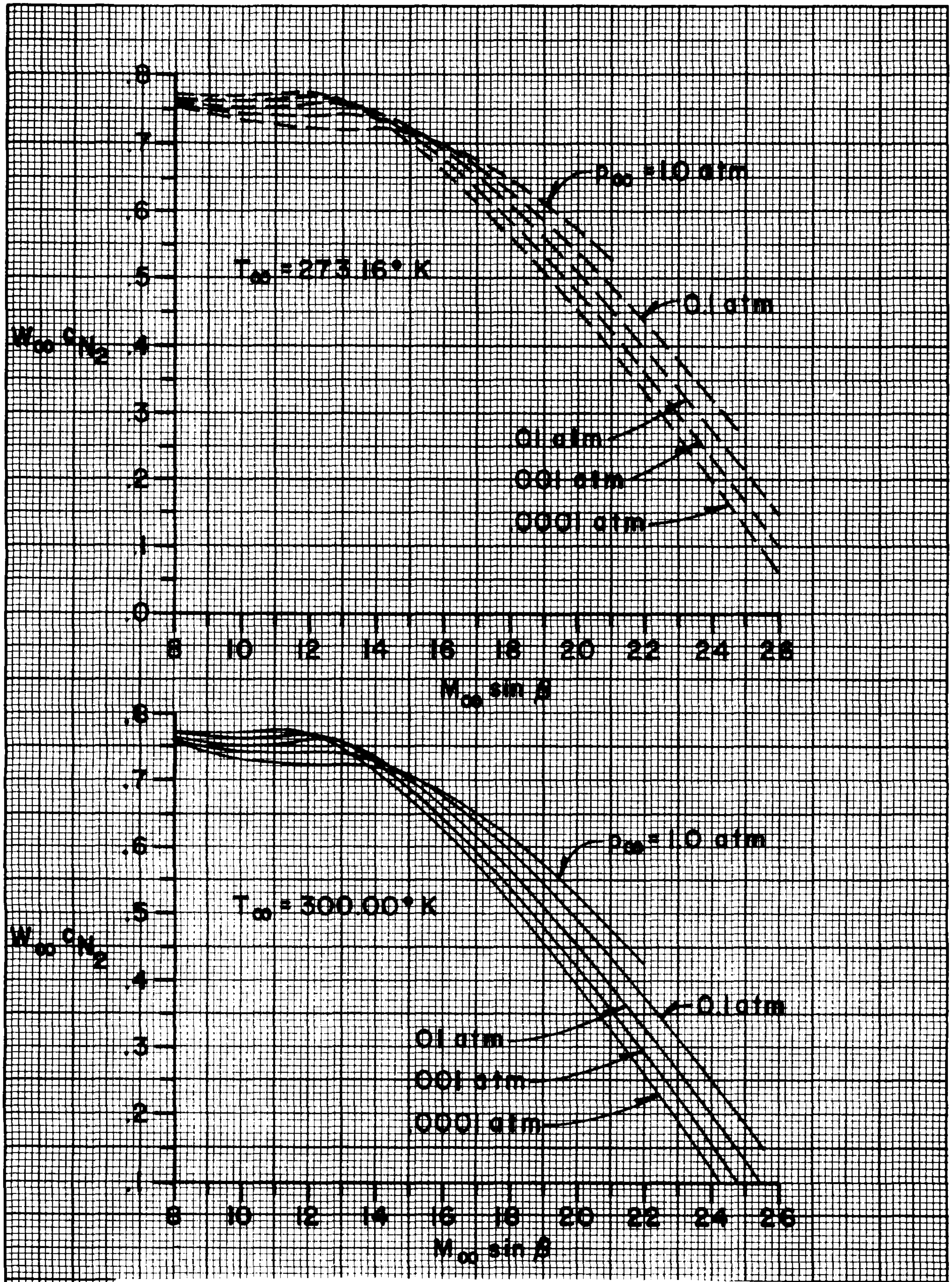


FIG. I.8. VARIATION OF N_2 CONCENTRATION ACROSS SHOCK WAVES
(W_∞ = 28.86 GM/MOLE)

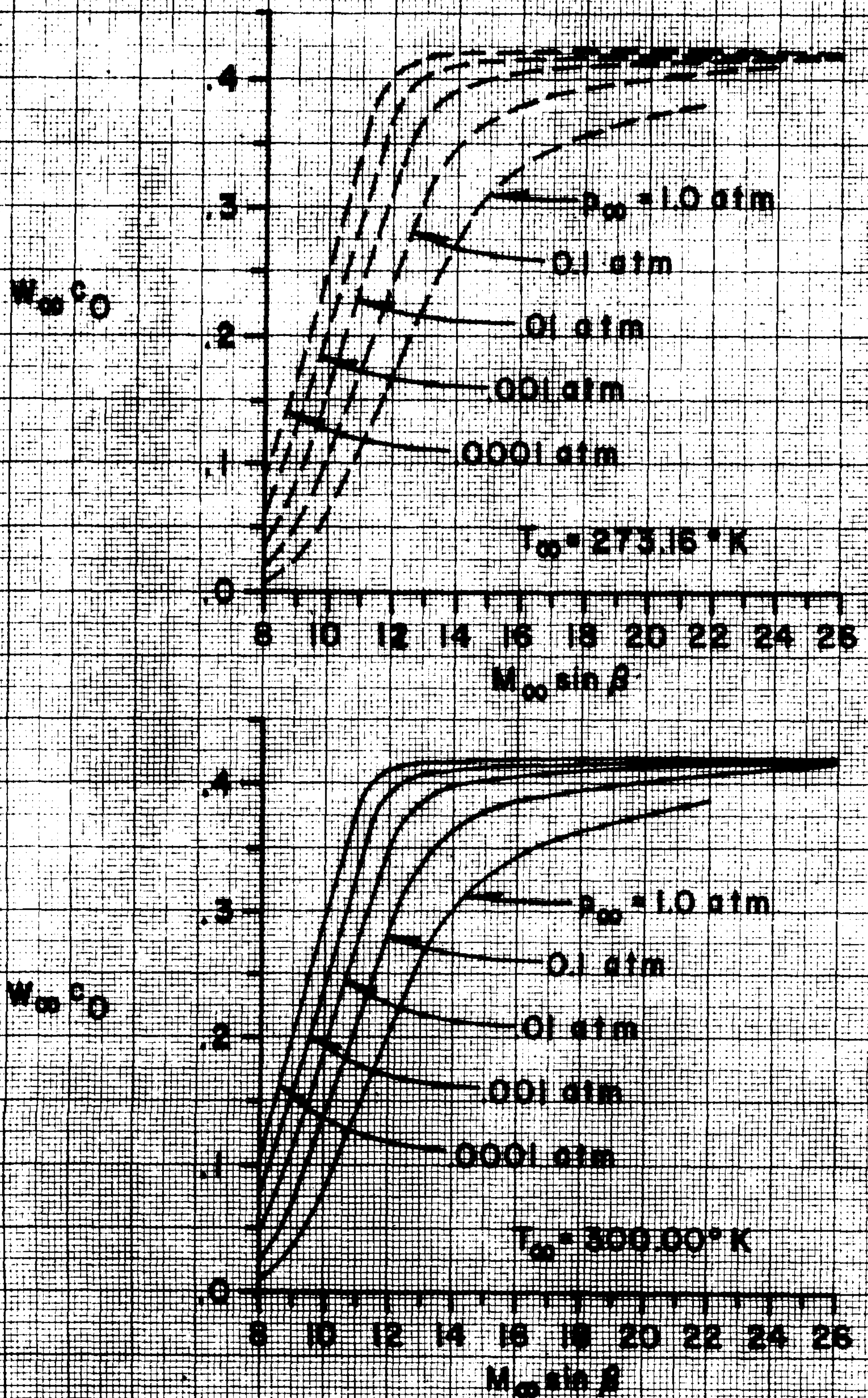


FIG. I.9. VARIATION OF O CONCENTRATION ACROSS SHOCK WAVES (W_∞ = 28.86 GM/MOLE)

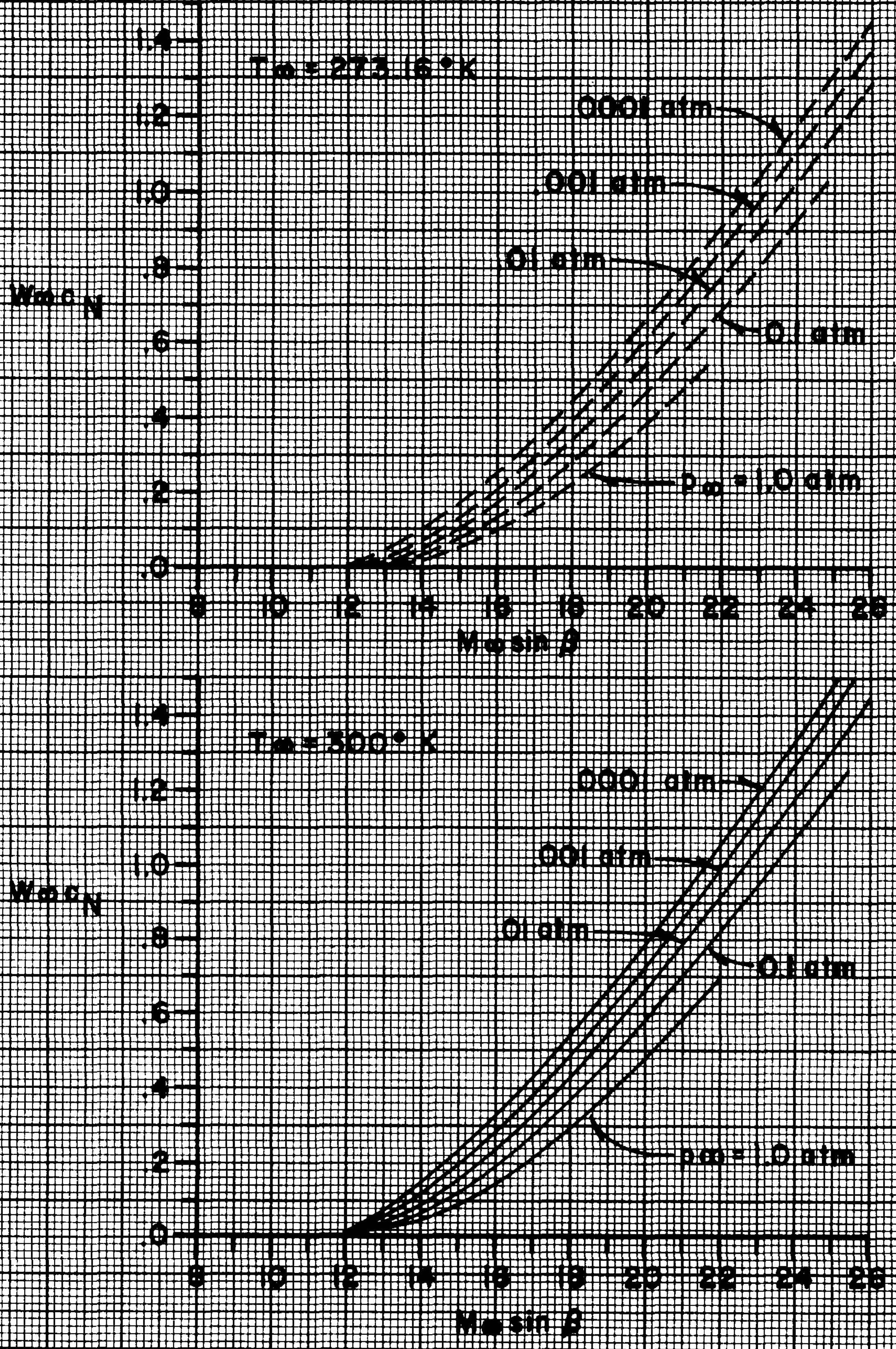


FIG. I.10. VARIATION OF N CONCENTRATION ACROSS SHOCK WAVES (W_{∞} = 28.86 GM/MOLE)

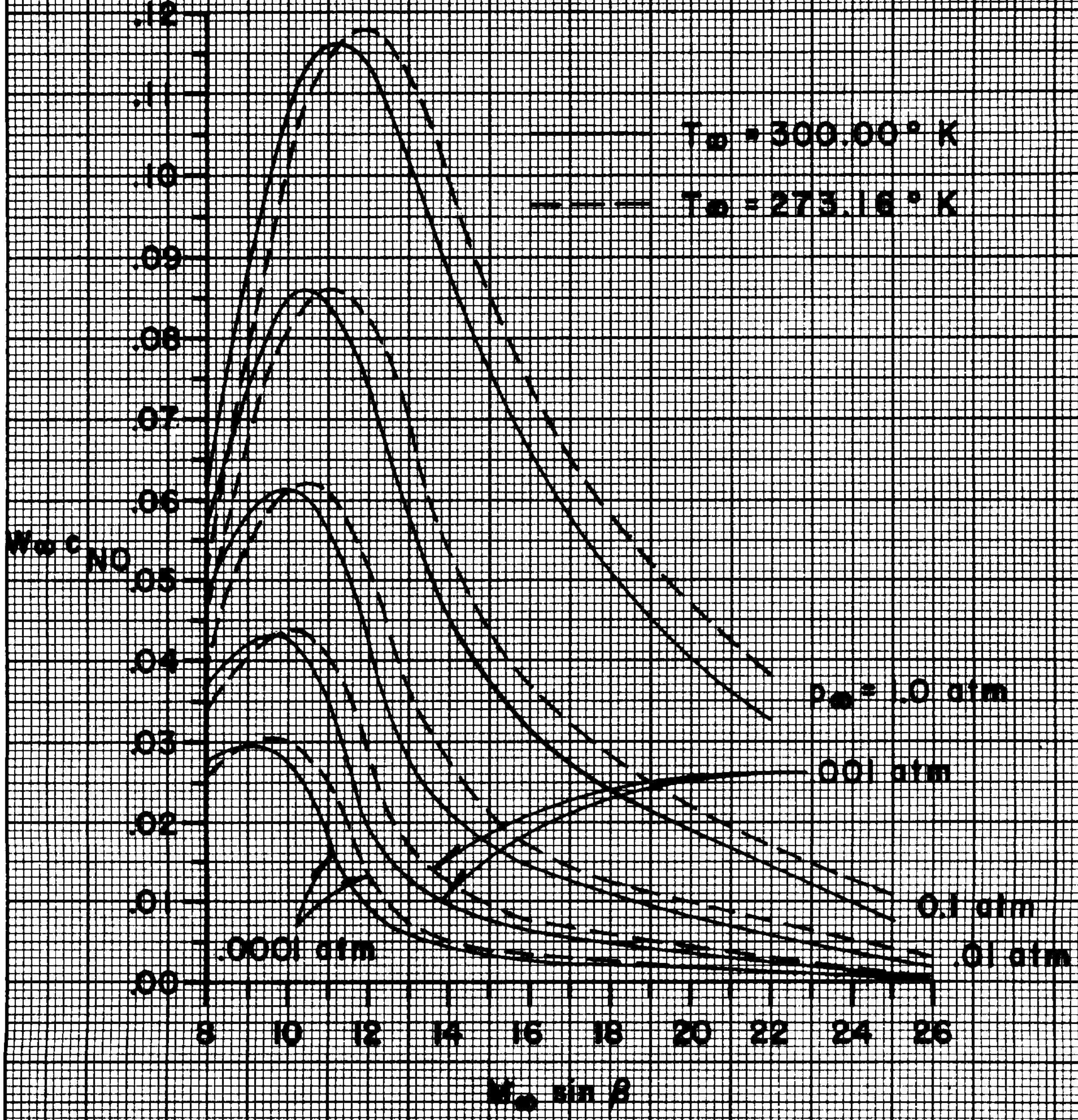


FIG. I.11. VARIATION OF NO CONCENTRATION ACROSS SHOCK WAVES (W_∞ = 28.86 GM/MOLE)

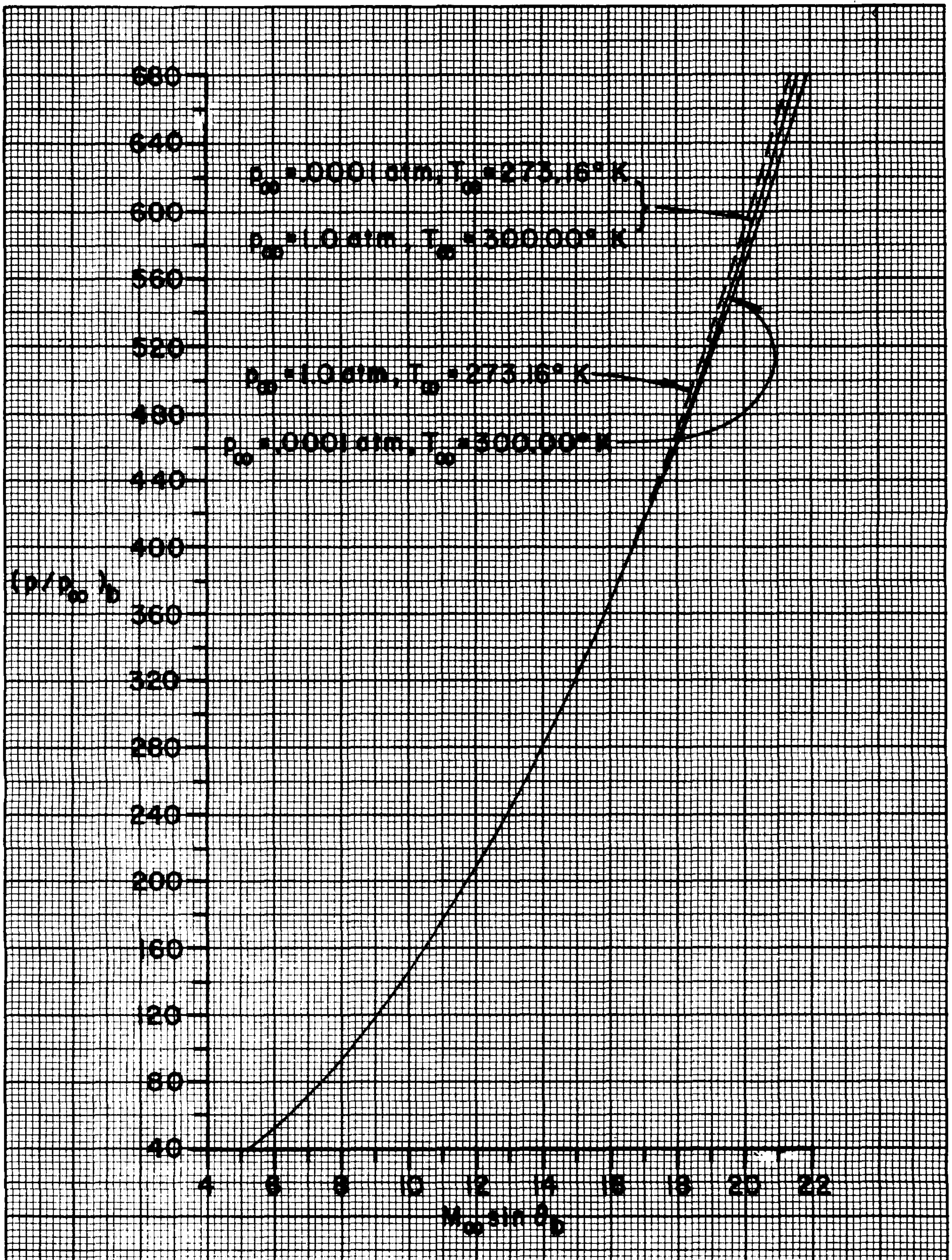


FIG. II.1. CONICAL FLOW - PRESSURE ON CONE SURFACE

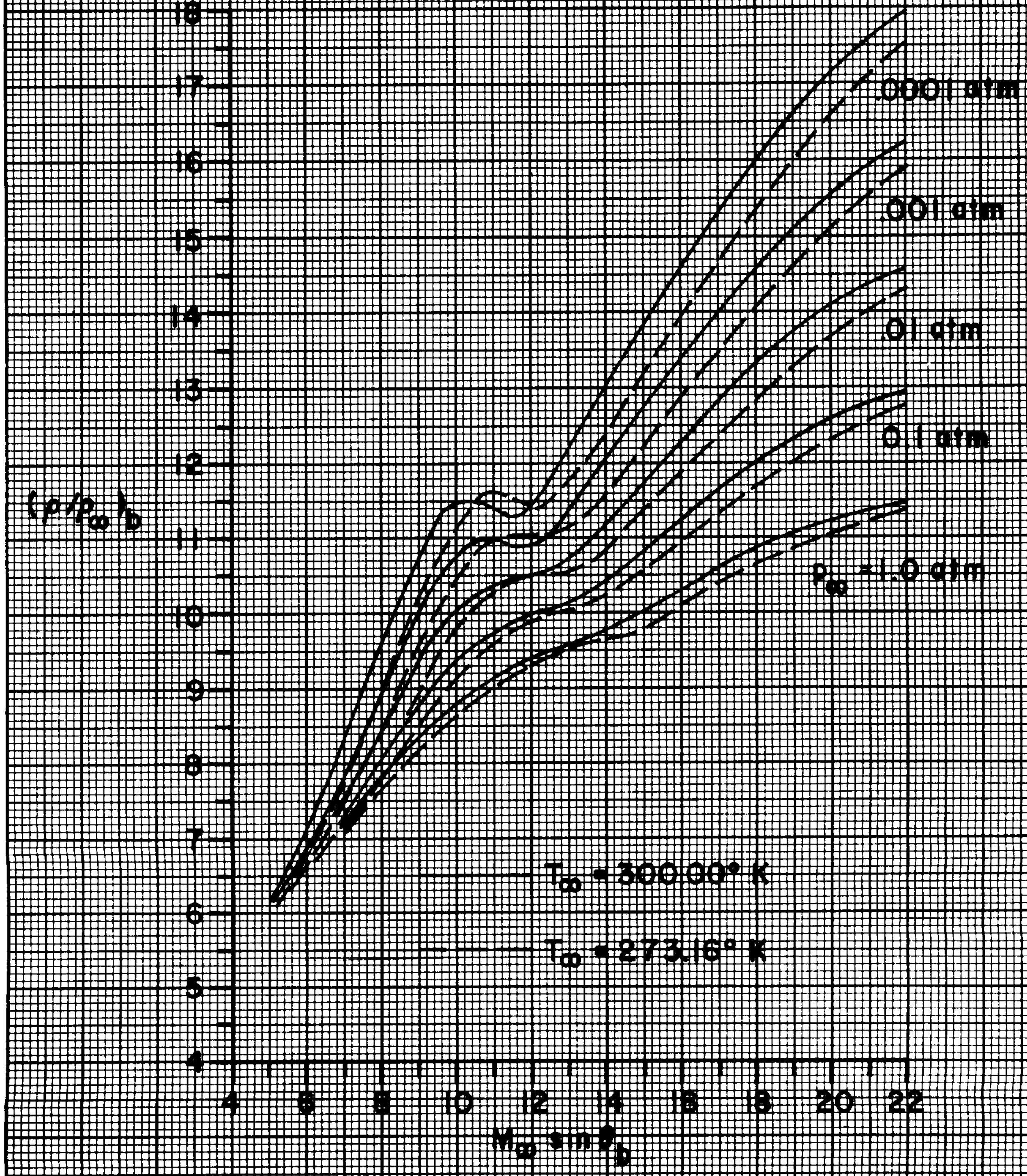


FIG. II.2. CONICAL FLOW - DENSITY ON CONE SURFACE

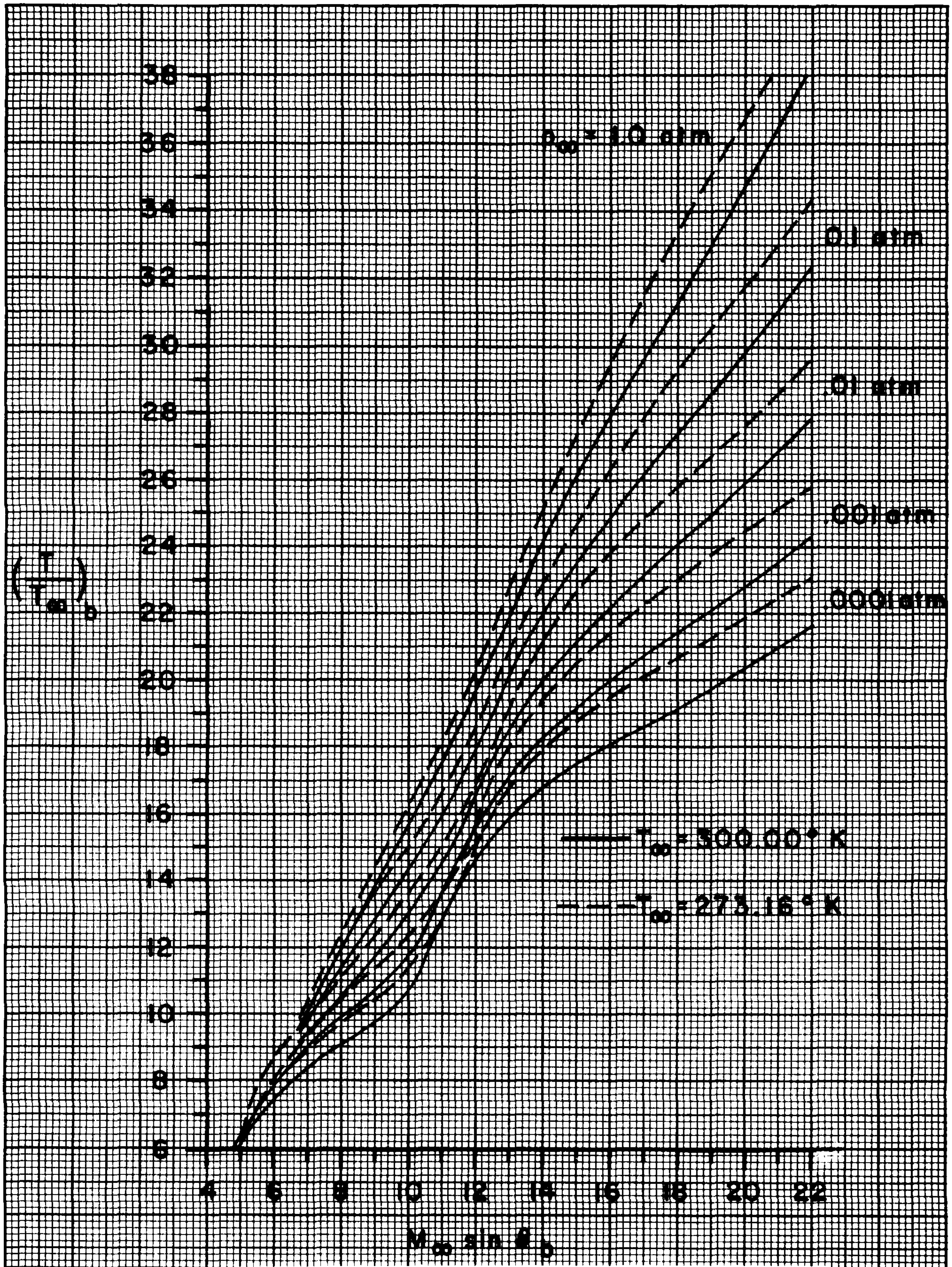


FIG. II.3. CONICAL FLOW - TEMPERATURE ON CONE SURFACE

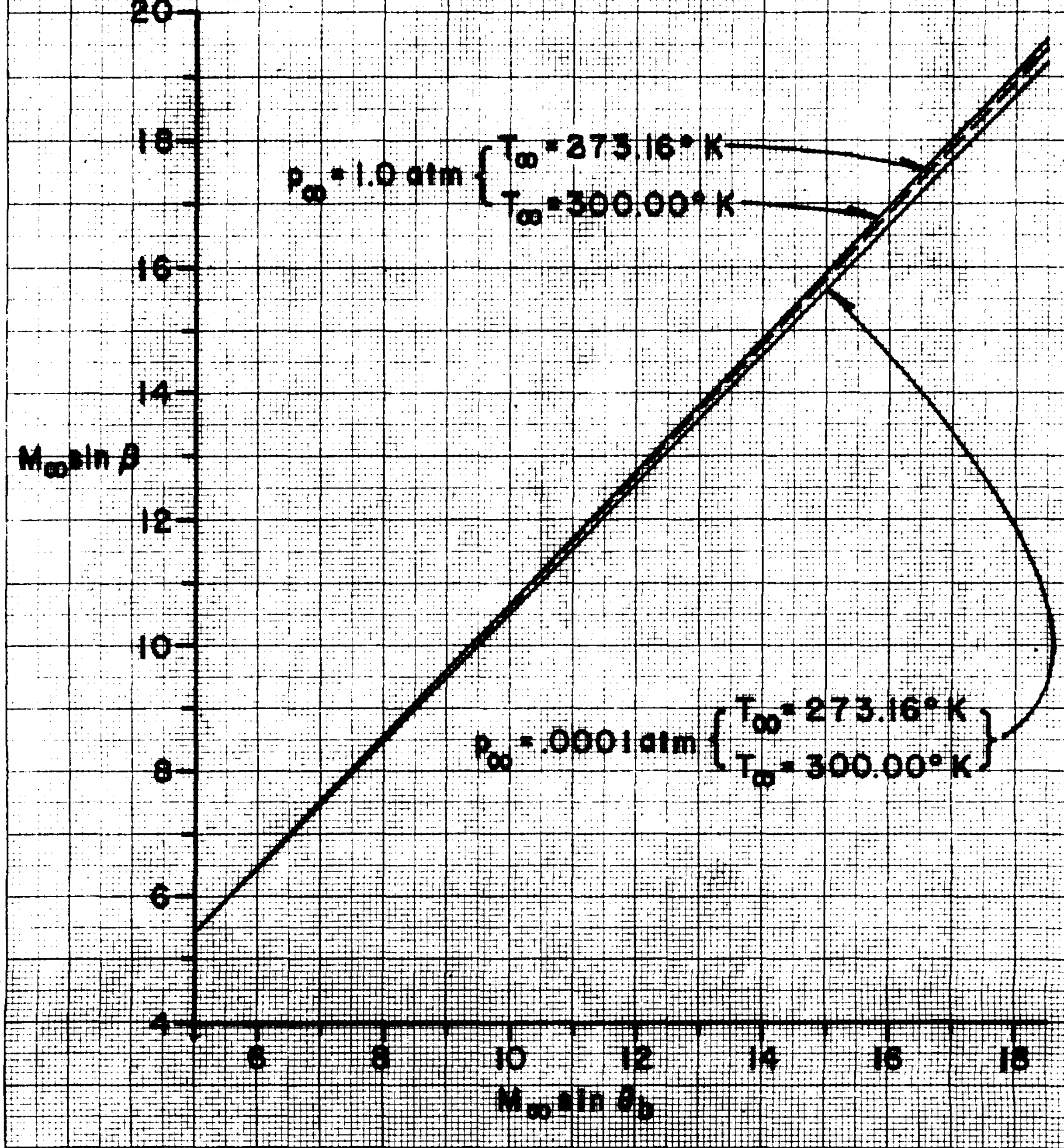


FIG. II.4. CONICAL FLOW - SHOCK WAVE ANGLE AS A FUNCTION OF GIVEN MACH NUMBER AND CONE ANGLE

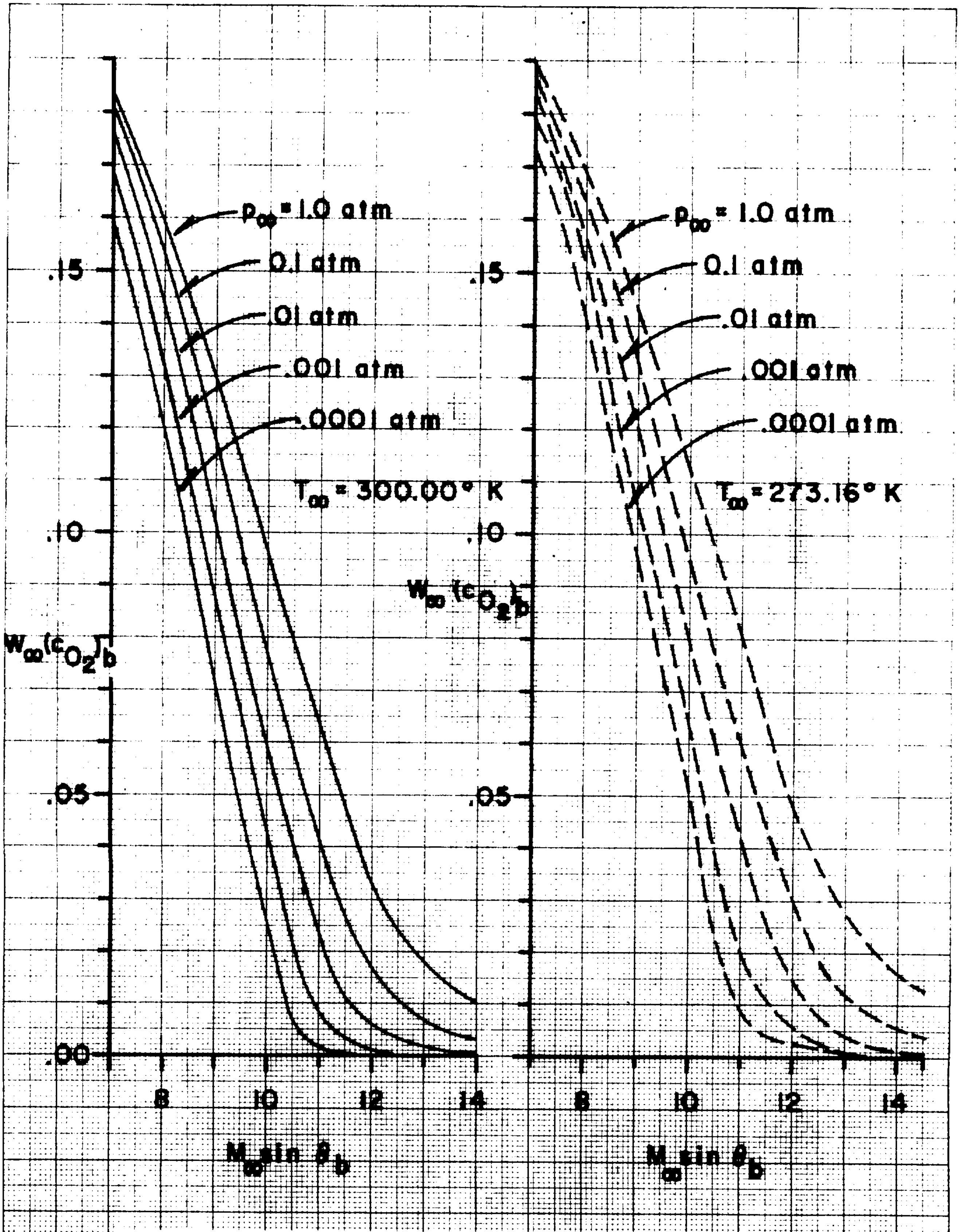


FIG. II.5. CONICAL FLOW - CONCENTRATION OF O_2 ON CONE SURFACE (W_∞ = 28.86 GM/MOLE)

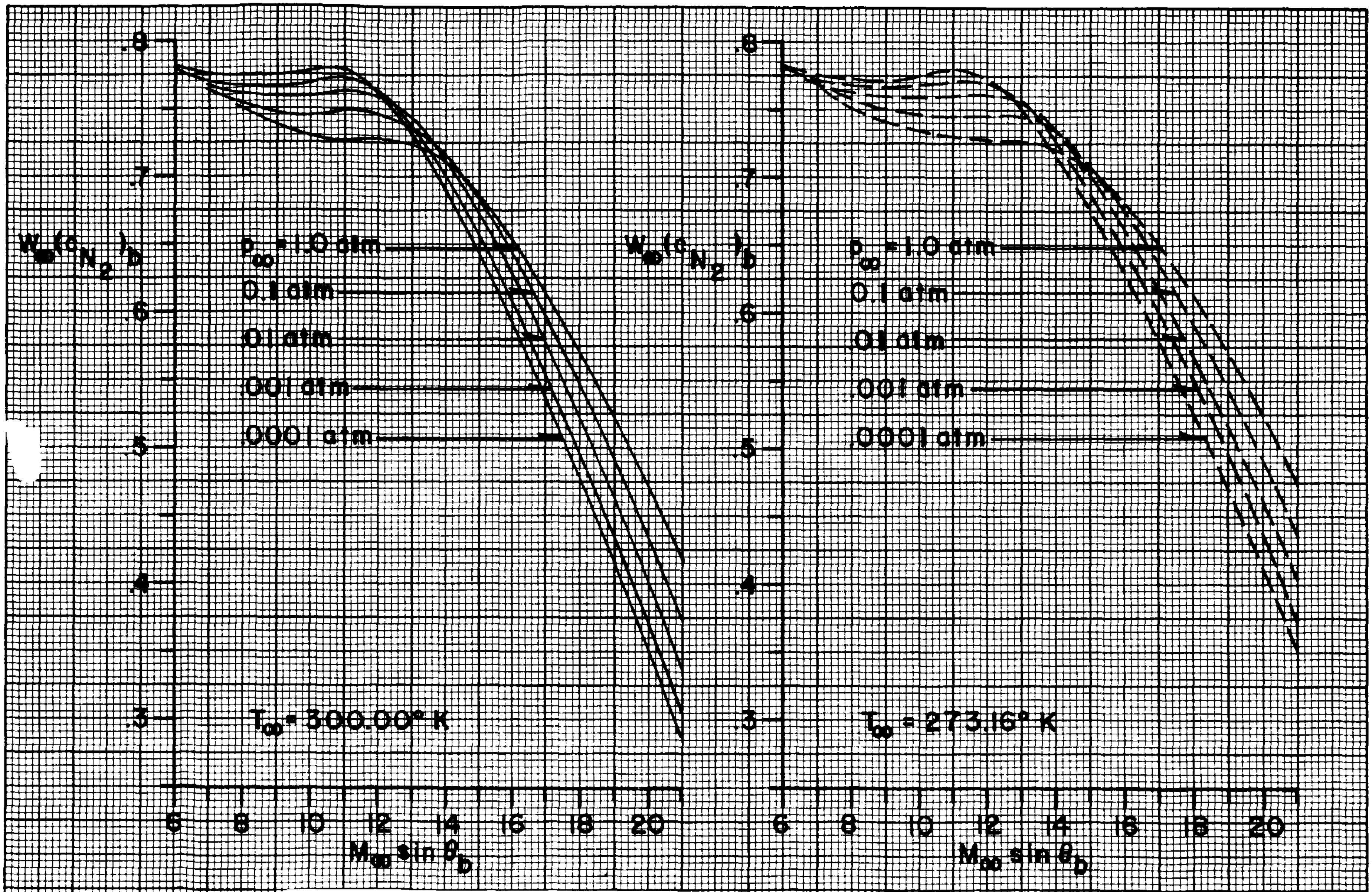


FIG. II.6. CONICAL FLOW - CONCENTRATION OF N_2 ON CONE SURFACE
(W_∞ = 28.86 GM/MOLE)

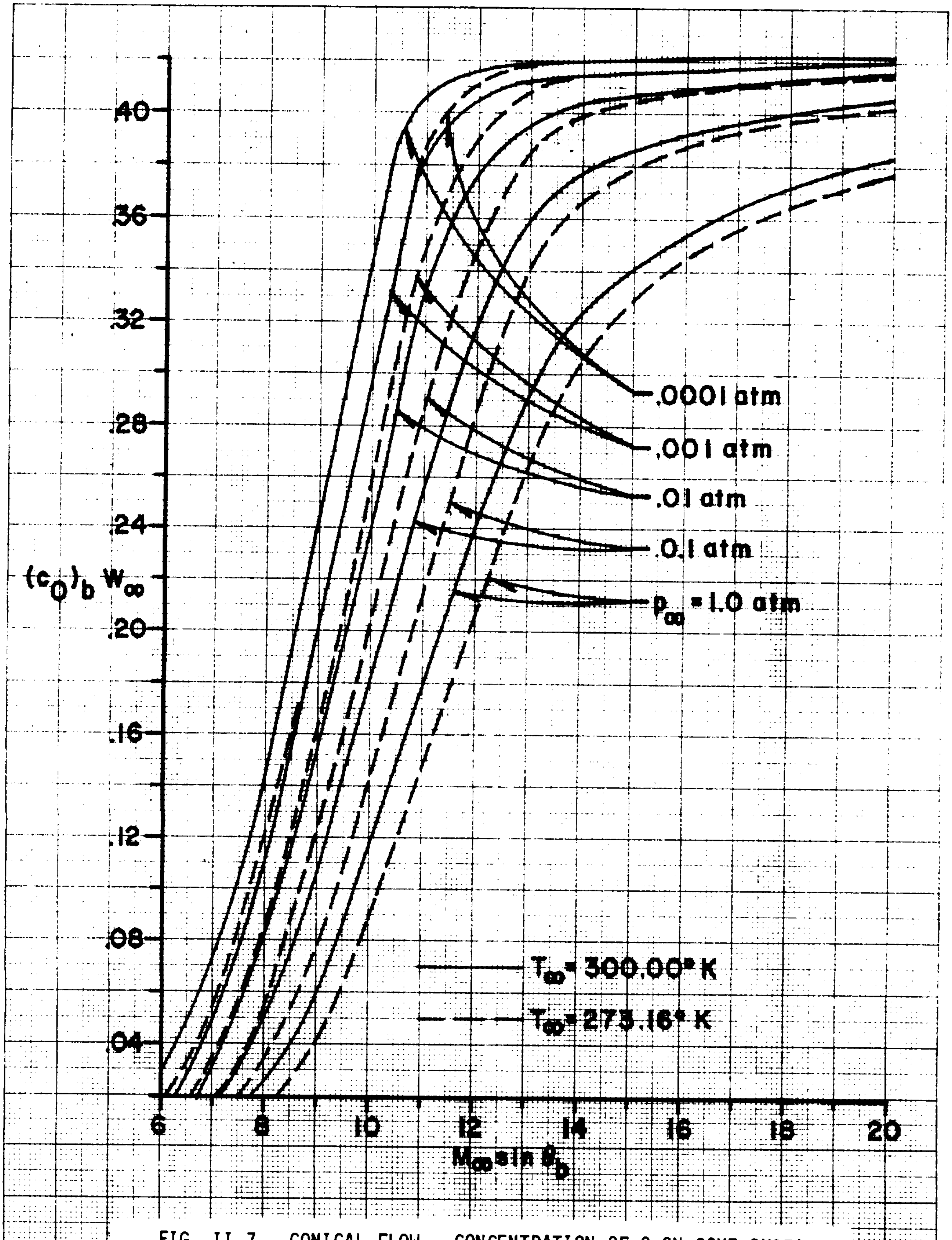


FIG. II.7. CONICAL FLOW - CONCENTRATION OF O ON CONE SURFACE (W_∞ = 28.86 GM/MOLE)

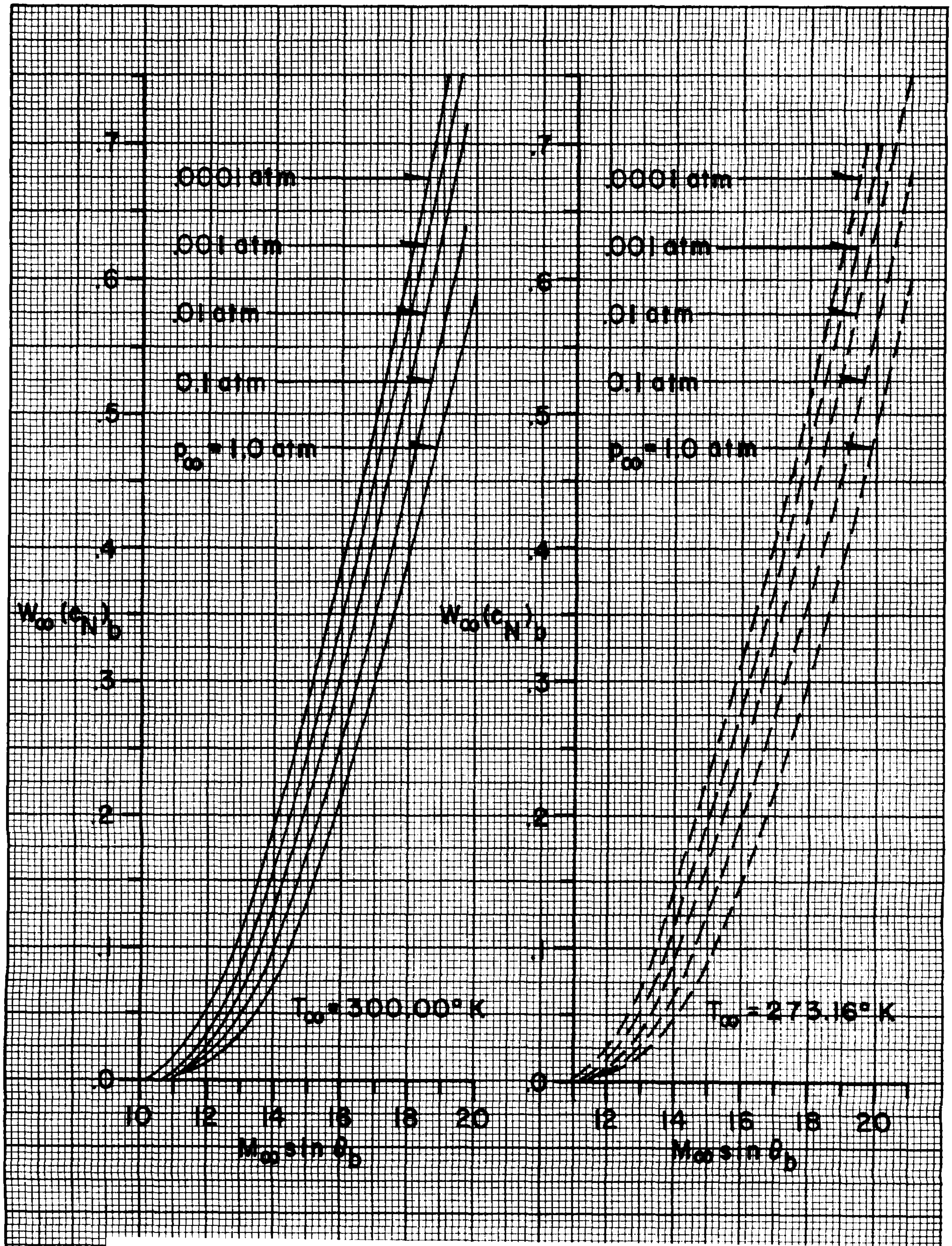


FIG. II.8. CONICAL FLOW - CONCENTRATION OF N ON CONE SURFACE (W_∞ = 28.86 GM/MOLE)

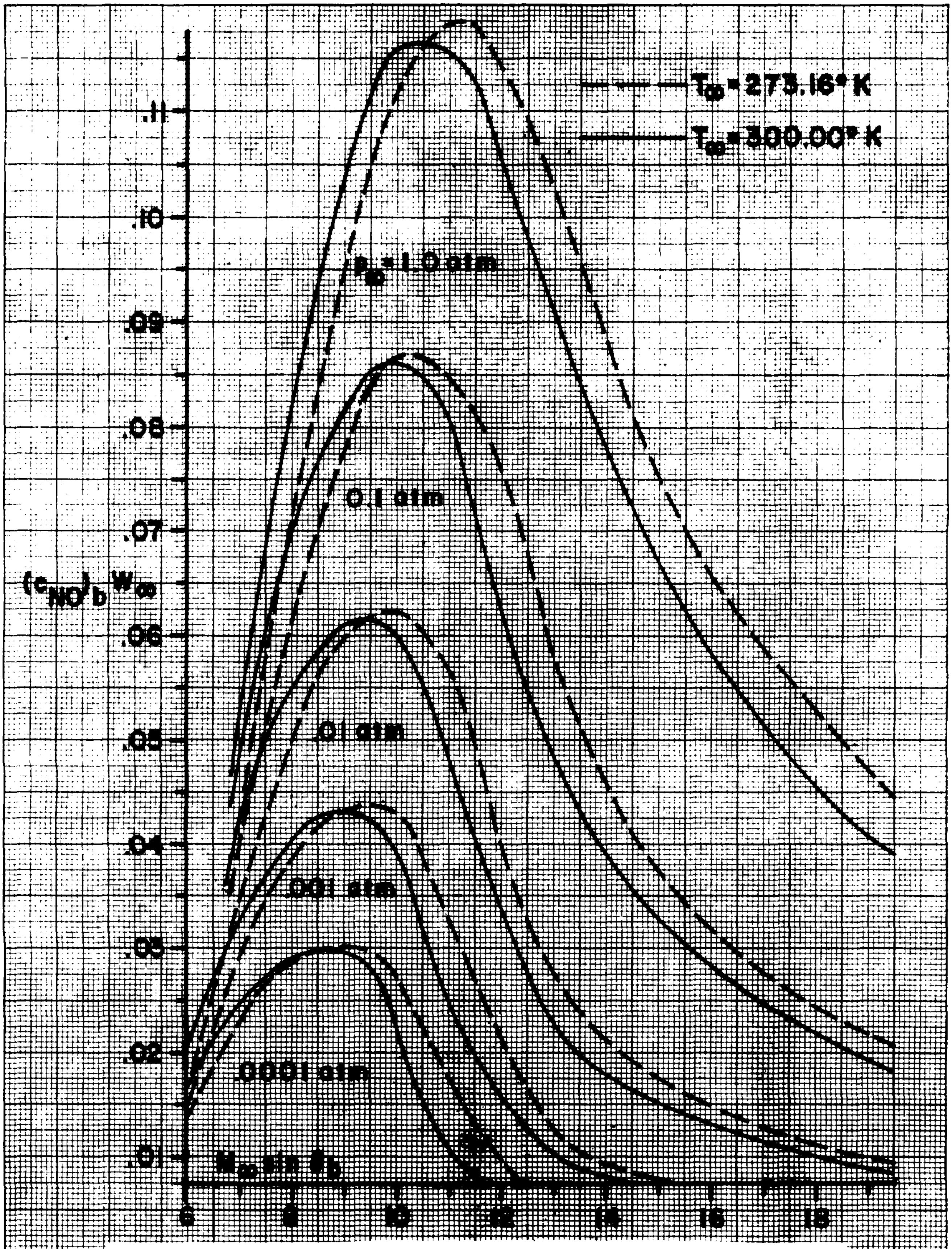


FIG. II.9. CONICAL FLOW - CONCENTRATION OF NO ON CONE SURFACE (W_∞ = 28.86 GM/MOLE)

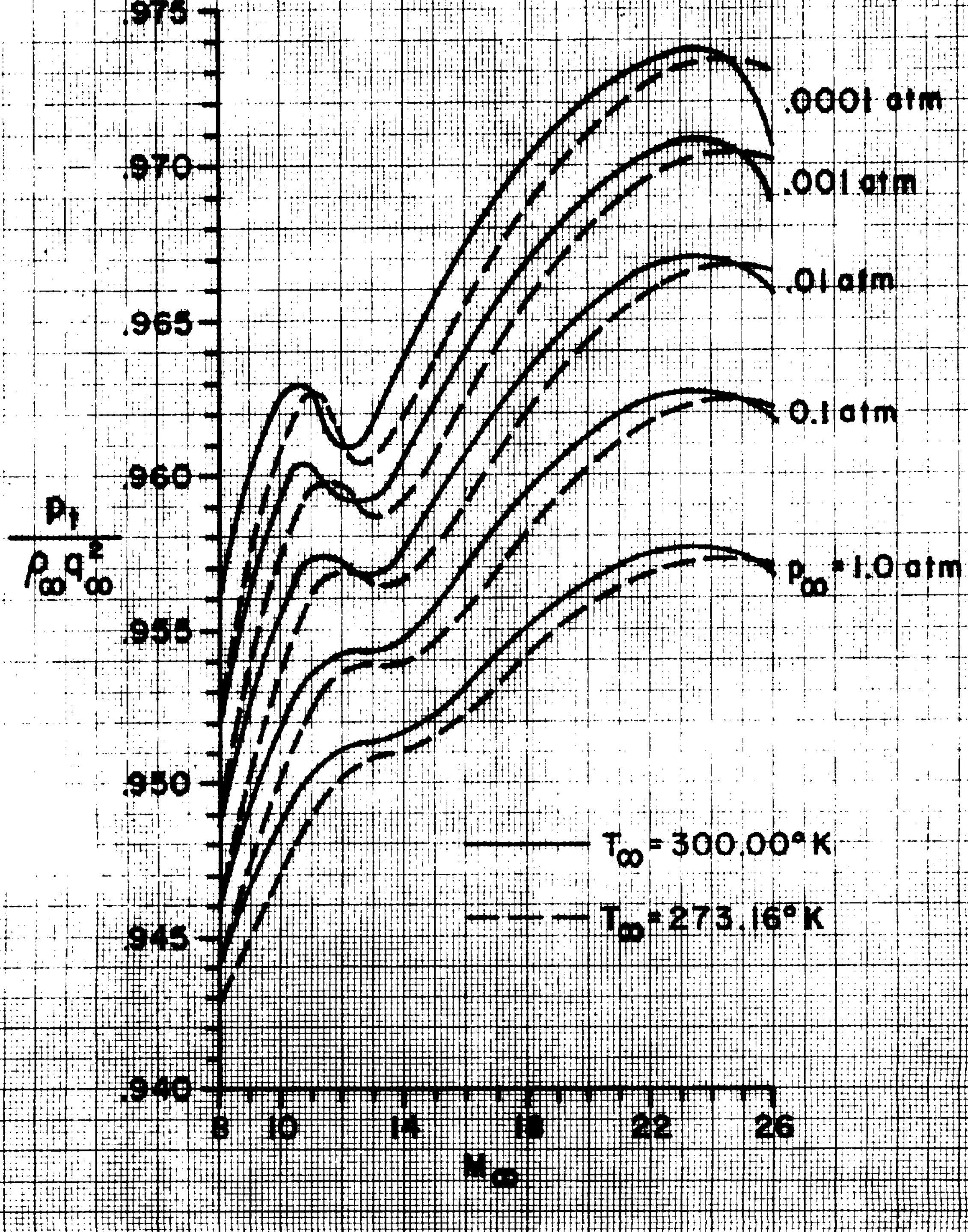


FIG. III.1. STAGNATION PRESSURE VS FREE STREAM MACH NUMBER

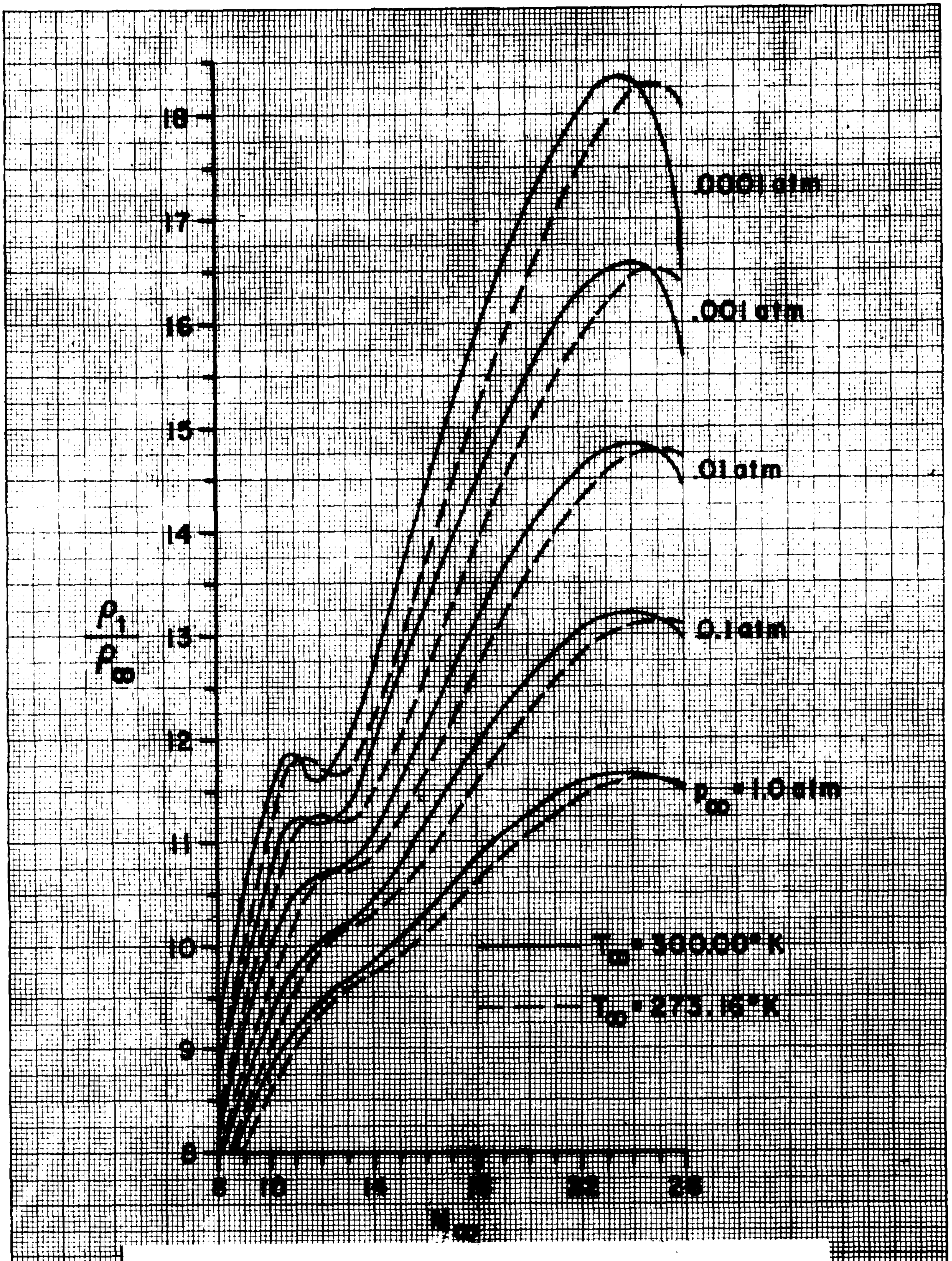


FIG. III.2. STAGNATION DENSITY VS FREE STREAM MACH NUMBER

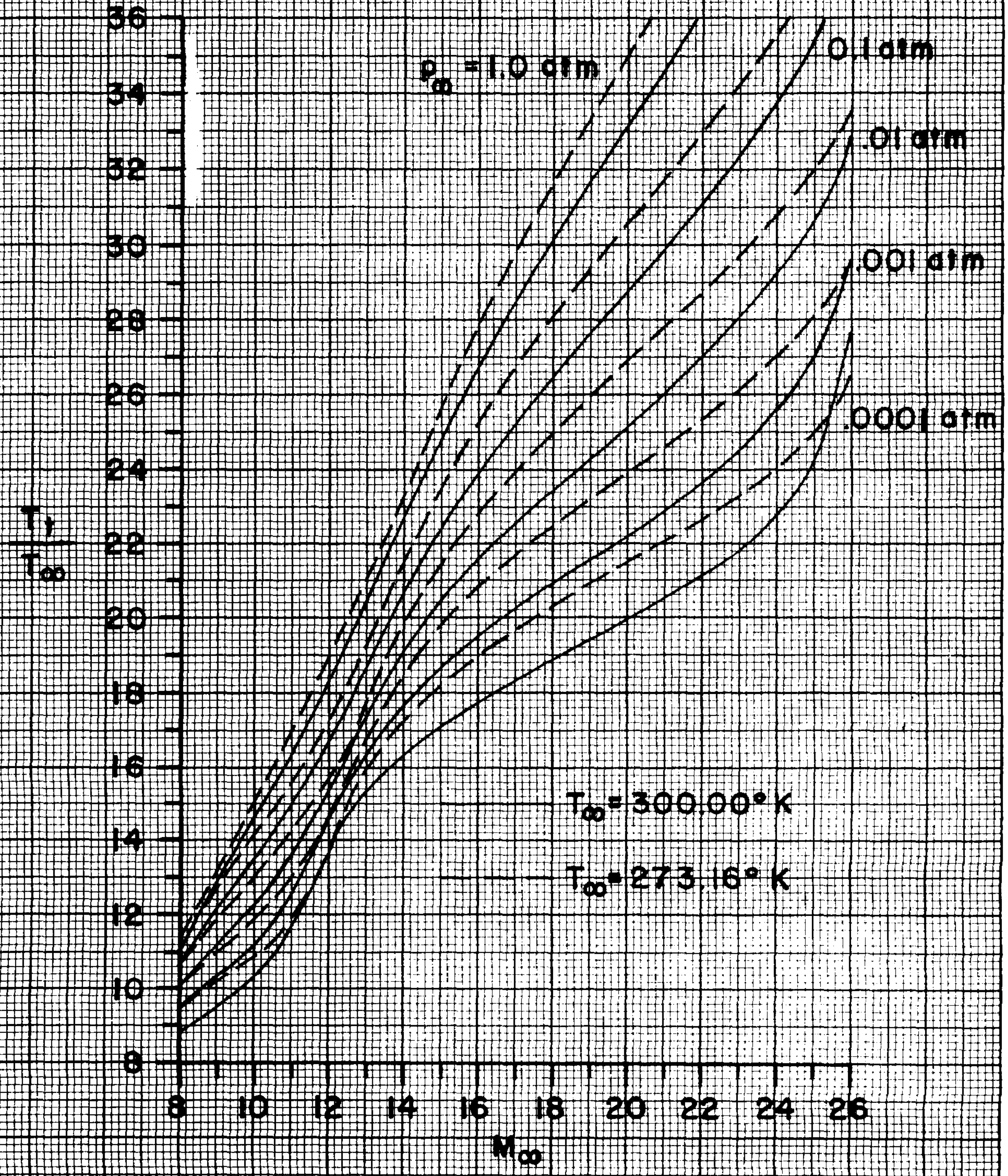


FIG. III.3. STAGNATION TEMPERATURE VS FREE STREAM MACH NUMBER

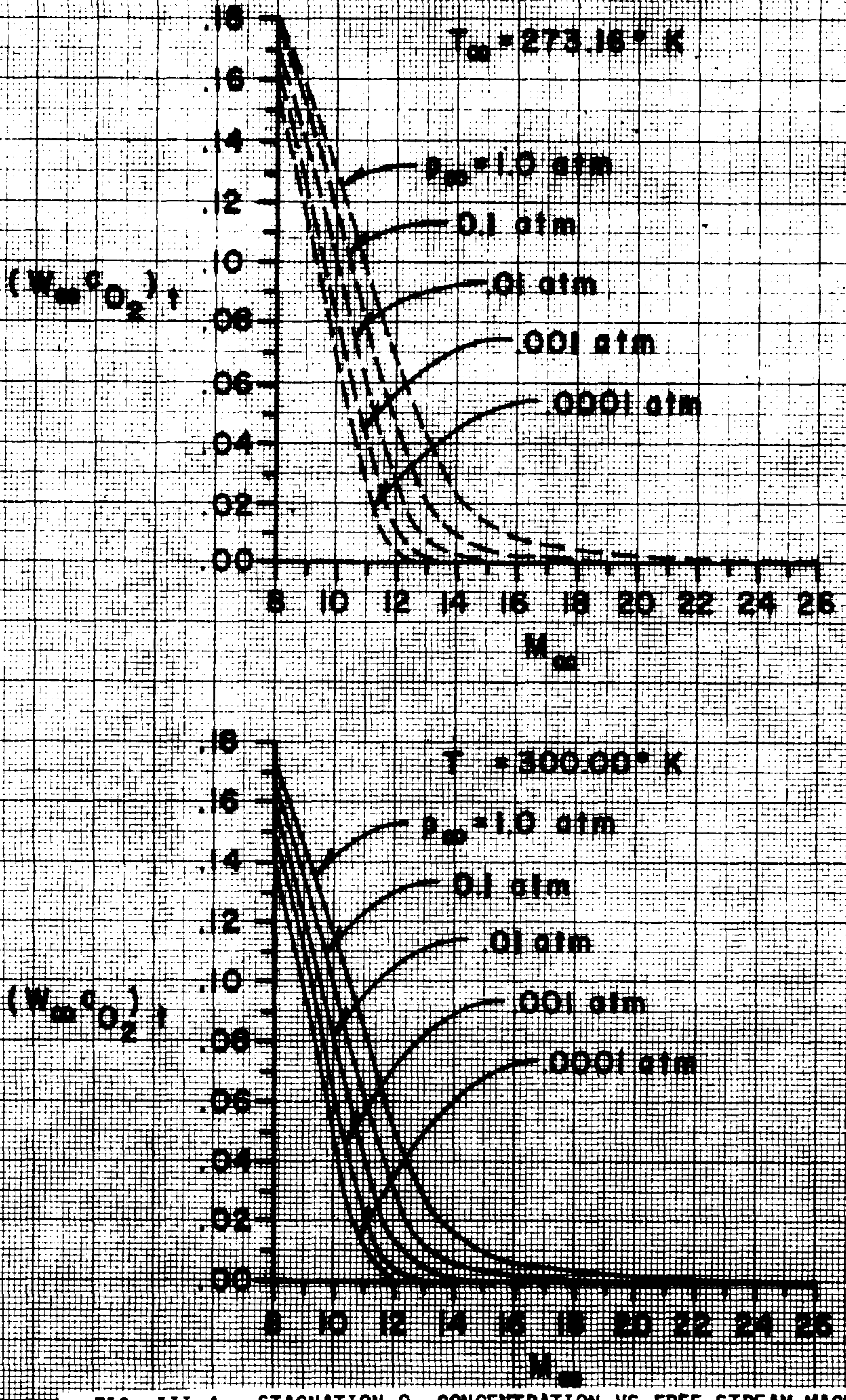


FIG. III.4. STAGNATION O_2 CONCENTRATION VS FREE STREAM MACH NUMBER (W_∞ = 28.86 GM/MOLE)

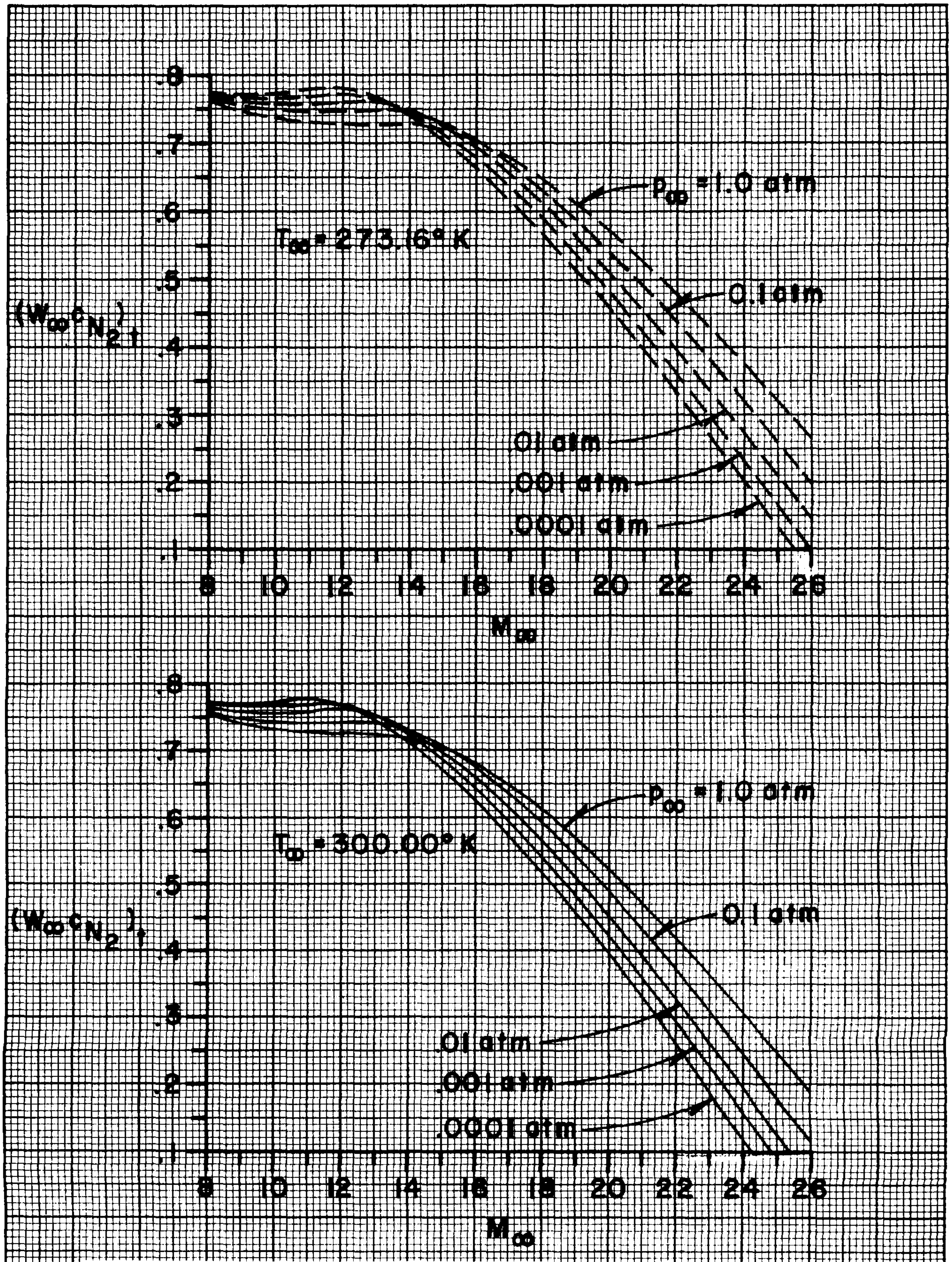


FIG. III.5. STAGNATION N_2 CONCENTRATION VS FREE STREAM MACH NUMBER (W_∞ = 28.86 GM/MOLE)

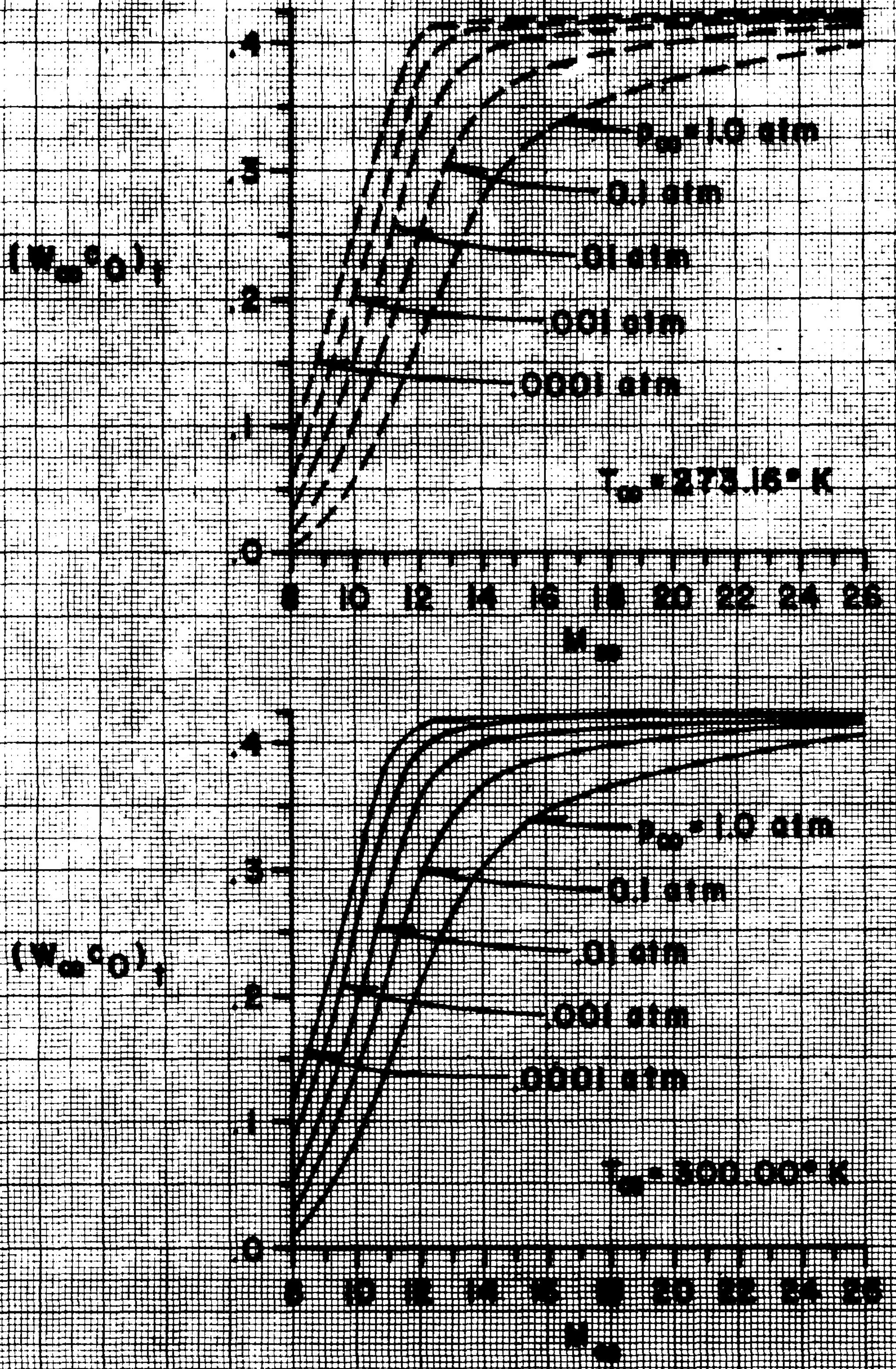


FIG. III.6. STAGNATION O CONCENTRATION VS FREE STREAM MACH NUMBER (W_∞ = 28.86 GM/MOLE)

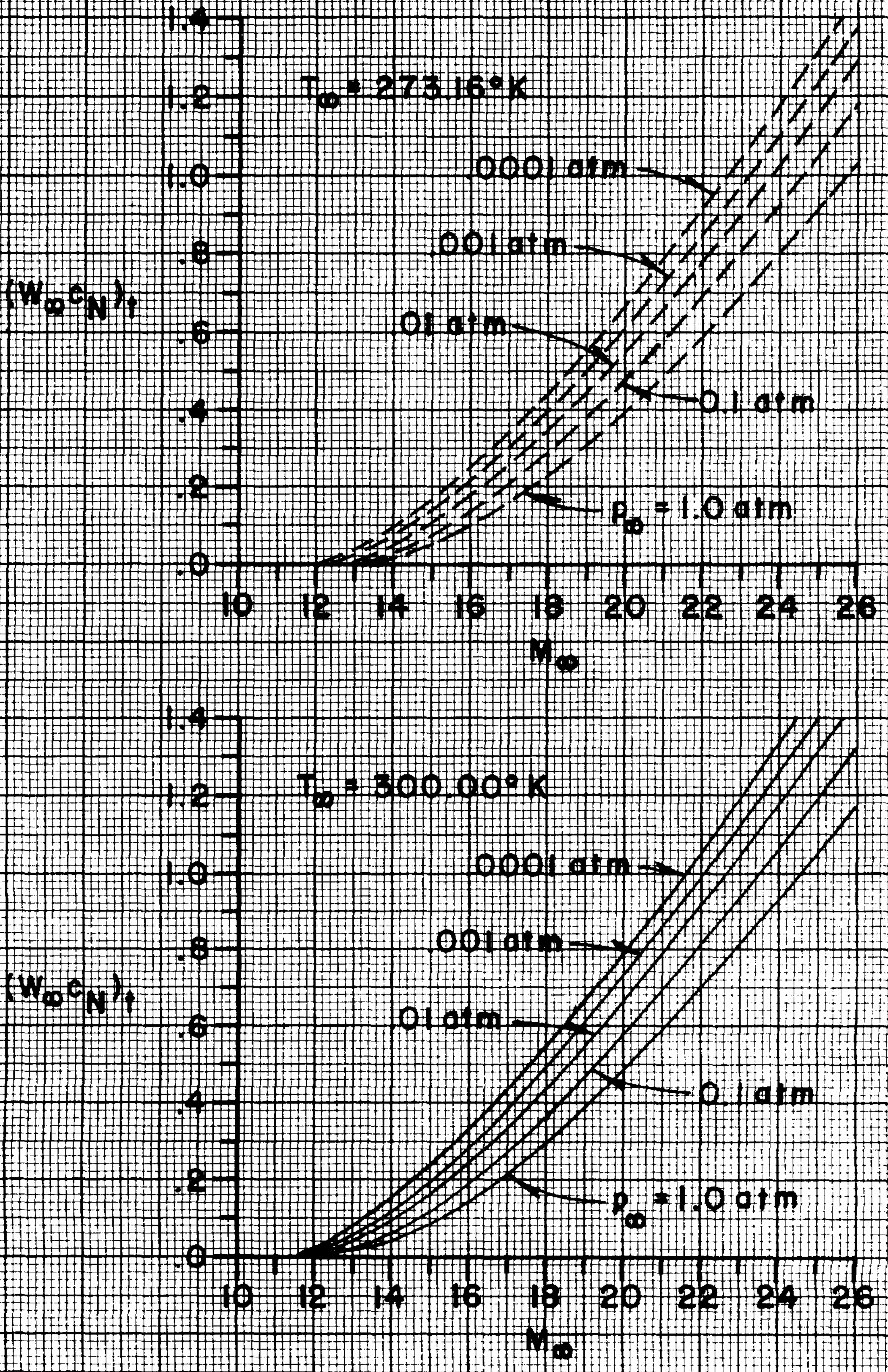


FIG. III.7. STAGNATION N CONCENTRATION VS FREE STREAM MACH NUMBER (W_∞ = 28.86 GM/MOLE)

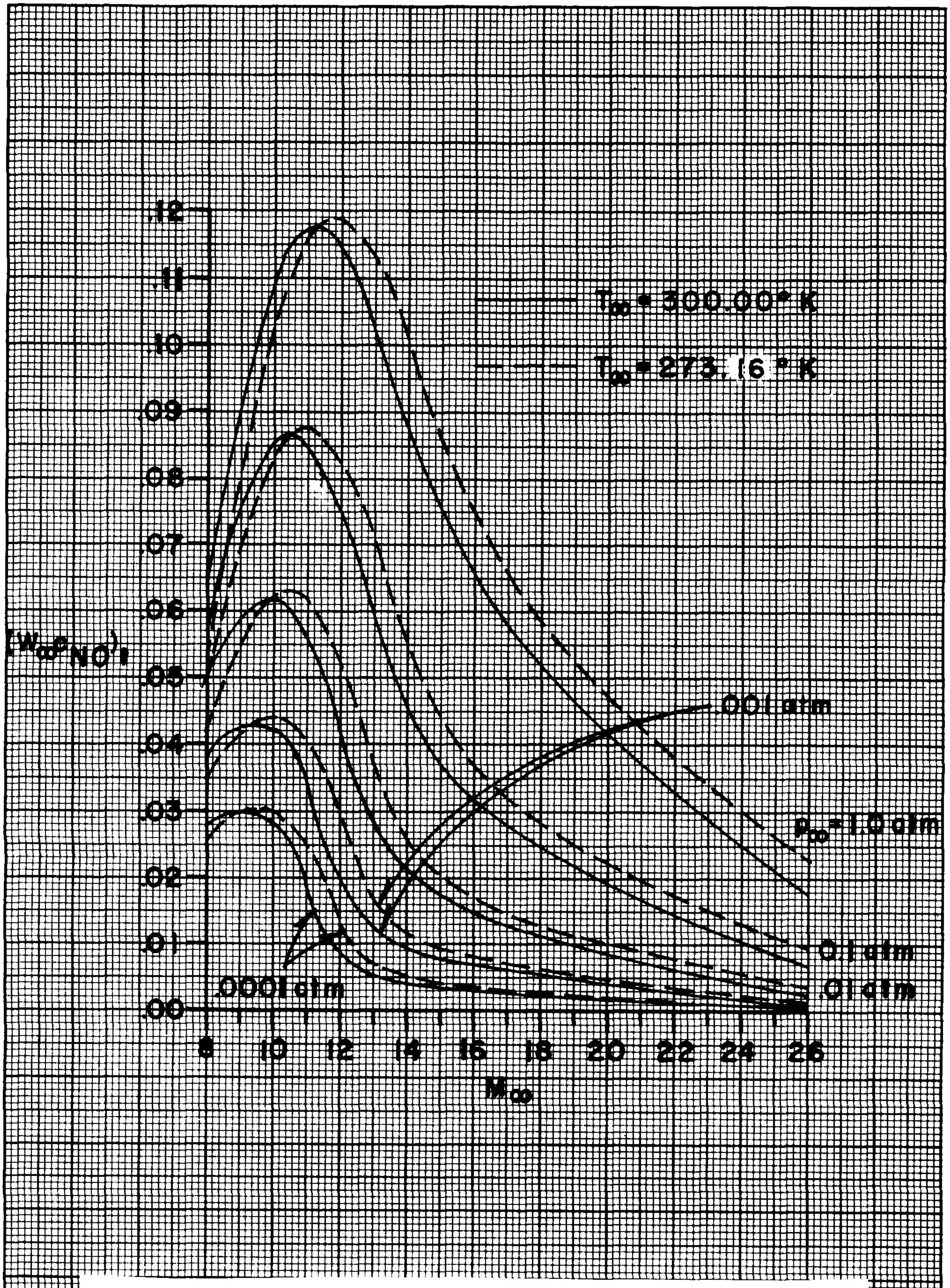


FIG. III.8. STAGNATION NO CONCENTRATION VS FREE STREAM MACH NUMBER (W_∞ = 28.86 GM/MOLE)

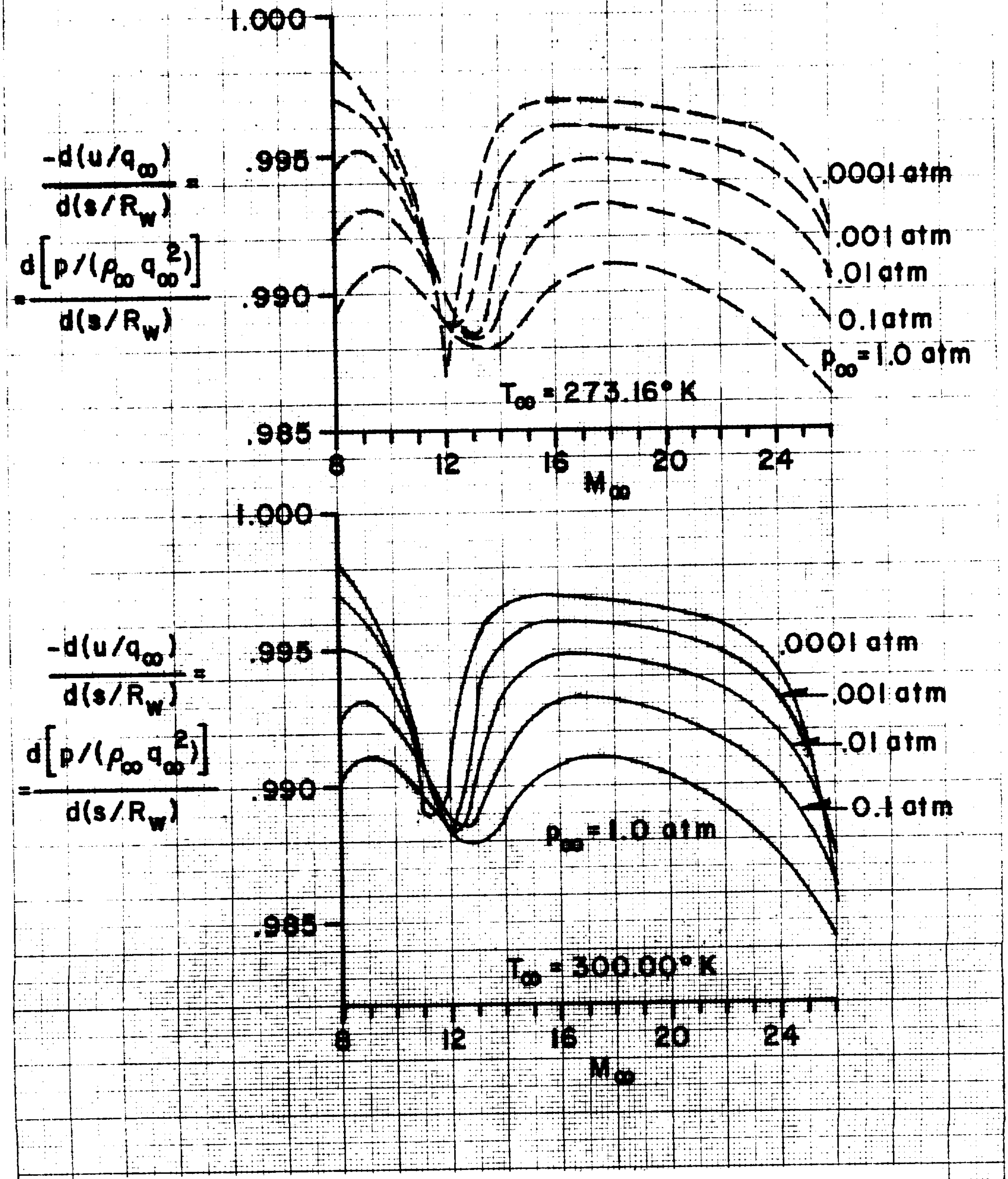


FIG. IV.1. VELOCITY AND PRESSURE GRADIENTS ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE

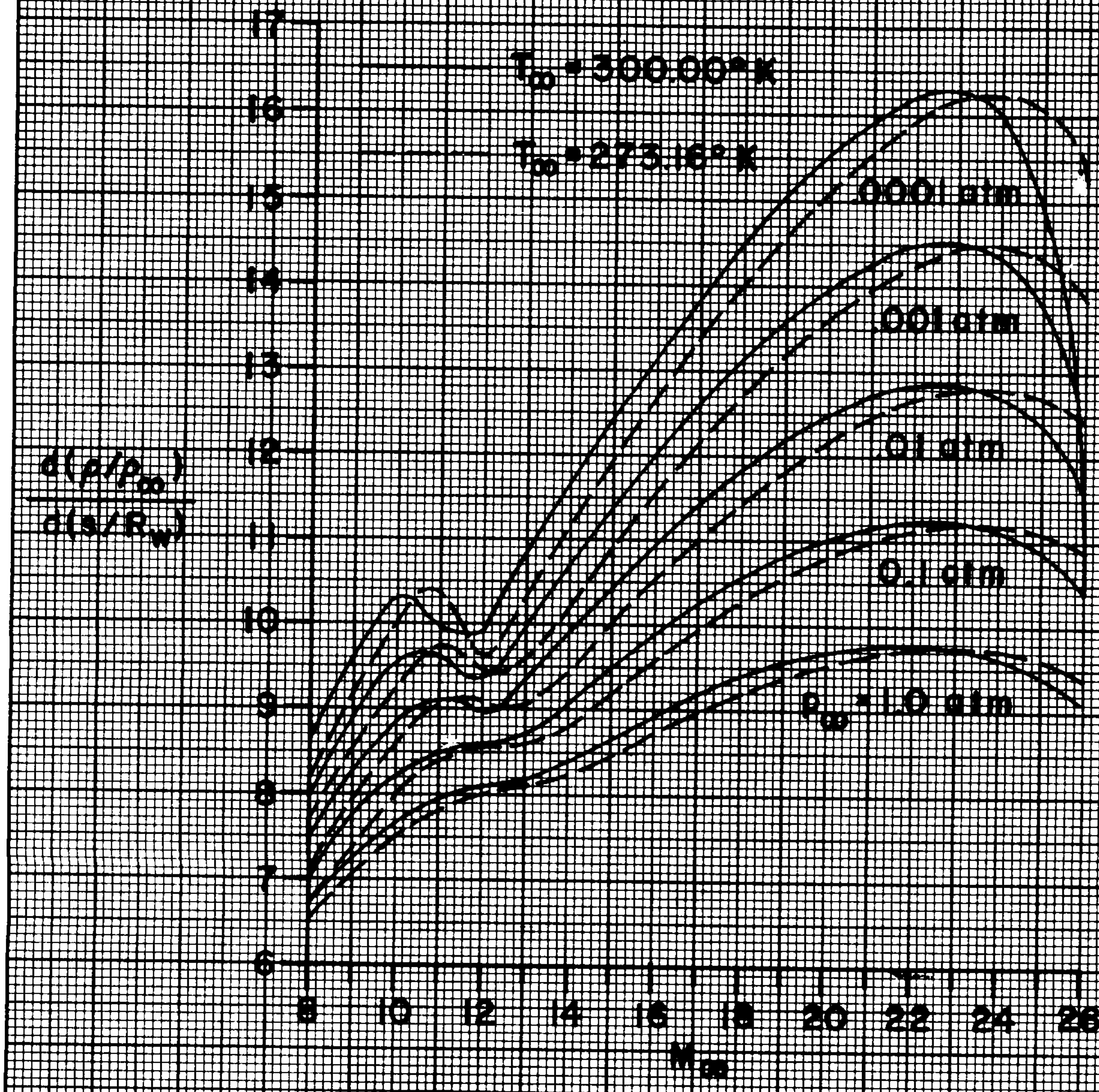


FIG. IV.2. DENSITY GRADIENT ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE

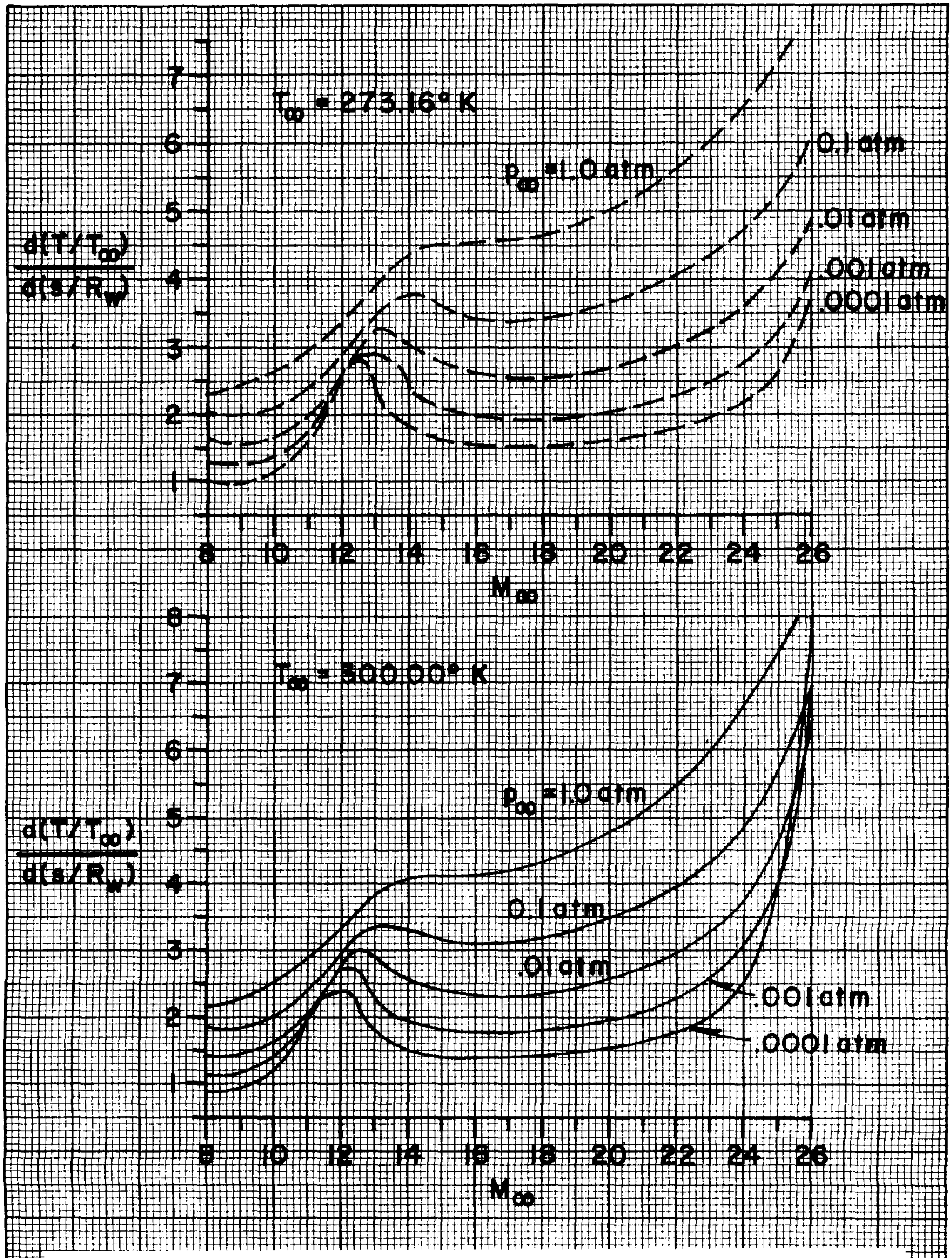


FIG. IV.3. TEMPERATURE GRADIENT ALONG STREAMLINE NORMAL TO CURVED SHOCK SHOCK WAVE

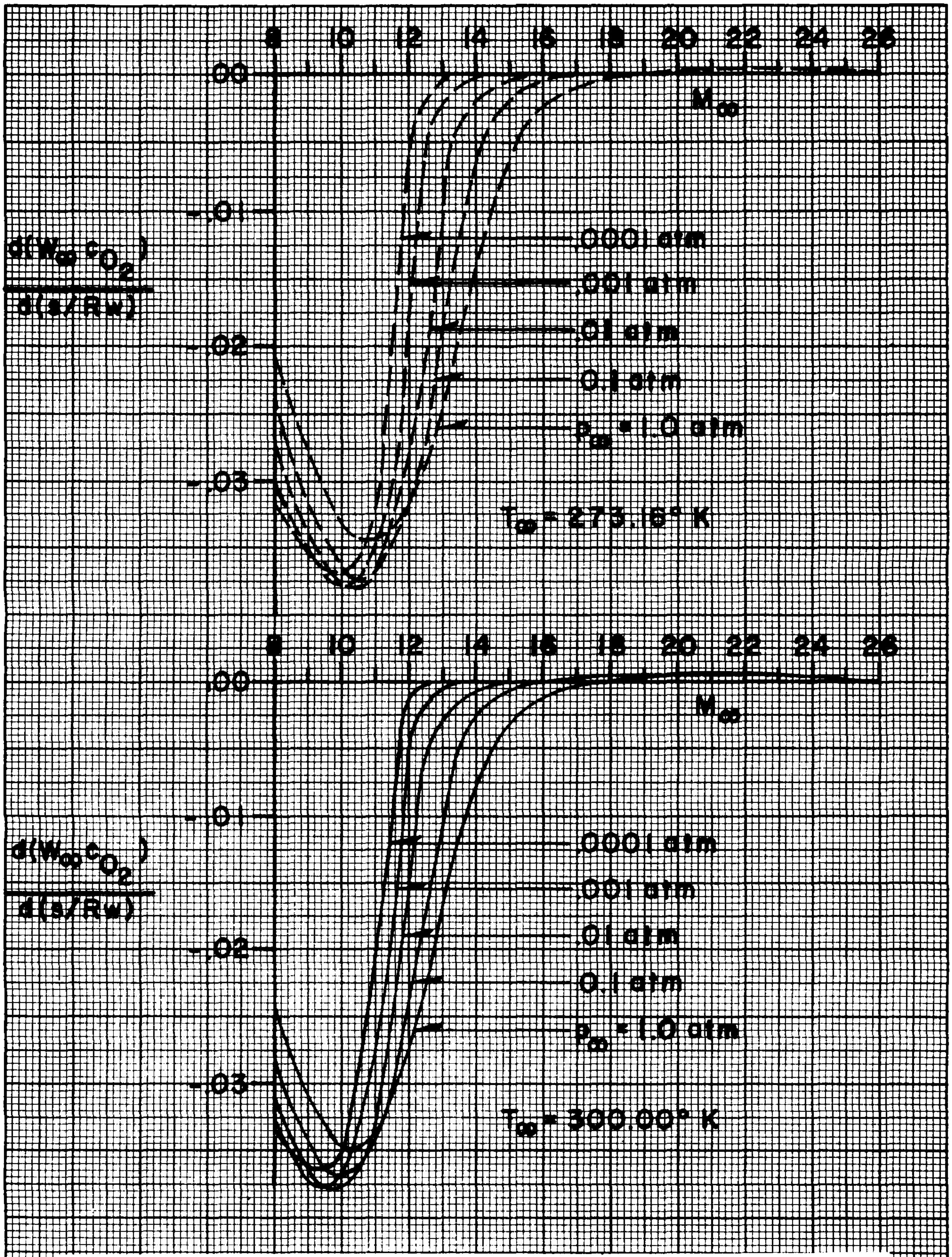


FIG. IV.4. GRADIENT OF O_2 CONCENTRATION ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE (W_∞ = 28.86 GM/MOLE)

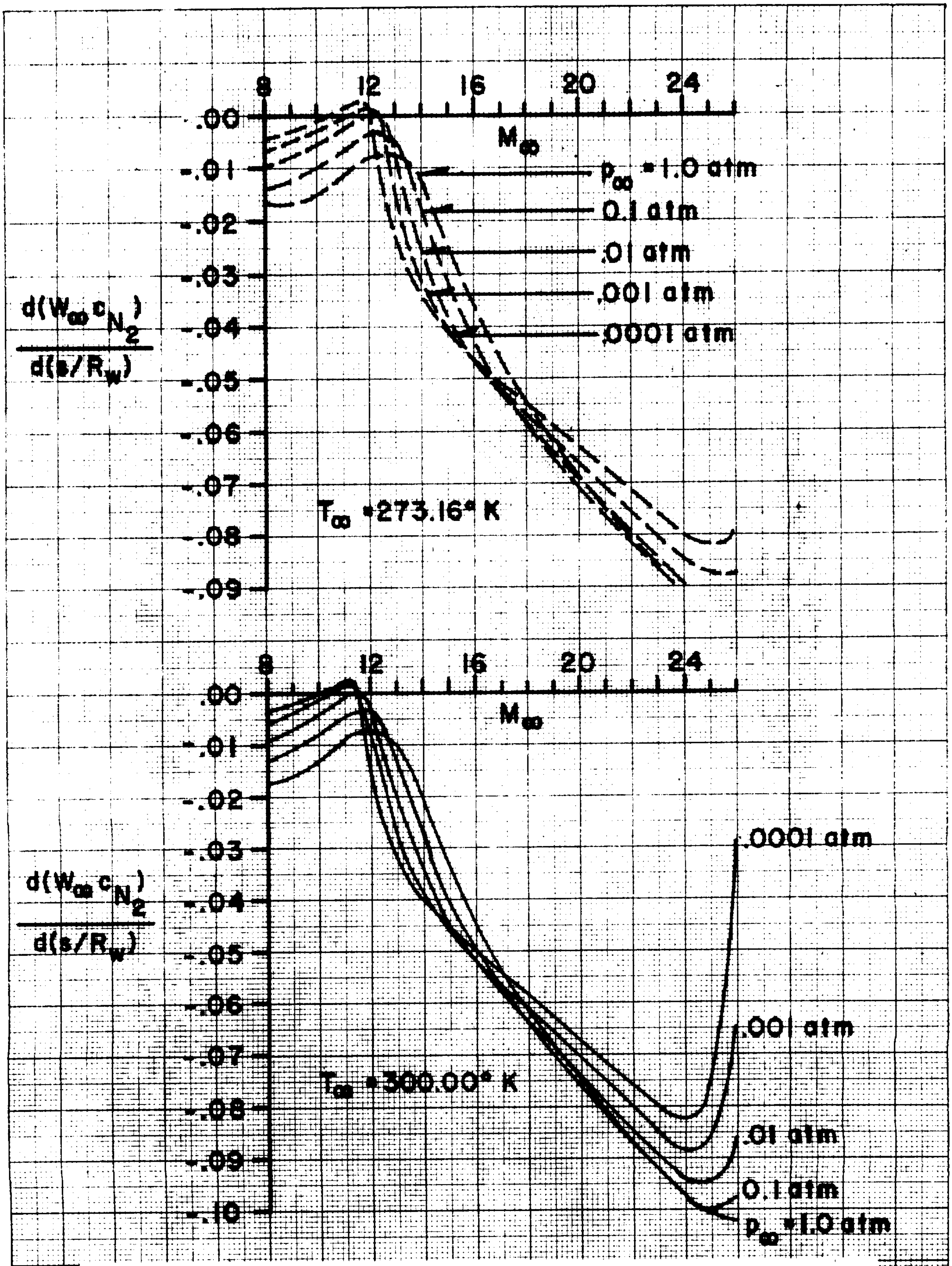


FIG. IV.5. GRADIENT OF N_2 CONCENTRATION ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE (W_∞ = 28.86 GM/MOLE)

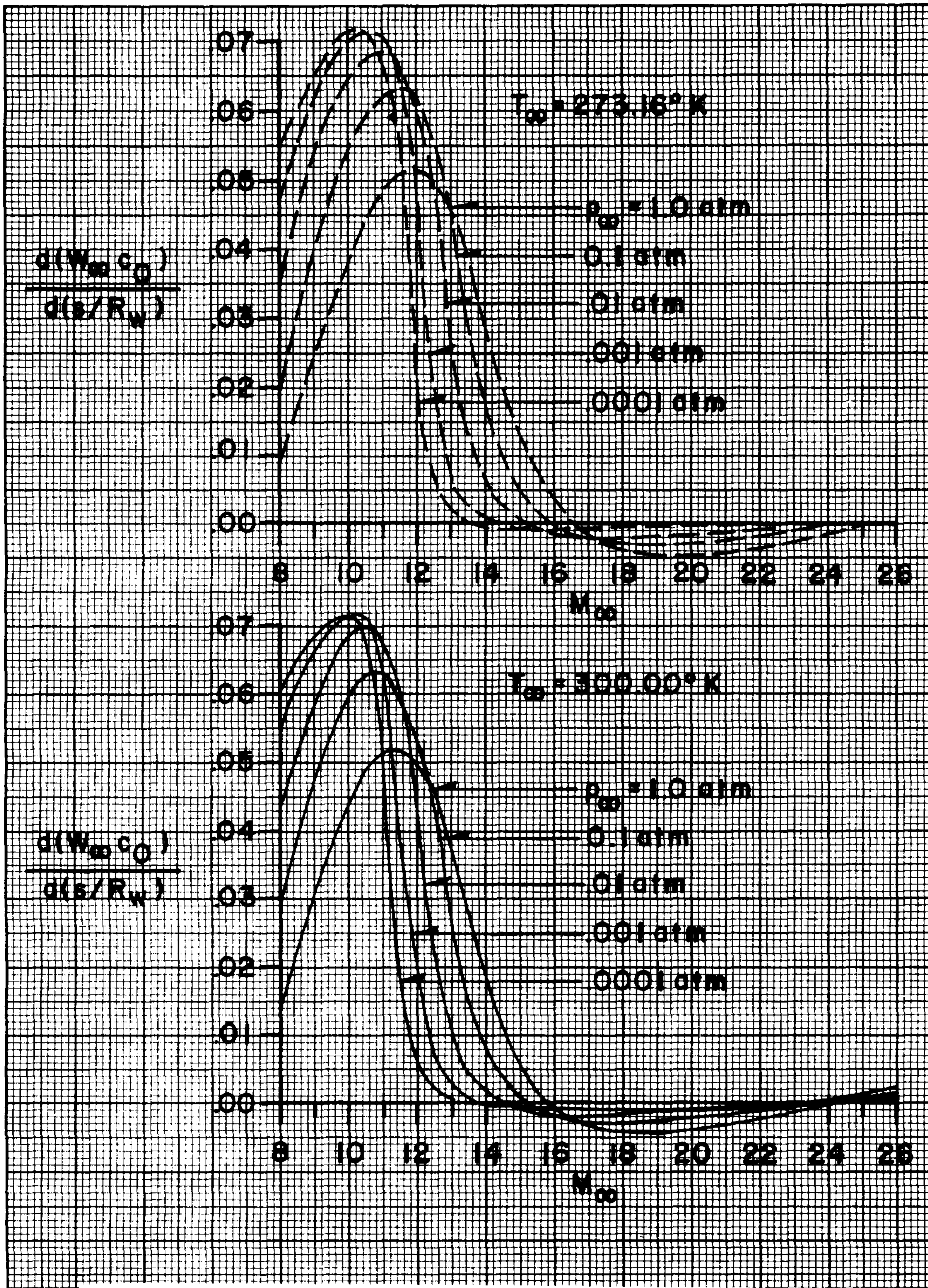
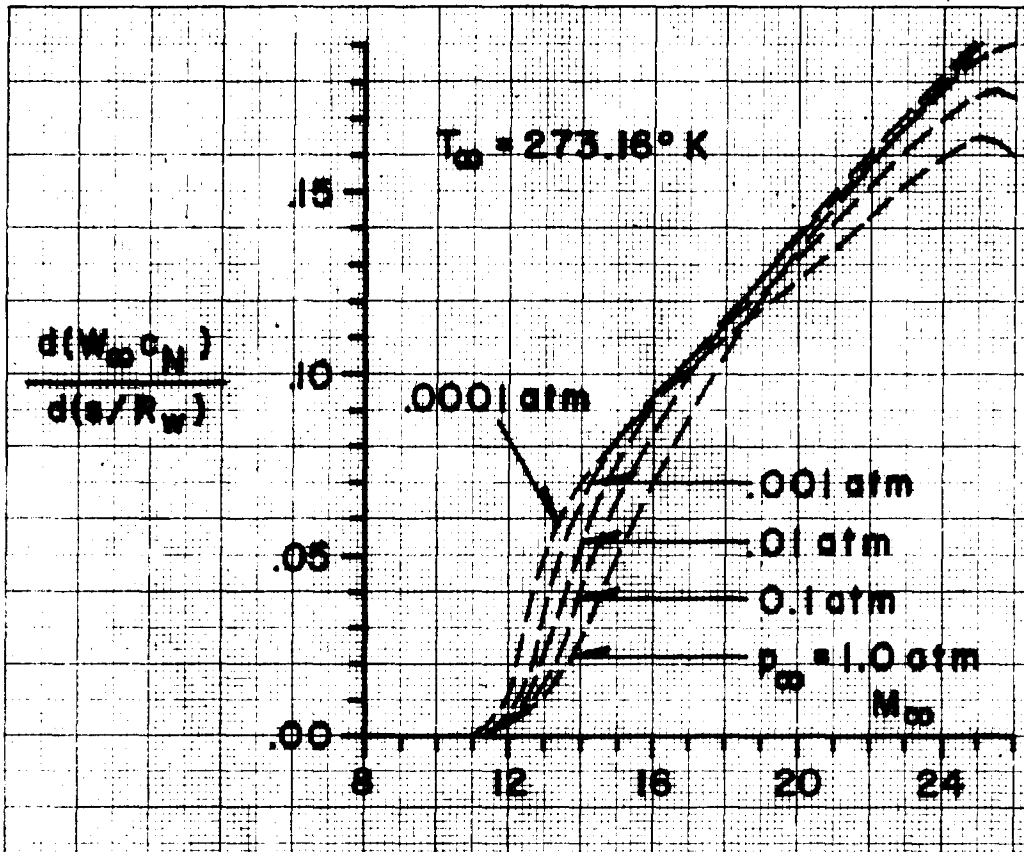


FIG. IV.6. GRADIENT OF O CONCENTRATION ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE (W_∞ = 28.86 GM/MOLE)



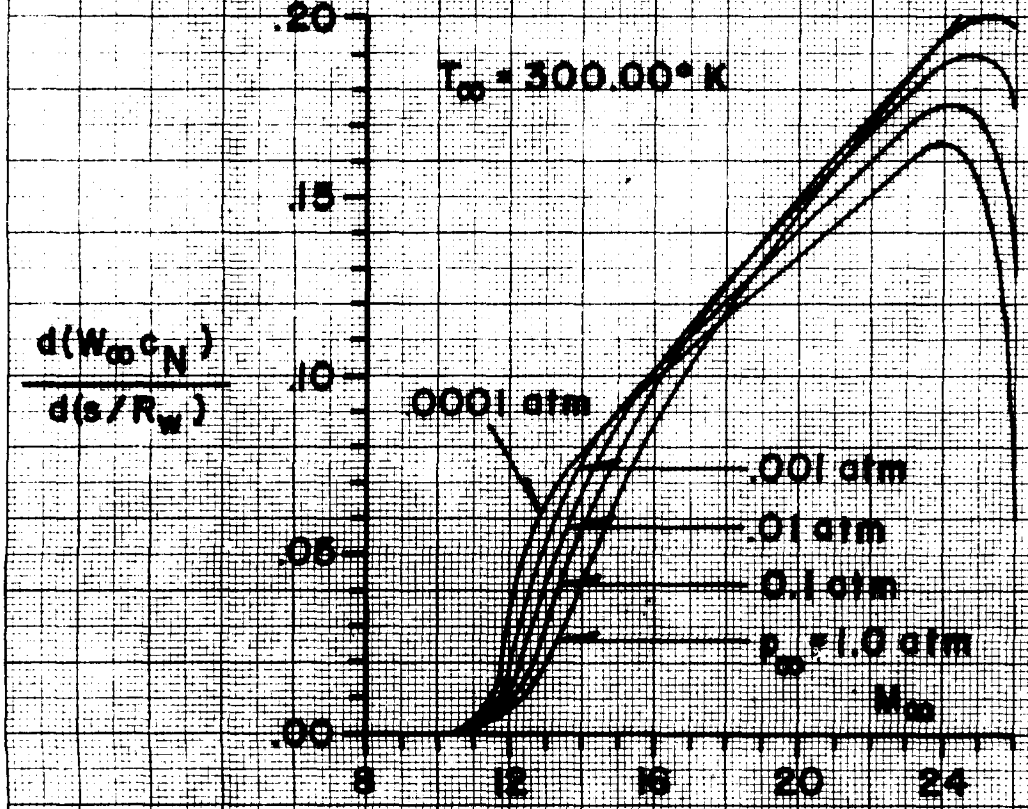


FIG. IV.7. GRADIENT OF N CONCENTRATION ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE (W_∞ = 28.86 GM/MOLE)

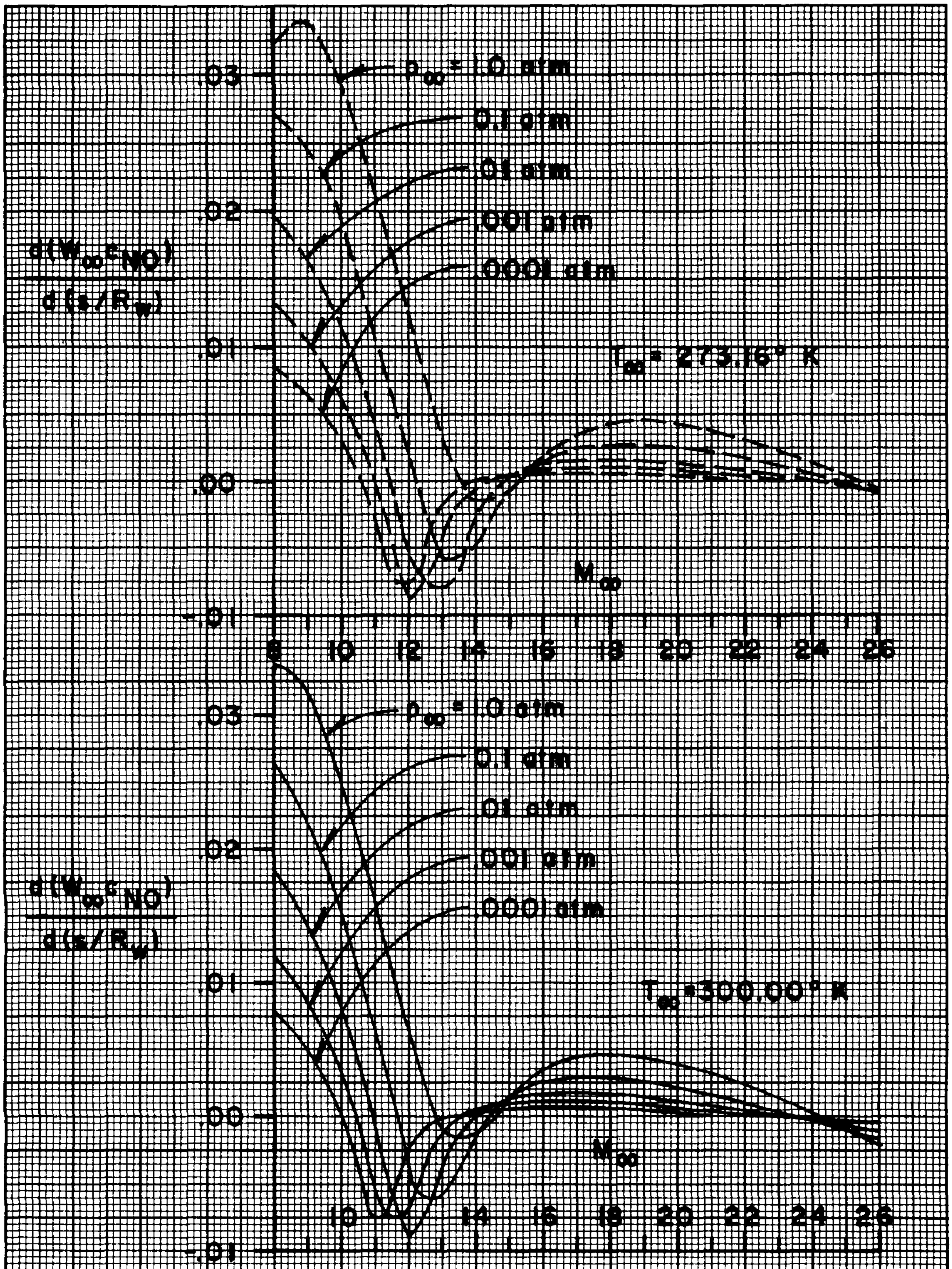


FIG. IV.8. GRADIENT OF NO CONCENTRATION ALONG STREAMLINE NORMAL TO CURVED SHOCK WAVE (W_∞ = 28.86 GM/MOLE)

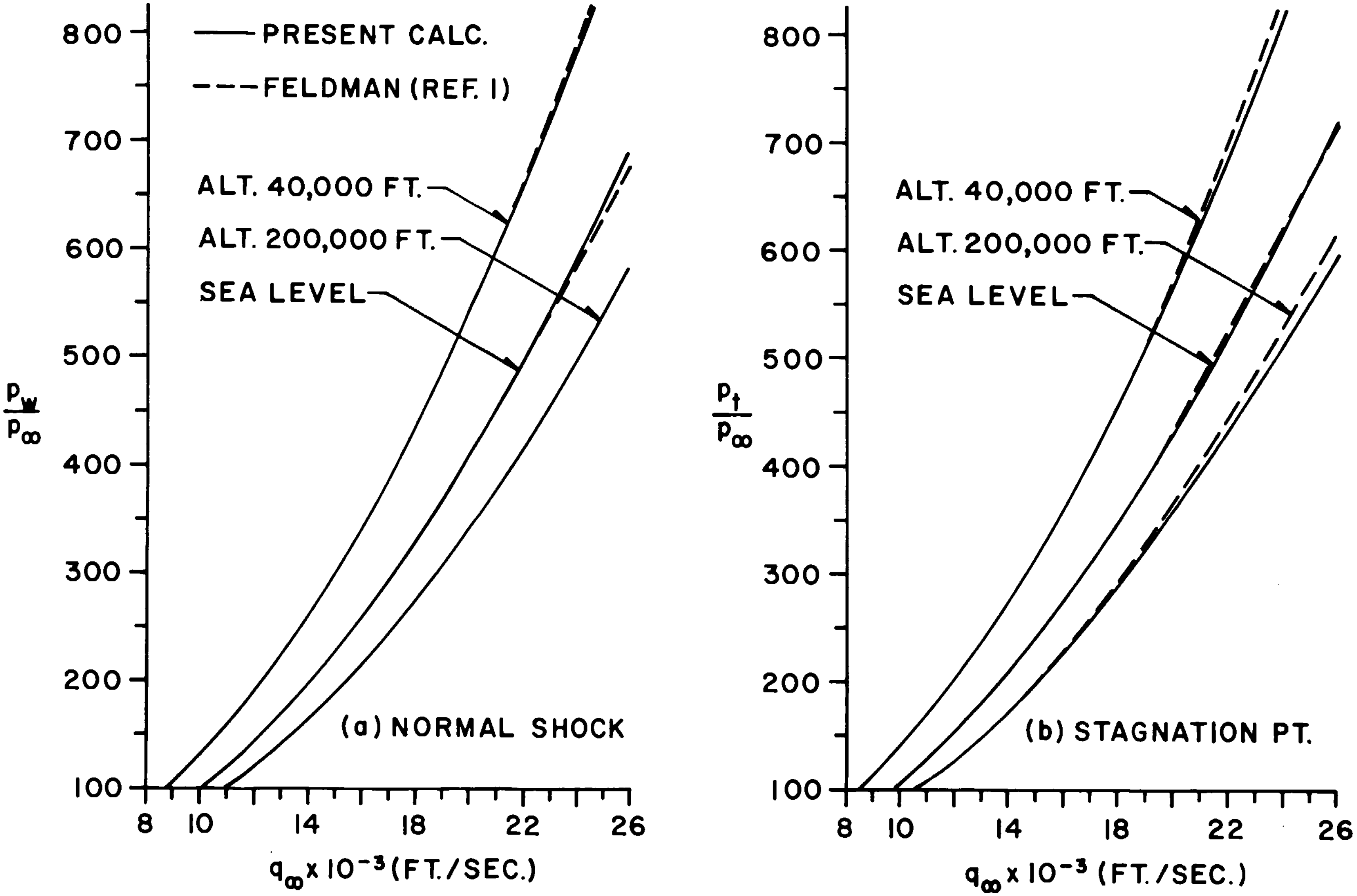


FIG. 7.1 COMPARISON OF PRESSURE CALCULATIONS WITH VALUES IN REF. 1.

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APPENDIX

COEFFICIENTS OF EQUATIONS (2.6) AND (2.9)

$$A_{11} = 2/\rho$$

$$A_{12} = A_{13} = 2/[c_O + c_N + (2/W_\infty)] \qquad A_{14} = 2/T$$

$$A_{21} = c_O\left[\frac{c_O}{K_1} + \frac{c_N}{2K_5}\right]$$

$$A_{22} = \frac{2\rho c_O}{K_1} + \frac{1}{2} + \frac{\rho c_N}{2K_5} \qquad A_{23} = \frac{\rho c_O}{2K_5}$$

$$A_{24} = -\rho c_O\left[\frac{c_O}{K_1{}^2}\ \frac{dK_1}{dT} + \frac{c_N}{2K_5{}^2}\ \frac{dK_5}{dT}\right]$$

$$A_{31} = c_N\left[\frac{c_N}{K_2} + \frac{c_O}{2K_5}\right] \qquad A_{32} = \frac{\rho c_N}{2K_5}$$

$$A_{33} = \frac{2\rho c_N}{K_2} + \frac{1}{2} + \frac{\rho c_O}{2K_5}$$

$$A_{34} = -\rho c_N\left[\frac{c_N}{K_2{}^2}\ \frac{dK_2}{dT} + \frac{c_O}{2K_5{}^2}\ \frac{dK_5}{dT}\right]$$

$$A_{41} = (c_O^2\ h_{O_2}/K_1) + (c_N^2\ h_{N_2}/K_2) + (c_N c_O\ h_{NO}/K_5)$$

$$A_{42} = (2\rho c_O\ h_{O_2}/K_1) + (\rho c_N\ h_{NO}/K_5) + h_O$$

$$A_{43} = (2\rho c_N\ h_{N_2}/K_2) + (\rho c_O\ h_{NO}/K_5) + h_N$$

$$A_{44} = \sum_i c_i c_{p_i} - \rho\left[\frac{c_O{}^2}{K_1{}^2}\frac{dK_1}{dT}\ h_{O_2} + \frac{c_N{}^2}{K_2{}^2}\ \frac{dK_2}{dT}\ h_{N_2} + \frac{c_O c_N}{K_5{}^2}\ \frac{dK_5}{dT}\ h_{NO}\right]$$

TABLE I

REACTION RATE COEFFICIENTS AND EQUILIBRIUM CONSTANTS

No.(j)	Reaction	Rate Coeff.,Equilib.Const.	Catalyst($\underline{M}$)
I	$O_2+\underline{M}\rightleftharpoons 2O+\underline{M}$	$(k_f)_1 = 1.2\times 10^{18}\, T^{-3/2}\exp(-59{,}380/T)$ $K_1 = 1.2\times 10^{6}\, T^{-1/2}\exp(-59{,}380/T)$	N_2,N,NO
II	$N_2+\underline{M}\rightleftharpoons 2N+\underline{M}$	$(k_f)_2 = 9.9\times 10^{17}\, T^{-3/2}\exp(-113{,}260/T)$ $K_2=18.0\times 10^{3}\exp(-113{,}260/T)$	O_2,O,NO
III	$O_2+O_2\rightleftharpoons 2O+O_2$	$(k_f)_3 = 3.6\times 10^{18}\, T^{-3/2}\exp(-59{,}380/T)$ $K_3=$ ----same as for I	----
IV	$N_2+N_2\rightleftharpoons 2N+N_2$	$(k_f)_4 = 3.0\times 10^{18}\, T^{-3/2}\exp(-113{,}260/T)$ $K_4=$ ----same as for II	----
V	$NO+\underline{M}\rightleftharpoons N+O+\underline{M}$	$(k_f)_5 = 5.2\times 10^{18}\, T^{-3/2}\exp(-75{,}490/T)$ $K_5 = 4.0\times 10^{3}\exp(-75{,}490/T)$	O_2,O,N_2,N,NO
VI	$O+N_2\rightleftharpoons NO+N$	$(k_f)_6 = 5.0\times 10^{10}\exp(-38{,}000/T)$ $K_6 = 4.5\exp(-37{,}750/T)$	----
VII	$N+O_2\rightleftharpoons NO+O$	$(k_f)_7 = 1.0\times 10^{9}\, T^{1/2}\exp(-3{,}120/T)$ $K_7 = 4.166667\exp(+16{,}120/T)$	----
VIII	$O_2+O\rightleftharpoons 3O$	$(k_f)_8 = 2.1\times 10^{15}\, T^{-1/2}\exp(-59{,}380/T)$ $K_8=$ ----same as for I	----
IX	$N_2+N\rightleftharpoons 3N$	$(k_f)_9 = 1.5\times 10^{19}\, T^{-3/2}\exp(-113{,}260/T)$ $K_9=$ ----same as for II	----
X	$N_2+O_2\rightleftharpoons 2NO$	$(k_f)_{10} = 9.1\times 10^{21}\, T^{-5/2}\exp(-65{,}000/T)$ $K_{10}=19.0\exp(-21{,}640/T)$	----

Dimensions: $(k_f)_j$ -- $m^3/(kmol\ sec)$;

K_j for 3 body reactions -- $kmol/m^3$.

TABLE II

SPECIFIC ENTHALPIES AND SPECIFIC HEATS

$$h_{O_2} = 7RT/2 + (R\bar{\theta}_{O_2})/ [\exp(\bar{\theta}_{O_2}/T)-1] + \bar{h}_{O_2}$$

$$h_{N_2} = 7RT/2 + (R\bar{\theta}_{N_2})/ [\exp(\bar{\theta}_{N_2}/T)-1] + \bar{h}_{N_2}$$

$$h_O = 5RT/2 + \bar{h}_O$$

$$h_N = 5RT/2 + \bar{h}_N$$

$$h_{NO} = 7RT/2 + (R\bar{\theta}_{NO})/ [\exp(\bar{\theta}_{NO}/T)-1] + \bar{h}_{NO}$$

$$(C_p)_{O_2} = 7R/2 + R(\bar{\theta}_{O_2}/T)^2 \exp(\bar{\theta}_{O_2}/T)/[\exp(\bar{\theta}_{O_2}/T)-1]^2$$

$$(C_p)_{N_2} = 7R/2 + R(\bar{\theta}_{N_2}/T)^2 \exp(\bar{\theta}_{N_2}/T)/[\exp(\bar{\theta}_{N_2}/T)-1]^2$$

$$(C_p)_O = 5R/2$$

$$(C_p)_N = 5R/2$$

$$(C_p)_{NO} = 7R/2 + R(\bar{\theta}_{NO}/T)^2 \exp(\bar{\theta}_{NO}/T)/[\exp(\bar{\theta}_{NO}/T)-1]^2$$

No.(i)	Species	$\bar{\theta}_i$(°K)	$\bar{h}_i$(Dyn m/k mole)
1	O_2	2256	0
2	N_2	3374	0
3	O	--	$2.467\,65 \times 10^8$
4	N	--	$4.710\,63 \times 10^8$
5	NO	2719	$0.898\,655 \times 10^8$

1 Dyn. = 10^5 dynes

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Results of calculations carried out for a model of air in dissociation equilibrium are presented in graphical form. The quantities computed are i) flow variables (including species concentrations) behind normal and oblique shock waves, ii) flow variables in axisymmetric conical flow fields, iii) stagnation point values of flow variables on the 'stagnation' streamline behind two-dimensional and axisymmetric detached shock waves, and iv) flow variable gradients at the shock wave on stagnation streamlines. Computations are given for free stream temperatures of 273.16°K and 300°K, free stream pressures of 1.0, .1, .01, .001, and .0001 atmospheres, and a range of initial Mach numbers and cone angles to provide flow field temperatures in the range 3000°K - $10,000^{\circ}$K. Brief derivations of the equations employed are given.

The present calculations are oriented toward application in experiments in hypersonic flow with ground facilities such as shock tubes and ballistic ranges. In addition, they furnish important supplementary information to theoretical studies of nonequilibrium flows.

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