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Oscillatory Combustion in Rockets

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NOMENCLATURE

Symbol	Meaning
A,B	Species A and B
c	Molar density
c_p	Specific heat at constant pressure
D_{AB}	Coefficient of binary diffusion
$\bar{H}_i$	Partial molal enthalpy of component i
k	Thermal conductivity of the mixture
N_i	Molar flux of species i with respect to stationary coordinates
P	Total pressure
Q	Energy flux defined by Eq. (15)
r	Radial distance in spherical coordinates
r_o	Droplet radius
S	Droplet surface
T	Temperature
t	Time
V	Droplet volume
v	Molar average velocity
x_i	Mole fraction of component i
Superscripts	
ℓ	Liquid
v	Vapor

I Introduction

The research being conducted under this grant is aimed at obtaining a more fundamental understanding of some of the aspects of oscillatory combustion. The investigations dealing with size and velocity distributions in sprays and heat transfer in a non-flow system were completed previously and the resulting publications listed in past reports. During this reporting period the investigation dealing with heat transfer in a flow system has been completed and reported in Contractor Report CR-72443, "The Effect of Periodic Shock-Fronted Pressure Waves on the Instantaneous Heat Flux at the End-Wall of a Tube".

This report thus gives a summary of progress during the period on the investigation of vaporization in the region of the critical point. The work is divided into three projects; a theoretical investigation of droplet vaporization, an experimental investigation of vaporizing droplets suspended from a thermocouple in a flowing air stream, and an experimental investigation of vaporizing droplets falling through a hot stagnant gas.

The work on the theory of a spherically symmetric drop vaporizing at steady state has been completed for a CO_2-N_2 system. A paper covering this work has been submitted for publication in a technical journal. A program for calculating unsteady histories of a sub-critical droplet has been written and a few histories have been computed.

The suspended droplet experiments have yielded data on Freon 13 droplets which show liquid temperatures much higher than those calculated from simple theory. In order to establish a better understanding of the data a program has been initiated to obtain heptane droplet data at pressures from 1.5 to 100. atm. Data taken for pressures up to 10 atm. shows good agreement with the simple theory.

The falling droplet experiments have been concerned with improving the drop forming apparatus to prevent initial disturbances of the droplet geometry. The apparatus was also modified to allow formation of CO_2 droplets, thus allowing data to be taken with lower gas temperatures than those required when using n-heptane.

II Droplet Vaporization Theory

A mathematical model for unsteady droplet vaporization at high ambient pressures has been formulated during this reporting period.

The model includes the effects of non-ideal mixtures, variation of the physical properties through the boundary layer, rate of surface regression and transient effects. In order to simplify the analysis, a continual formation of completely fresh surface is assumed. Furthermore, the liquid temperature is considered to be uniform.

Under these postulates, the conservation equations for mass and energy are sufficient to describe the evolution with time of the one-dimensional temperature and composition profiles in the gaseous phase surrounding a droplet. For spherical symmetry, these equations can be written in the following form

$$c\frac{\partial x_A}{\partial t} + cv\frac{\partial x_A}{\partial r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 cD_{AB}\frac{\partial x_A}{\partial r}\right) \tag{1}$$

$$\frac{\partial c}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 cv) = 0 \tag{2}$$

$$cx_A\frac{\partial \bar{H}_A}{\partial t} + cx_B\frac{\partial \bar{H}_B}{\partial t} + N_A\frac{\partial \bar{H}_A}{\partial r} + N_B\frac{\partial \bar{H}_B}{\partial r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k\frac{\partial T}{\partial r}\right) \tag{3}$$

$$N_A = x_A cv - cD_{AB}\frac{\partial x_A}{\partial r} \tag{4}$$

$$N_B = x_B cv + cD_{AB}\frac{\partial x_A}{\partial r} \tag{5}$$

$$c = c(x_A, P, T) \tag{6}$$

Species A and B refer to those of the diffusing vapor and inert environment, respectively. Equation (6) is the equation of state for the mixture. The Redlich-Kwong equation of state has been adopted throughout this work.

The initial and boundary conditions are

$$x_A(r,0) = f(r) \qquad \text{for } r \geq r_o(0) \tag{7}$$

$$T(r,0) = g(r) \qquad \text{for } r \geq r_o(0) \tag{8}$$

$$x_A(r_o,t) = x_{Ao} \tag{9}$$

$$T(r_o,t) = T^{\ell}(t) \tag{10}$$

$$x_A(\infty,t) = 0 \tag{11}$$

$$T(\infty,t) = T_\infty \tag{12}$$

$$v(r_o,t) = \frac{dr_o}{dt} - \frac{D_{AB}}{1 - x_A} \frac{\partial x_A}{\partial r} \tag{13}$$

Equation (9) is determined by the vapor-liquid equilibrium relationship $x_{Ao} = x_{Ao}(T,P)$. Equations (11) and (12) are specified by the ambient conditions. In this work the initial conditions, (7) and (8), are determined from the numerical solution of a porous sphere supplied with liquid from its interior and kept at the injection temperature $T^{\ell}(0)$ under ambient conditions T_∞ and P.

In addition to the foregoing equations, mass and energy balances require that

$$\frac{dT^{\ell}}{dt} = \frac{S}{V} \frac{Q}{c^{\ell} c_p^{\ell}} \tag{14}$$

where

$$Q = k\frac{\partial T}{\partial r} - N_A(\bar{H}_A^{V} - \bar{H}_A^{\ell}) \Big| \quad r = r_o(t) \tag{15}$$

and

$$N_A \Big| r = r_o(t) = - c^{\ell}\frac{dr_o}{dt} - \frac{r_o}{3} \frac{\partial c^{\ell}}{\partial T} \frac{dT^{\ell}}{dt} \tag{16}$$

Equations (1) through (16) are being solved simultaneously by a numerical explicit technique. The technique in numerically stable if Fourier's modulus, based on the difference values of time and space evaluated at the ambient conditions, is equal to or less than 0.5.

In order to test the computer program, the temperature response of a CO_2, 1000-micron-radius, porous sphere vaporizing in N_2 at 815°K and 72.9 atmospheres was calculated for different mesh sizes. The steady state temperature predicted with a space increment of 400 microns was found to be 280°K whereas for a 200 micron increment the steady state temperature was found to be 277°K. The computing time in the latter case is prohibitively long. Previous steady state calculations with a more accurate numerical technique show a value of 275°K for these conditions. This discrepancy is primarily caused by the inability of the relatively large finite differences to portray accurately the large temperature and composition gradients existing in the film at the droplet surface. A six-point Lagrange formula is used to determine the temperature and composition derivatives there. It is of interest to note that for a 1000-micron-radius droplet with a steady state temperature equal to $0.9T_c$ and a total pressure equal to the critical, the temperature and mole fraction gradients at the droplet surface are of the order of 3000°K/cm(0.3°K/micron) and 6/cm, respectively. The larger the mesh size the larger the error introduced in the calculations. As a consequence of this error, the computations tend to predict consistently higher energy rates into the droplet.

Preliminary history calculations are shown in Figures 1 and 2 for a carbon dioxide droplet vaporizing in nitrogen under a pressure of 72.9 atmospheres and temperatures of 1400°K and 815°K, respectively.

For the conditions illustrated in Figure 2 the liquid temperature converges asymptotically towards its steady state value up to a point where the surface to volume ratio becomes appreciable. However, some care must be exercised in interpreting the last part of the vaporization process until further data are obtained for the reasons mentioned above. During the last part of the vaporization process the term dT^{ℓ}/dt exhibits small random variations.

For the near critical conditions illustrated in Figures 1 and 2 the rate of surface regression is not a significant factor in the vaporization process.

It is planned to obtain vaporization histories under higher pressure conditions where steady state conditions cannot be obtained. Comparisons with the quasi-steady state theory will be carried out.

III Suspended Drop Experiment

During the reporting period minor modifications were made to the probe, an air cooler was built to dry the high pressure air supply, and the instrumentation and optics were completed. An experimental technique has been developed. Water, Fr-13, and n-heptane drop vaporization data have been obtained. The purpose of the water experimentation was to test the apparatus. The Fr-13 data is considered provisional at this time because of the substantial deviation from simple steady state theory. As a result the program of n-heptane was undertaken to investigate any systematic deviations between experimental results and simple theory at increasing pressures. At pressures up to 10 atm. no significant departures from theory have been found for n-heptane in air.

Rig Development and Instrumentation

Two further probe modifications were made during the reporting period. One was to change the probe tube tip from stainless steel to teflon. This change provided thermal insulation for the drop from the cooled portion as well as electrical insulation for the probe thermocouple lead wires. A chromel-constantan thermocouple was substituted for the copper constantan probe thermocouple. The average thermal conductivity of the 0.005 in. diameter probe lead wires was reduced by a factor of 10 by this change. The optics

including the timer and the instrumentation are complete and have been used for data acquisition during the last half of the reporting period.

One new problem that was encountered was water vapor condensation from the high pressure air on the probe when it was fed with Fr-13. Under some circumstances ice formed on the probe. This was eliminated by designing and building a high pressure air cooler. It is located after the final stage of the 2000 psi air compressor. Previously the air was cooled to about 150°F at 1800 psi. Now the Fr-12 cooler cools the 1800 psi air to 32°F. It consists of a converted home type dehumidifier.

Mr. Lee D. Alexander has completed his master's degree research. The following quotation is the abstract from his master's thesis.

> Existing apparatus was modified and instrumentation was developed in order to study the vaporization of droplets suspended in a high pressure air stream. Water droplets were suspended at pressures of up to 60 atmospheres and at air temperatures of up to 275°F. Steady-state liquid temperatures were obtained from the thermocouple upon which the droplet was suspended. The experimental results were compared with a theoretical model and were found to be consistently slightly higher.
>
> In addition, the feasibility of droplet simulation, in the region of the critical temperature was investigated.[1]

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[1]Lee D. Alexander, "The Experimental Performance of an Apparatus Designed to Study the Vaporization of a Suspended Droplet in the Vicinity of Its Critical Point," Master's Thesis, U. of Wisconsin (1968).

Water Drop Data

Water Drops were evaporated in heated air at 20, 40, and 60 atm. pressures. It might be added that no droplets experiments would be complete without trying water. The steady state results are shown on Fig. 3 where they are compared with simple steady state theory calculations. The meagre data agrees in trend with the calculations, and the measured values are about 10, 7, and 5 °F above the calculated values for the pressures of 20, 40, and 60 atm., respectively. The water drop results were obtained with 0.005 in. diameter Fe-Con thermocouple wires which offer an improvement of about 4 times over the Cu-Con wires. Data obtained with Cu-Con thermocouple wires (not shown) resulted in plateau temperatures about 10°F above the data shown.

We believe that there is insufficient water data to infer anything about the effect of pressure on the relation of measured to calculated drop temperatures. However, the agreement is good and attests the rig and temperature instrumentation performance. No drop size regression measurements were obtained, and consequently no mass transfer rate comparisons were possible.

Fr-13 Drop Data

The initial Fr-13 in air data taken showed quite a scatter in plateau versus air temperature. This was eliminated by changing the drop-making from an interupted air

flow to a continuous air flow technique. Making drops with an uninterupted air flow has the further advantage that drops are stable at a higher Weber Number than if they are formed in a non-flow field and then subjected to a sudden rapid transient in air flow.

Fr-13 drop data has been obtained at reduced pressures of 1, 1.5, and 2 and air temperatures of 70 - 200 °F. The droplet plateau temperatures as a function of air temperature are shown on Fig. 4. The values of liquid temperatures calculated from simple steady state theory are overlayed on the figure. All of the data and calculations shown correspond to a reduced pressure of 1 (560 psi) except for point A. which is a data point for P_r=1.5 (840 psi). A measured temperature history is shown on Fig. 5. This history corresponds to data point B. on Fig. 4. This data is considered very provisional for a number of reasons:

a. The temperatures show a large deviation from simple theory.
b. Frequent droplet behavior included spinning, oscillation and drops hanging from the bottom of the thermocouple bead rather than enveloping it.
c. Mass transfer rates predicted from simple theory for specific data were as much as an order of magnitude less than observed rates.
d. The effects of free convection due both to temperature and concentration gradients were present but are difficult to estimate.

e. The droplet lifetimes were on the order of a fraction of a second which raises questions about the ability of the thermocouple to follow the temperature histories.

Despite these difficulties, distinct temperature plateaus occured and the data is fairly reproducible and self-consistant. A small 0.001 in. diameter wire ring was attached to the probe thermocouple bead in order to better support the Fr-13 drops. This addition maintained the droplet around the bead, and this arrangement produced similar temperature data to that without the ring.

Calculations were made which showed that the contributions from thermal radiation and thermocouple lead conduction should total less than 10% of the heat being transferred to a typical drop by forced convection. Data on heat transfer to oscillating drops indicates that at most the heat transfer rates could be inhanced by 50% over the quiescent case. The mass transfer rates would be enhanced as well.

Errors in the application of simple theory in the range of $P_r = 1$ and $T_r = 0.92$ are expected. Absorption of air in Fr-13 and real gas effects are not properly accounted for by the simple theory.

The calculated[2] critical mixing line for Fr-13 in air is shown on Fig. 6. The range of data points at P_r = 1, 1.5 and 2 is overlayed. Two data points labeled C. were obtained at P_r = 2. These points which fall above the P-T dome were unsteady histories. The temperature and size histories were poorly defined and are not reported. It should be pointed out that the critical mixing line was calculated from an equation developed for nonpolar hydrocarbon mixtures and thus may be in substantial error. For example, the critical mixing line similarly calculated for Co_2-N_2 gave pressures 60% too low when compared to data and/or calculations based on fugacity values.

We believe that the Fr-13 data can be improved by going to a smaller thermocouple bead and wires and by using improved experimental techniques.

It has been demonstrated that supercritical data, i.e. above the critical mixing line and not merely at supercritical pressures, can be obtained.

n-Heptane Drop Data

In order to clarify the status of the Fr-13 in air data, it was decided to make vaporization measurements with a hydrocarbon fuel over a wide range of pressures. Thus, it would be possible to compare data at low pressures and

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[2]P.L. Church, J.M. Prausnitz,"Vapor-Liquid Equilibria at High Pressure: Calculation of Critical Temperatures, Volumes and Pressures of Non Polar Mixtures," AIChE J., 13, 6, 1107-1113, (1967).

investigate any systematic variation between simple steady state theory and experimental values at increasing air pressures. This program has been partially completed. About 65 individual droplet histories have been recorded in the following range of conditions:

n-heptane drops in air

pressures; 1.5, 5, 10 atm. abs.

air temperature range; 100-300°F

The results of steady state calculations for atmospheric pressure are compared with both theory and calculations of earlier workers[3] in Fig. 7. It wasn't possible to maintain adequate air flow rates in the rig at pressures below 1 1/2 atm. abs., so a one to one comparison with data at 1 atm. wasn't possible. The present calculations are in excellent agreement with the former calculations, and agree well with the 1 atm. experimental data of Priem.

Figures 8, 9, and 10 show data points and calculated steady state temperatures at 1 1/2, 5, and 10 atm. abs. for the n-heptane in air system. A comparison between measured and calculated droplet vaporization rates in the steady temperature region will provide a further check between theory and experiment. When the movies have been analyzed

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[3] R. J. Priem et al, "Experimental and Calculated Histories of Vaporizing Fuel Drops," NACA TN 3988, 1957.

it is expected that this variable will be more sensitive to deviations at increasing pressures than is droplet temperature.

The possibility of reaching the critical mixing line for a n-heptane in air mixture at high pressures was considered. Figure 11 shows a calculated critical mixing line for n-heptane in air mixture. Point A. designates the maximum design condition of the rig, i.e. 2000 psi and 300°F air temperature. This operating point is well within the P-T dome for the mixture, so it would not be expected that supercritical conditions could be reached.

IV Falling Drop Experiment

The experimental goal of this project is to obtain motion, mass, diameter, and temperature histories of single droplets falling freely through an atmosphere of temperature and pressure such that the liquid will approach its critical temperature. During this report period the work has been divided between acquiring background relevant to the theory of droplet vaporization and improving the experimental apparatus and technique. The object and general method remain the same as described in previous reports though some of the details have changed.

Some additions have been made to the drop forming probe assembly. A shield which retracts to permit viewing the formation of the droplet on the probe tip and then positions itself to protect the droplet from being shoved up the probe tip by the relative airflow was added to the probe assembly. Experiments were performed using rubber cushions of various thicknesses to determine how fast the droplet should be decelerated to release the droplet suitably from the probe tip. In conjunction with this a latching mechanism was constructed which catches the probe at the height of its rebound from the oven in order to protect the probe tip from the high temperature.

Many of the droplets tend to either break up and quickly leave the field of view as they are released from the probe tip or to oscillate or gyrate so that the two

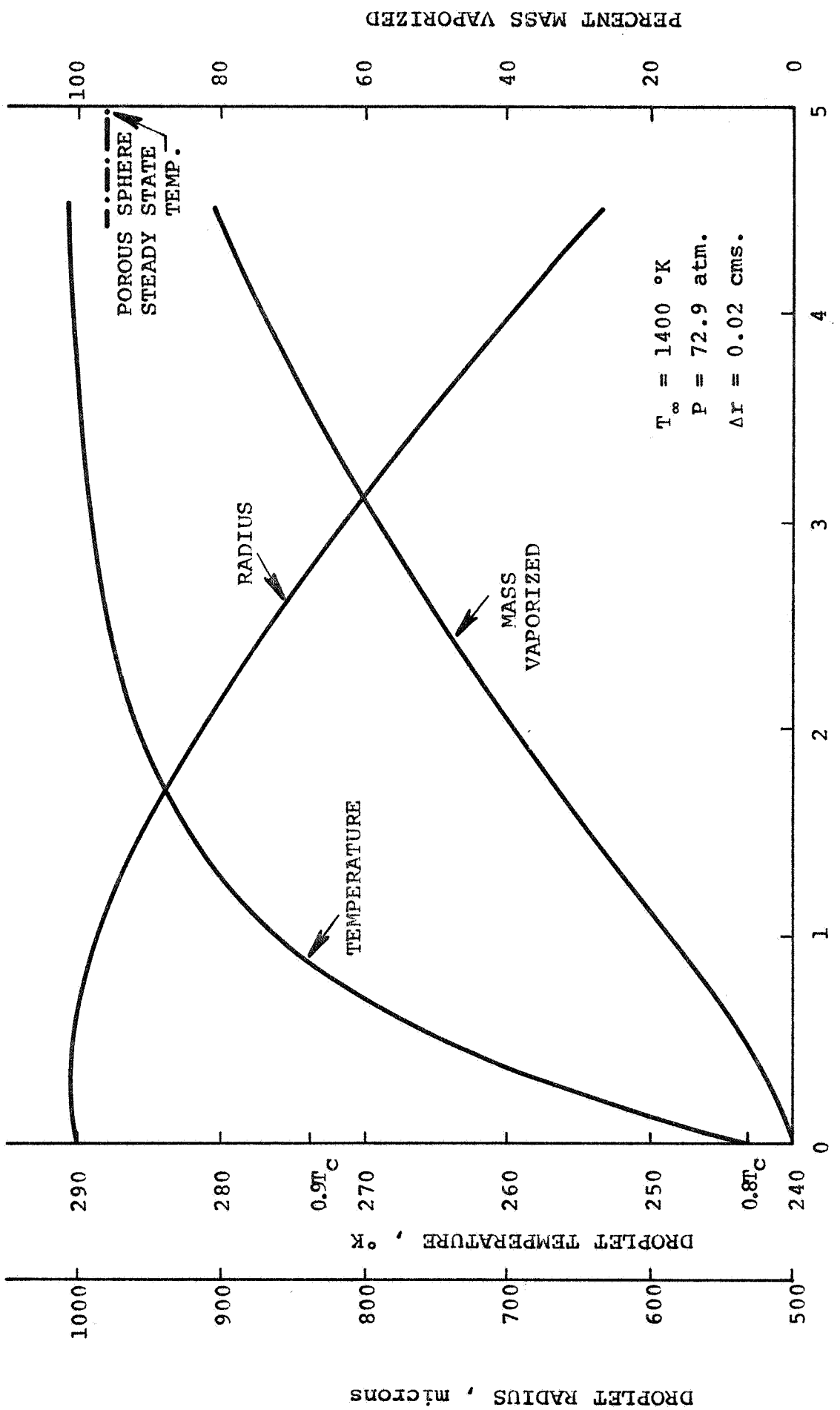
dimensional view available on the film is not sufficient to permit a determination of size. Because simple remedies have not corrected this, a systematic study of the formation of droplets on and their release from the probe tip is in progress.

The oven was originally intended to be operated by setting the input power level and waiting until the gas inside reached its steady state temperature. This proved unsatisfactory because the insulating material reaches excessive temperatures, and because the long periods which are required to reach high steady state temperatures permit metal vapors to plate the internal windows and make them quickly unusable. Because of this the oven is now to be operated at high power for a short time and the individual data runs made when the oven reaches the required temperature. New parts have been fabricated to adapt the oven to this use.

In addition, the fact that metal vapors from the heater cloud the windows at high temperatures make it desirable to obtain useful data at lower temperatures. This may be accomplished by using materials with lower critical temperatures than normal heptane. To explore this possibility a cooling system using ice water was added to the apparatus and other modifications were made so that carbon dioxide could be used as the droplet fluid. With these preparations some carbon dioxide droplets have been successfully formed in Nitrogen gas and photographed using the present probe

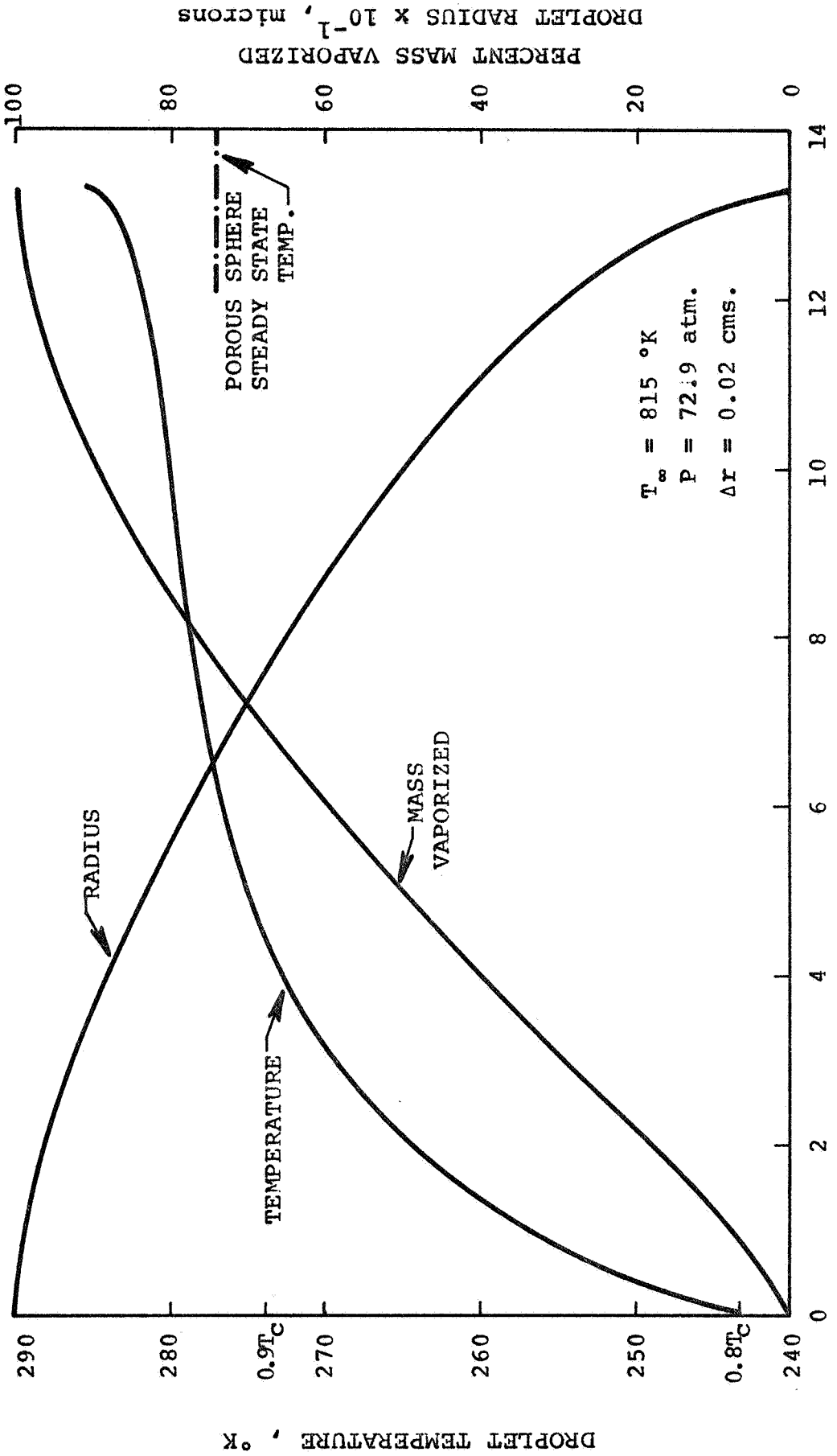
assembly. This was accomplished by filling the probe reservoir with solid carbon dioxide at atmospheric pressure, then melting it under pressure in the apparatus. Although this technique might be used to obtain a limited amount of data it requires rapid handling and is very fussy. Because of this some thought has been given to developing a probe which will conveniently handle materials which are not easily handled fluids at atmospheric pressure. Such a drop forming probe will be fabricated if required.

Future plans include finishing the drop forming study in order to improve the initial droplets, further testing of the oven assembly, and some minor work on the camera to improve the quality of the photographs.



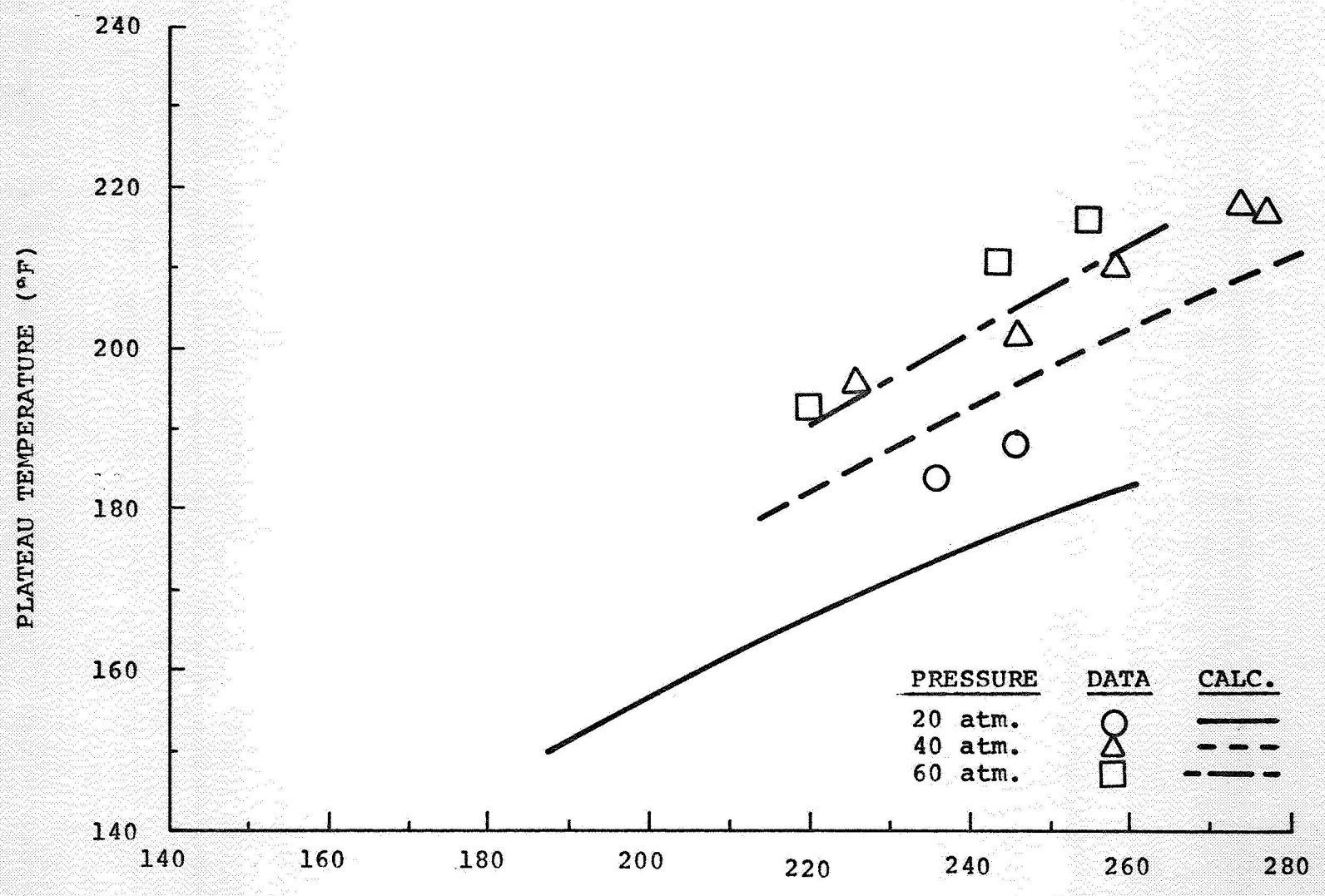
Calculated Vaporization Histories of CO_2 Drop in 1400 °K Nitrogen at 72.9 atm.

Fig. 1



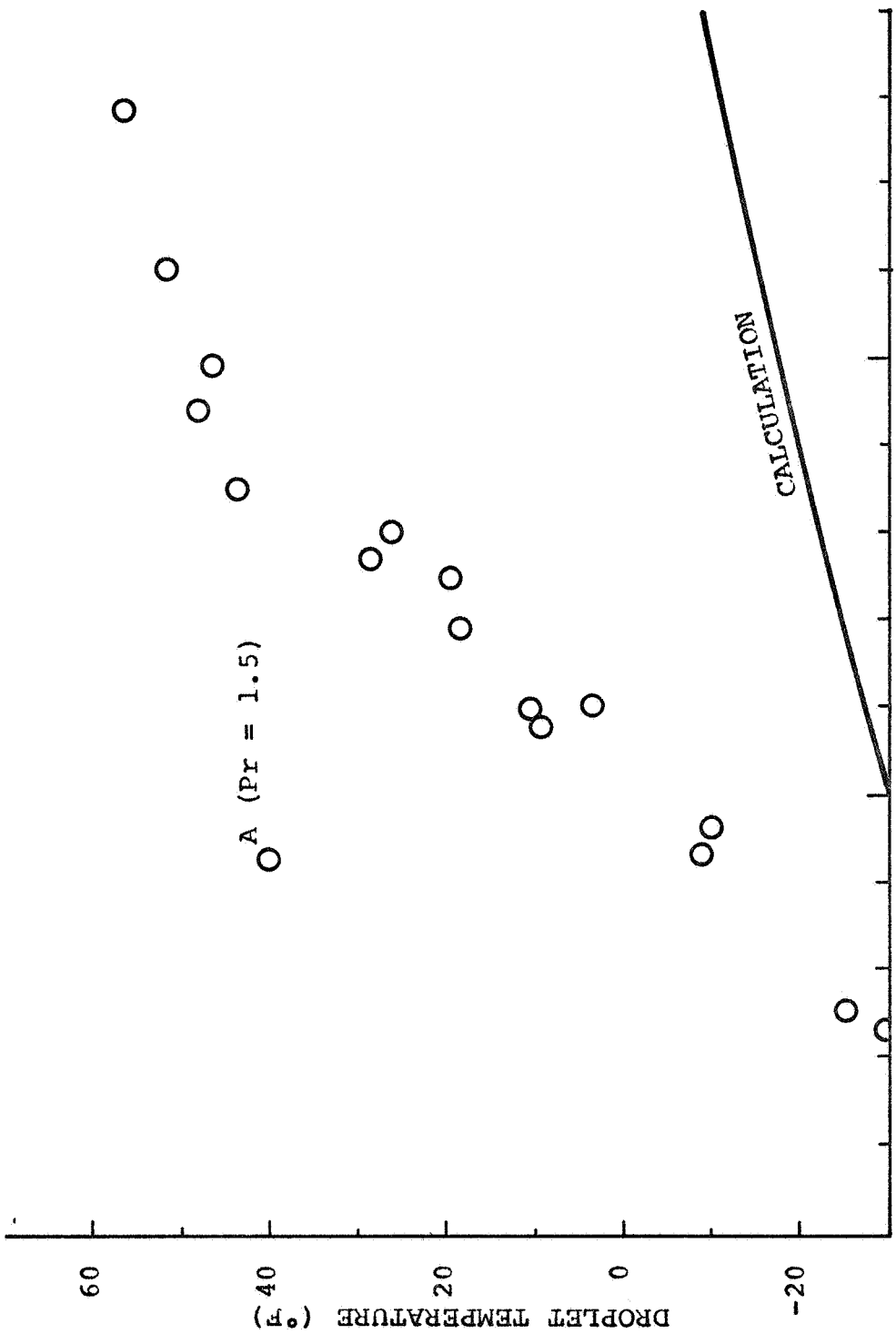
Calculated Vaporization History of CO_2 Drop in 815 °K Nitrogen at 72.9 atm.

Fig. 2



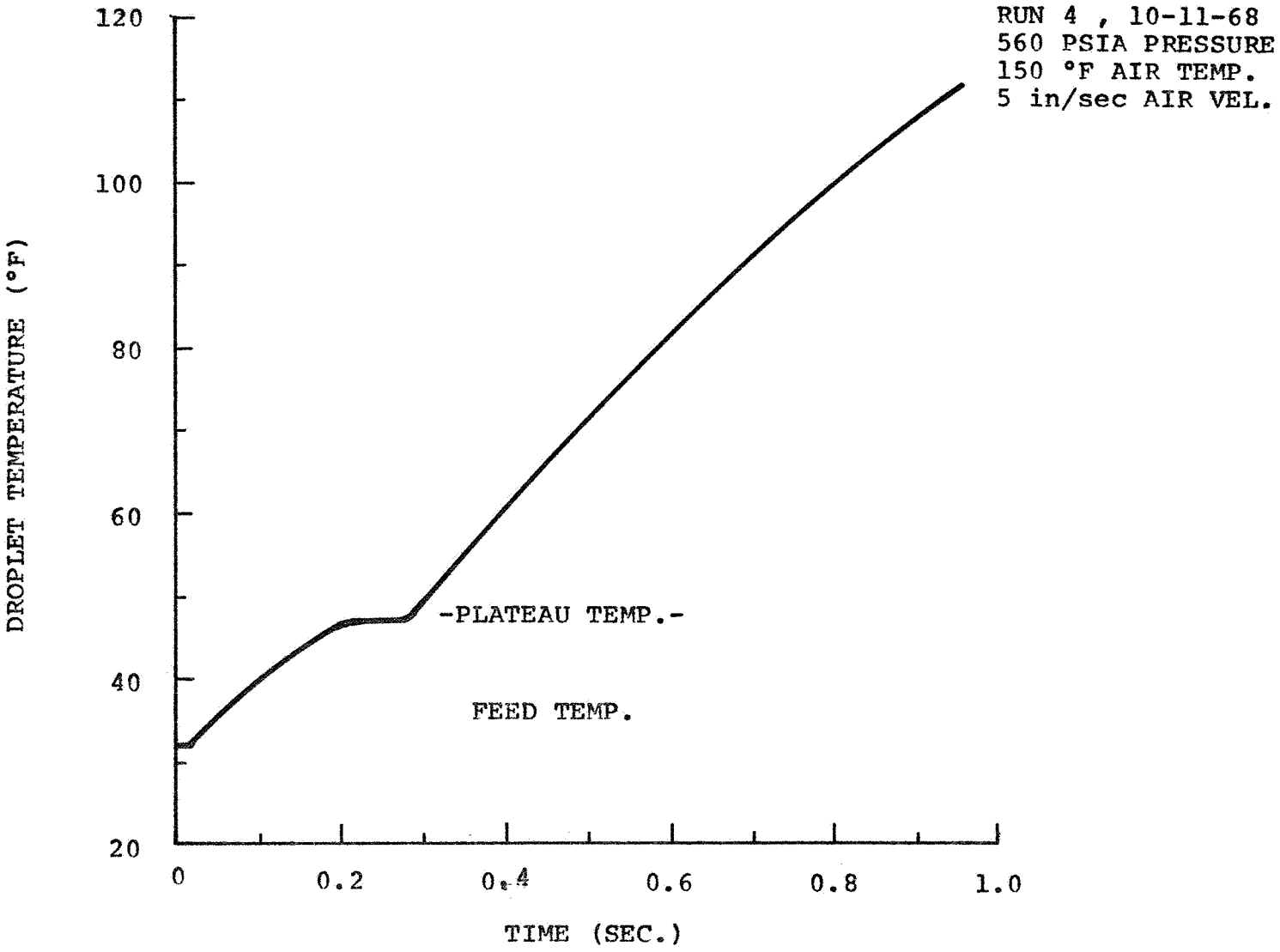
Liquid Temperatures of Water Droplets Vaporizing in Air.

Fig. 3



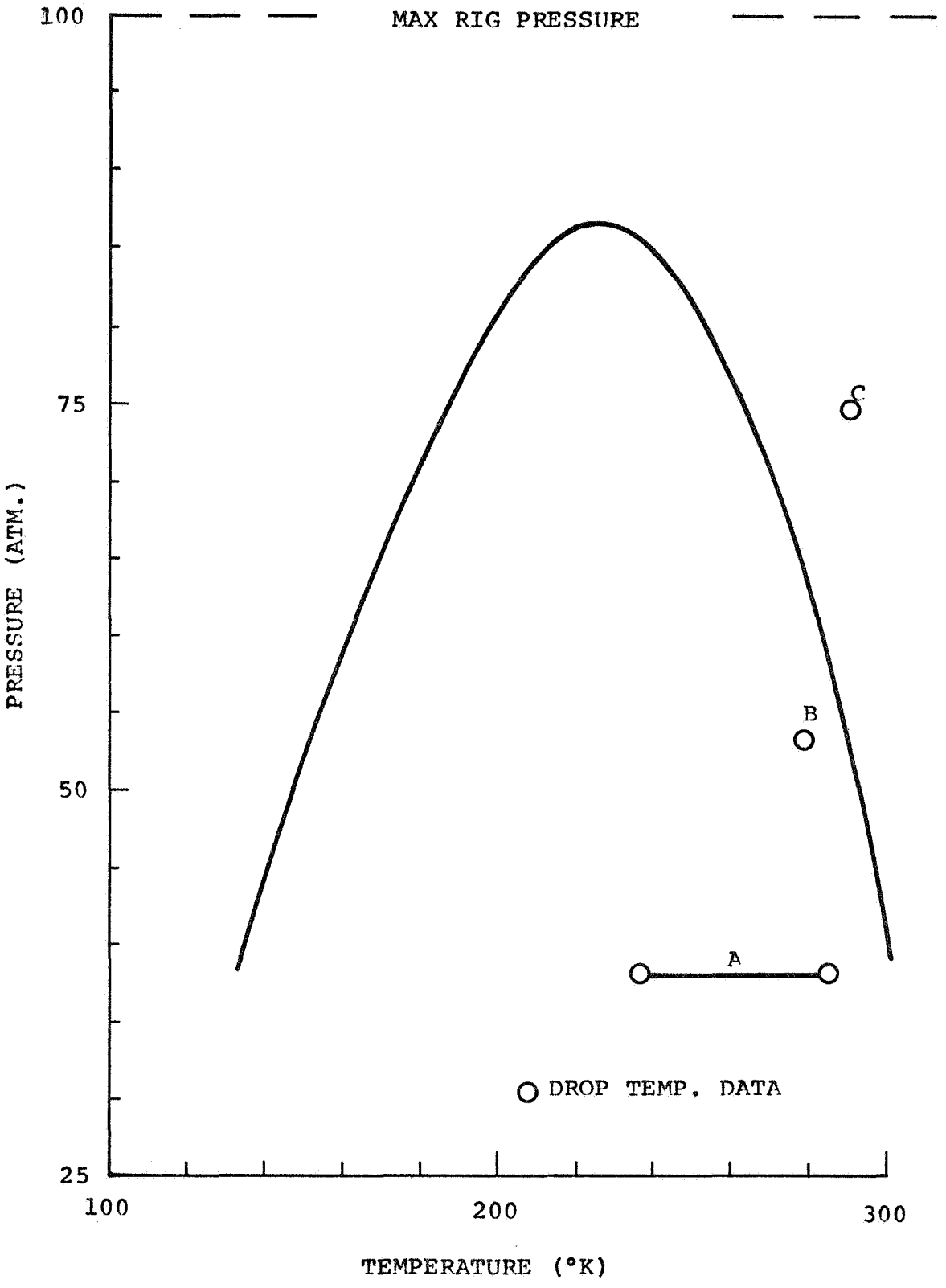
Liquid Temperatures of Fr-13 Droplets Vaporizing in Air at $P_{reduced} = 1.$

Fig. 4



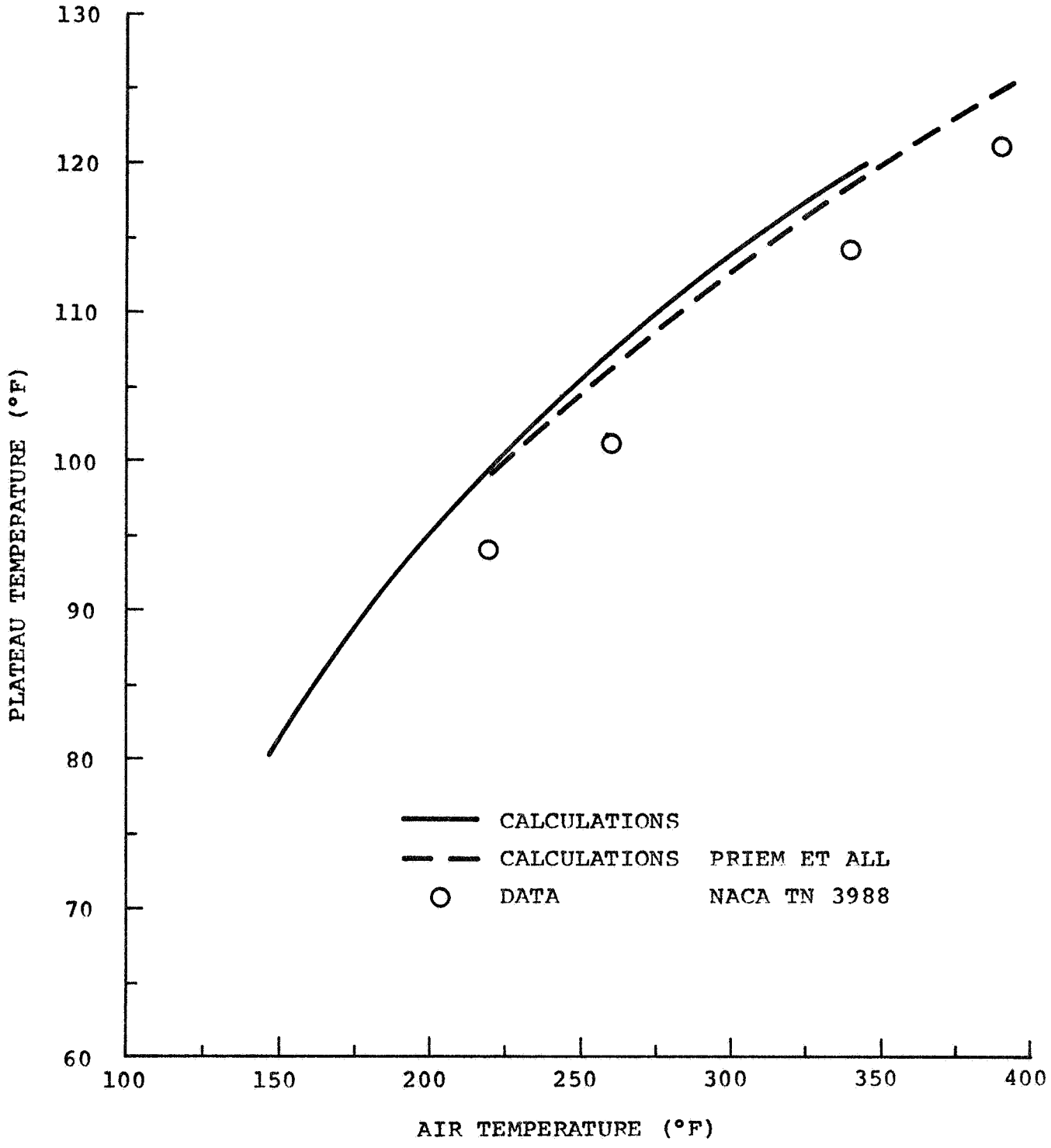
Measured Temperature History for Fr-13 Droplet Vaporizing in Air at 560 psia and 150 °F.

Fig. 5



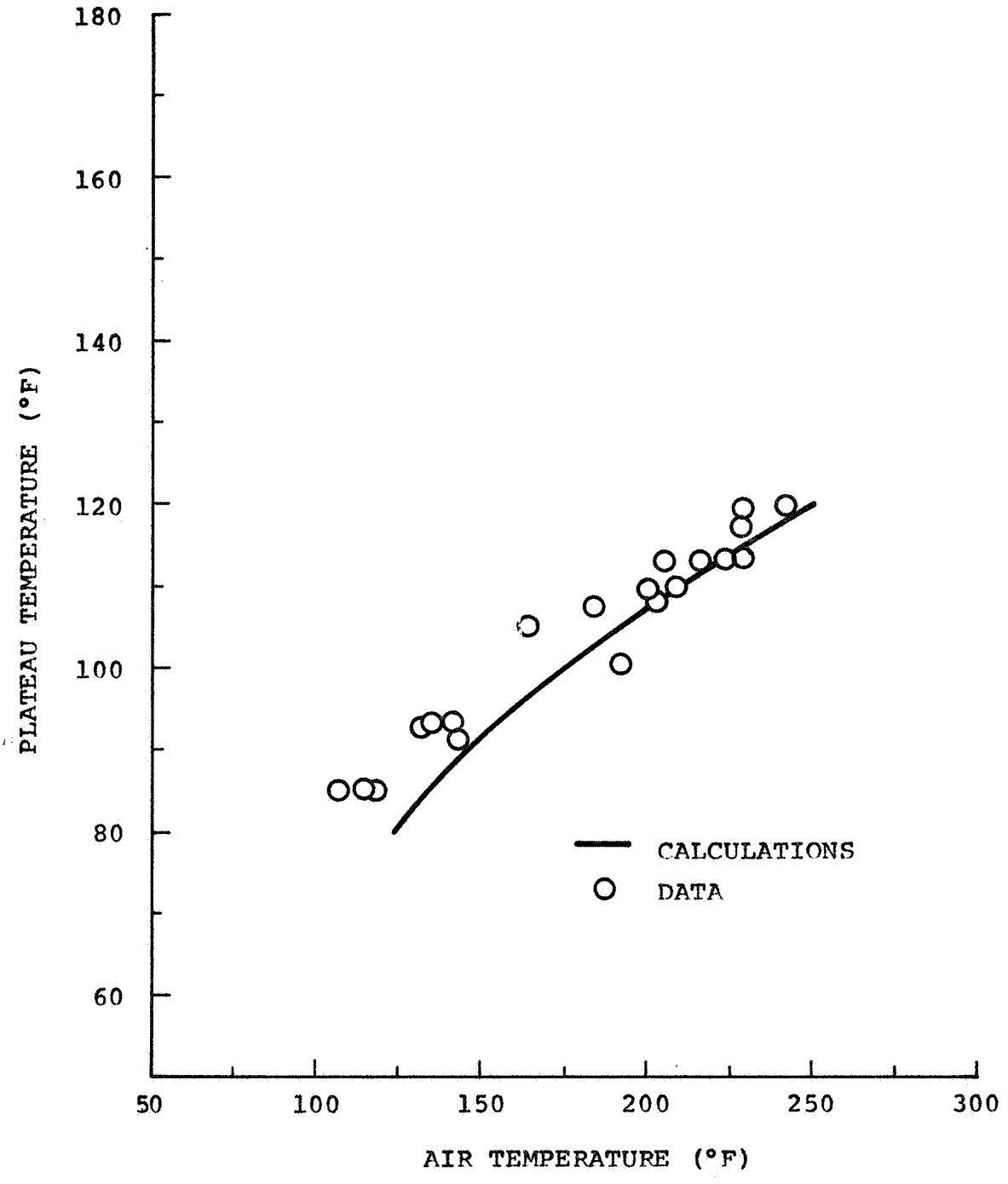
Calculated Pressure-Temperature Relation for Critical Mixtures of Fr-13/air.

Fig. 6



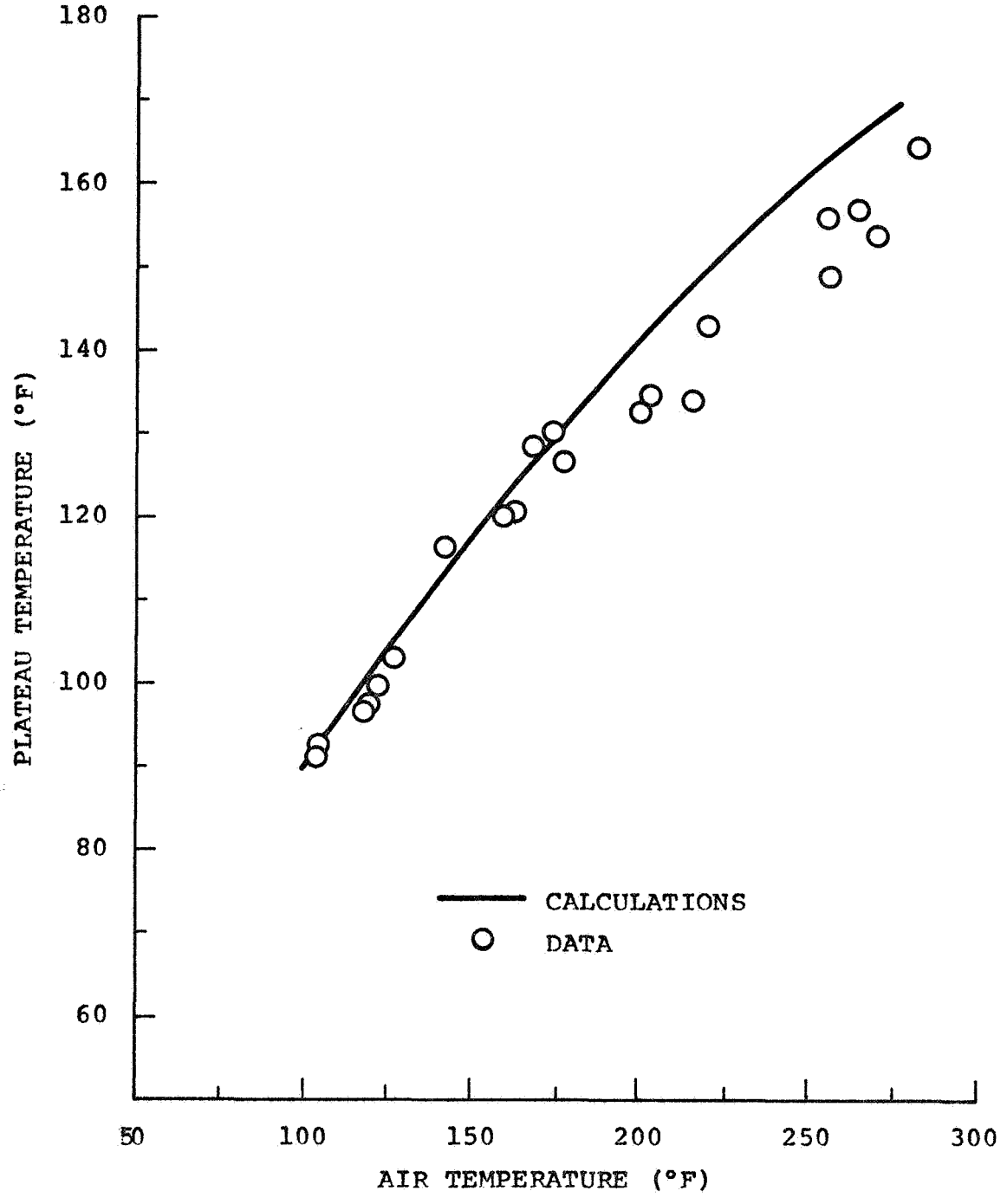
A Comparison of Data and Calculations for n-Heptane Droplets Vaporizing in Air at 1 atm. abs. Pressure. Data Taken from NACA TN 3988.

Fig. 7



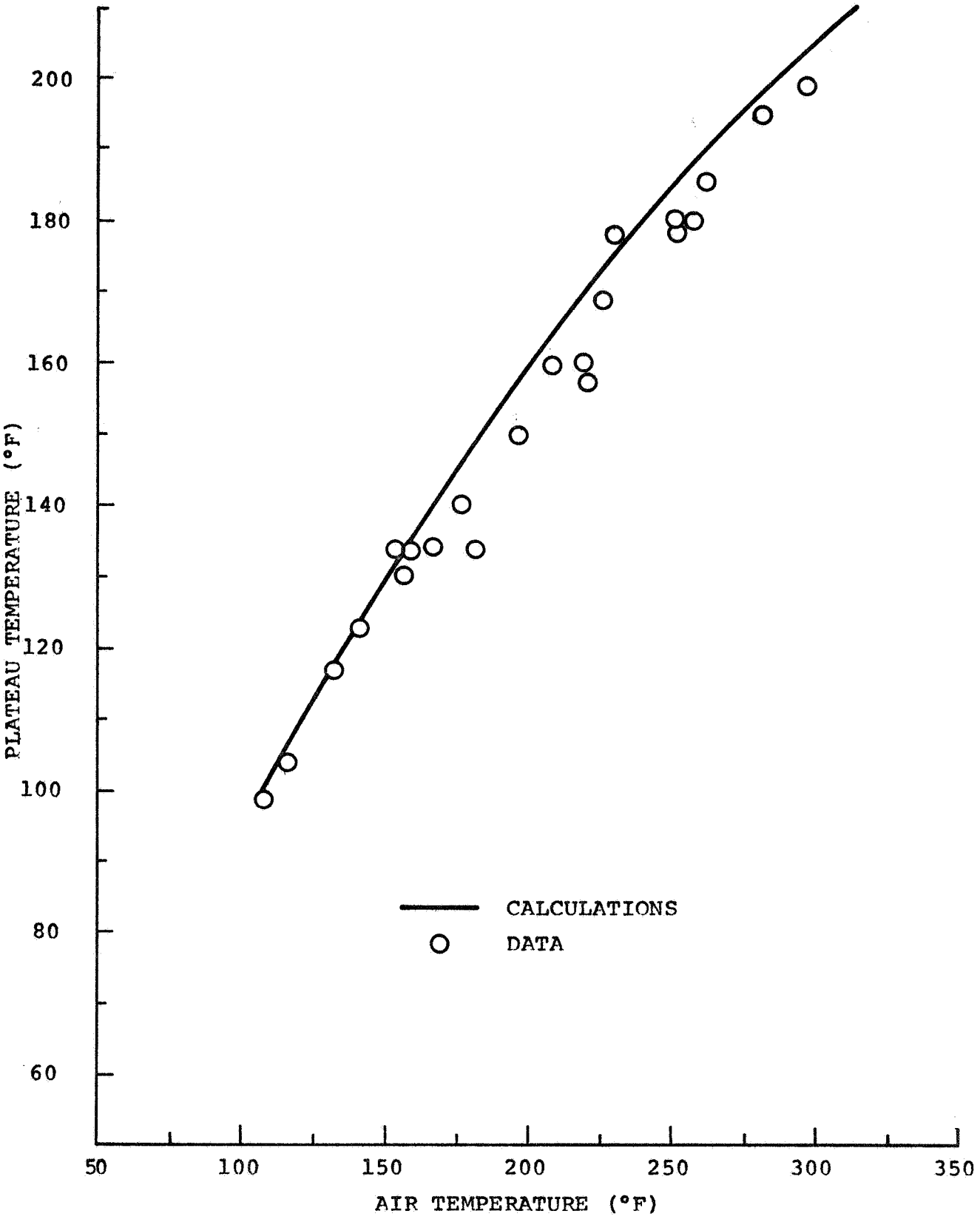
Liquid Temperatures of n-Heptane Droplets Vaporizing in Air at 1 1/2 atm. abs. Pressure.

Fig. 8



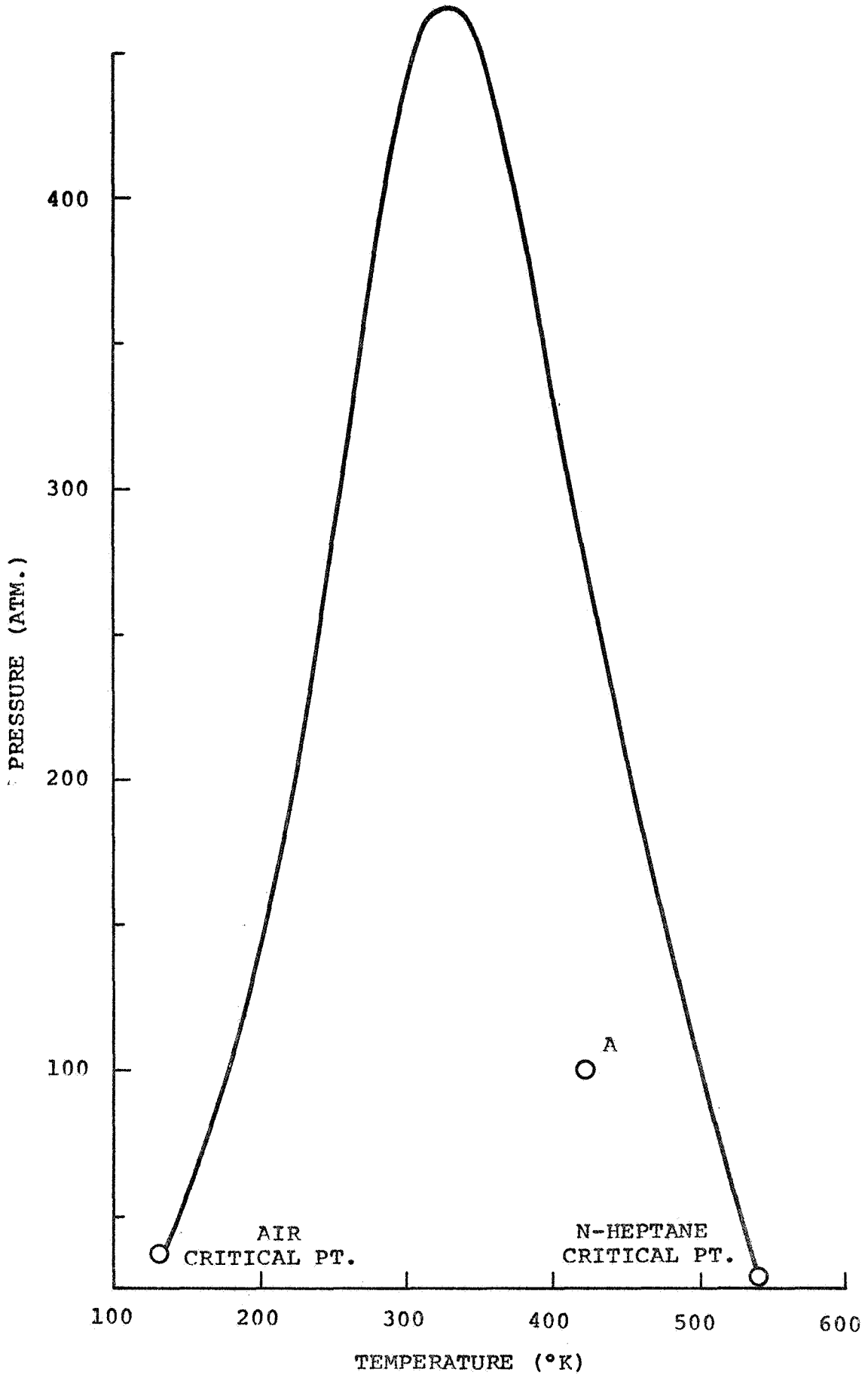
Liquid Temperatures of n-Heptane Droplets Vaporizing in Air at 5 atm. abs. Pressure.

Fig. 9



Liquid Temperatures of n-Heptane Droplets Vaporizing in Air at 10 atm. abs. Pressure.

Fig. 10



Calculated Pressure-Temperature Relation for
Critical Mixtures of n-Heptane/Air.
Fig. 11