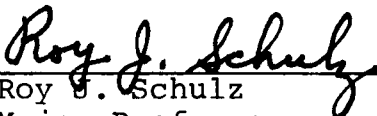
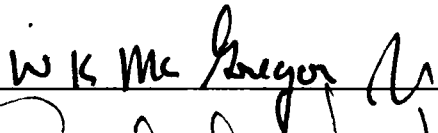
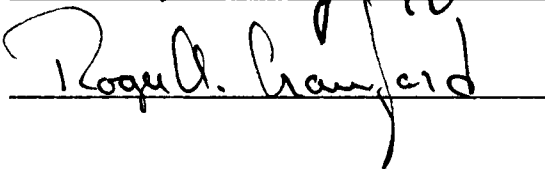


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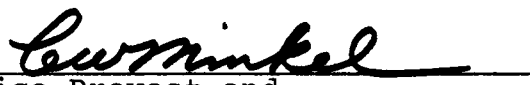
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THE MODELING OF LIQUID SPRAYS
FROM THE BASE OF CYLINDRICAL BODIES
IN SUBSONIC FLOW

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

John J. Melescue, Jr.

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ABSTRACT

The following thesis is an experimental and theoretical study on the flow field downstream of a cylindrical body aligned with a low Mach number air stream with liquid mass ejecting from the base of the body. The objectives of this study are two-fold: one, to modify a single-phase flow model of a flow field downstream of a cylindrical body to include liquid mass ejection at the base of the body; and two, to gather experimental data of such a flow field enabling an evaluation of the model to be performed. Experimental data from previous work were gathered which measured the total mass concentrations of the liquid and its vapor in the two-phase flow at 12 and 41 X/D downstream of the cylindrical body which measured 2.5 inches in diameter and 5 inches in length. Droplet diameters of the liquid spray were also measured at 72 X/D downstream of the body. Additional data were gathered on the pressures at the base of the body with no liquid mass ejection taking place. All data were taken in an air stream of Mach number 0.4 or less. These data were used to evaluate the computer model which used the local homogeneous flow (LHF) approximation theory, described by Faeth in Reference 1, to model the ejected liquid spray. The LHF theory assumes that the liquid spray is a continuum phase (dense gas) transported like heat or

concentration in the mixing process. Local density thus represents a mixture density lying between the liquid and freestream gas densities, and whose value depends on the local liquid mass fraction.

The LHF model evaluation showed that the overall model uncertainty for the predicted liquid mass fractions at the centerline was on the order of 150 percent. The model invariably overestimated the diameters of the spray at 12 X/D and almost invariably underestimated the spray diameters at 41 X/D. The spray diameters at 12 X/D were overestimated by the model by as much as 150 percent, and were underestimated at 41 X/D by as much as 45 percent. The base pressure coefficients predicted by the model with no liquid ejection at the base were overestimated by 200 percent, but were constant for the range of tunnel air velocities used in the test as they should be.

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NOMENCLATURE

A	Area, m^2
C	Conserved Species
C_p	Base Pressure Coefficient
D	Cylindrical Body Diameter, m
d_i	Droplet Diameter of i th Droplet, μm
d_{30}	Volumetric or Mass Mean Diameter, μm
H	Total Enthalpy, J/kg
k	Turbulence Kinetic Energy
$\dot{m}$	Mass Flow Rate, kg/sec
MF_A	Mass Fraction of Air
MF_L	Mass Fraction of Liquid
MM	Math Model
MW	Molecular Weight, kg/kg-mole
M_∞	Tunnel Flow Free-stream Mach Number
N	Total Number of Spray Droplets
n	Power of the Power Law Velocity Profiles
N_i	Number Density of Spray Droplets
P	Static Pressure, Pa
P_b	Body Base Static Pressure, Pa
PML	Prandtl Mixing Lengths for Circular Pipes
P_∞	Tunnel Flow Free-stream Total Pressure, Pa
q_∞	Air Flow Dynamic Pressure, Pa
r	Radial Distance From Centerline, m

R_{body}	Cylindrical Body Radius, m
RESOR_{ϕ}	Residual Source Terms for the Variable ϕ
R_{jet}	Jet Spray Radius, m
R_{δ}	Radial Distance from the Centerline to the Top of the Body Boundary Layer, m
R	Universal Gas Constant, J/(kg-mole-°K)
S_{ϕ}	Source Term for Scalars
T	Static Temperature, °K
u	Axial Velocity, m/sec
U_{max}	Jet Spray Maximum Velocity, m/sec
U_{mean}	Jet Spray Mean Velocity, m/sec
$U(r)$	Local Axial Velocity, m/sec
URF_{ϕ}	Under-relaxation Factor for the Variable ϕ
v	Radial Velocity, m/sec
V	Spherical Cap Velocity Vector, m/sec
$V(r)$	Local Radial Velocity, m/sec
w	Swirl Velocity, m/sec
X	Axial Distance Downstream of Cylindrical Body, m
y	Coordinate Axis Defined for the Body Boundary Layer Velocity Profiles
y'	Coordinate Axis Defined for the Jet Spray Velocity Profiles
Δr_b	Distance Between the First Two Radial Grid Lines Above the Body Boundary Layer, m

Δr_j	Distance Between the First Two Radial Grid Lines Below the Jet Spray Radius, m
$\Theta_{\max}$	Angle of the Spherical Cap Velocity Vector, rads
δ	Body Boundary Layer Thickness, m
μ_L	Laminar Viscosity
γ	Ratio of Specific Heats
ϕ	A Set of Transported Scalar Quantities
ϕ_{next}	Next Guess of Solution
ϕ_{prev}	Previous Guess of Solution
ψ	Static Density, kg/m^3
μ_t	Total, Turbulent, or Effective Viscosity
Γ_ϕ	Transport Term for Scalars
ϵ	Turbulent Dissipation Rate

CHAPTER 1

INTRODUCTION AND BACKGROUND

A major objective of modeling sprays is to reduce the time and cost of design and development. Substantial development and experience with the use of spray models will be required before they become reliable design tools. There are two common types of spray models: separated phase models, and local homogenous flow (LHF) models [1]. Separated phase models take into account the effects of finite rates of transport between the phases of two-phase flow; LHF models assume there is no velocity difference between the phases (no slip) and that the phases are in thermodynamic and chemical equilibrium. Separated phase models are generally needed for quantitative predictions of practical sprays and are of the greatest practical importance. However, it may be desirable to use an LHF model rather than a separated phase model in some cases, since, in principle, they require the least computational effort.

If LHF models are capable of meeting the uncertainty requirement of the model predictions, then using an LHF model has several distinct advantages over separated phase models. The major advantages of LHF models are that they

require a minimum amount of information about injector characteristics since the initial drop size and velocity distributions play no role in the computations [1]. This simplification is important because injector properties are difficult to obtain for spray nozzles and the performance of elegant separated phase models is discouragingly poor in the absence of accurate initial conditions at the injector exit [1]. A second advantage of LHF models is that the computations for sprays are essentially identical to computations for single-phase flows; therefore, existing computer codes can be employed which require shorter computation time than the more complex separated phase procedures. A third advantage is that LHF models require far fewer empirical constants than separated phase models, which reduces the "art" involved in making predictions [1]. A disadvantage is they do not model the correct physics and therefore provide a limited description of the flow field.

Other theoretical studies have been performed to model the dispersion of particles from spray nozzles in various environmental conditions. A comprehensive review performed by Faeth in Reference 1 summarizes the use of LHF models of sprays. The applications include the evaporation or combustion of sprays in air with and without swirl, including axisymmetric, boundary layer flows and swirling flows with recirculation. The experimental methods used to

evaluate the LHF theory for noncombusting flows included ejecting a liquid spray vertically downward into still air. Generally, LHF spray models overestimate the rate of development of the flow, but do provide a reasonable first estimation of the extent and character of the spray profile [1-7]. However, one rare exception showed that LHF models have also underestimated flow widths due to enhanced turbulent dispersion of the liquid droplets [8].

The present study involves modeling a flow field downstream of a cylindrical body in a low Mach number air stream with liquid mass ejection at the base of the body (Fig. 1). This flow pattern involves axisymmetric boundary layer flows with separation and recirculation, and will provide additional evaluation of LHF spray models. Considered in the calculations are the effects of the spray radius and velocity, and the body boundary layer velocity profile. Model performance is correlated to various factors which include the simulated altitude and Mach number of the external flow field, the droplet diameters measured in the experiments, and the liquid ejection flow rate of the spray. The modeling of such flows may be useful in the design of many practical devices in resolving flow problems such as the effect of an airplane wake on the lateral dispersion of aerial sprays.

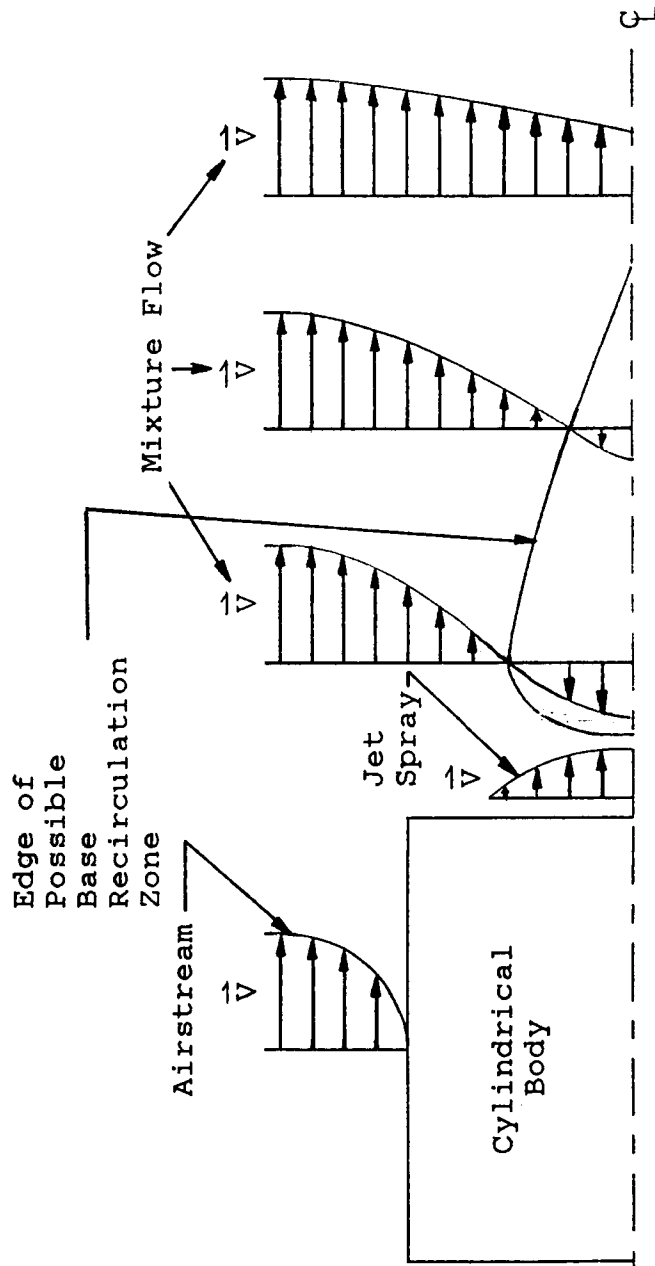


Figure 1. Flow Field Around Cylindrical Body with Liquid Mass Ejection at the Base

The mathematical model used in this study utilizes widely accepted methods for computing the convective fluxes of transported scalar quantities and the varying levels of turbulence. It is based on the Pantankar-Spalding "SIMPLE" method, the main ideas of which have been embodied into the "TEACH" computer program [9], which is a single-phase flow code, and utilized in other axisymmetric problems [10-12]. Further advances to the TEACH algorithm have been made and applied elsewhere [13-16]. The k - ϵ turbulence model is commonly accepted as representing a reasonable compromise between complexity and realism for single-phase recirculating flow fields [17]. A detailed description of the theoretical foundation of the model is presented in Chapter 4.

CHAPTER 2

PURPOSE OF RESEARCH AND APPROACH

The purpose of this study is two-fold: one, to modify a single-phase flow model of the flow field downstream of a cylindrical body to include liquid mass ejection at the base of the body; and two, to use existing experimental data of such a flow field enabling an evaluation of the model to be performed. This will not only provide an evaluation of the overall flow model, but will also provide an evaluation of the LHF modeling technique for an application to sprays into wake-type flows. Experimental data were gathered on the flow field downstream of a cylindrical body aligned with a low Mach number air stream with liquid mass ejecting from the base of the body. The cylindrical body measured 5 inches long and was 2.5 inches in diameter. The experimental data consists of total mass concentrations of the ejected liquid and its vapor at 12 and 41 X/D downstream of the cylindrical body, droplet diameters of the liquid spray, and base pressures at the base of the body with no liquid mass ejection [18,19]. The boundary layer on the cylindrical body and the initial flow profiles of the ejected liquid were not defined in the experimental data. Therefore, they were treated as variables in the model and were varied in

order to obtain the best approximation of the model predictions when compared to the experimental data for one randomly chosen test case. Boundary layers were modeled to simulate power law type profiles which might be obtained for round-nosed bodies, and wake type profiles which might be obtained for sharp-edged-nosed bodies. The boundary layer thickness was related to the body radius since it is physically dependent on the displacement effect of the body. After optimization of the predictions were obtained for the mass concentration at 12 and 41 X/D for a specific test case, the boundary layer and liquid spray profiles were fixed and the remainder of the test cases were run using these same profiles. Finally, an evaluation of the utility and physical adequacy of the model was performed. Since this computational flow model utilizes the LHF theory to model the liquid spray, which assumes single-phase gaseous flow, a determination was also made of the accuracy and limitations of the physical submodels used in the code for flow and transport in two-phase phenomenon. Since the flow system modeled in this study is general in nature, no tolerances for the model accuracy could be determined which would deem this model "useful" since these tolerances are functions of the physical applications. However, since a major objective of analytical models is to reduce the time and cost of design and development, it is felt that a

tolerance of 20% is reasonable for this model to have the potential for design applications. A comment on the iteration control and convergence of the code is given, plus recommendations for further study.

CHAPTER 3

EXPERIMENTAL METHODS

3.1 MASS CONCENTRATIONS OF THE EJECTED LIQUID3.1.1 Test Apparatus

The T-6 wind tunnel at Arnold Engineering Development Center (AEDC) was one of the facilities used to produce the air velocities and simulated altitudes for this experiment, as shown in Fig. 2 [19]. A liquid injection strut carried liquid n-butyl alcohol to a nozzle mounted on the downstream base of a cylindrical body located on centerline of the tunnel (Fig. 3). The tunnel total air temperature was set at about 0°C to prevent evaporation of the liquid droplets. The mass concentration of the liquid was measured radially across the tunnel flow at 12 and 41 X/D. A sampling probe was used to sample air-alcohol concentrations and was jacketed with steam lines to vaporize all the entrained liquid entering the probe (Fig. 4). Analysis of the air/vaporized liquid mixture was accomplished using a Beckman Model 402 hydrocarbon analyzer which uses the flame ionization method of detection to determine the mass concentration of the liquid. The Beckman Model 402 can measure the liquid mass concentration within a 5% uncertainty. The system schematic is shown in Fig. 5. When

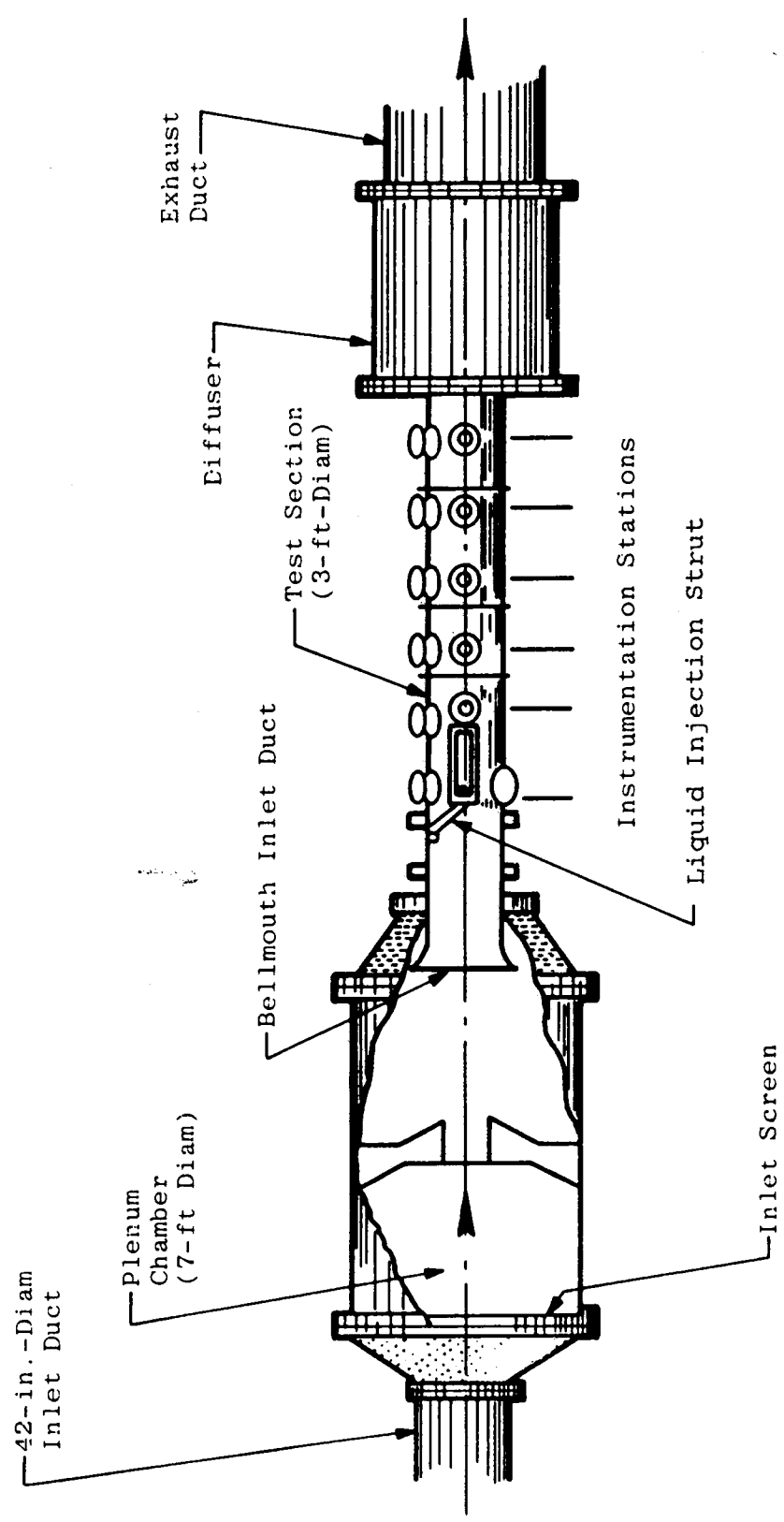


Figure 2. Research Cell T-6

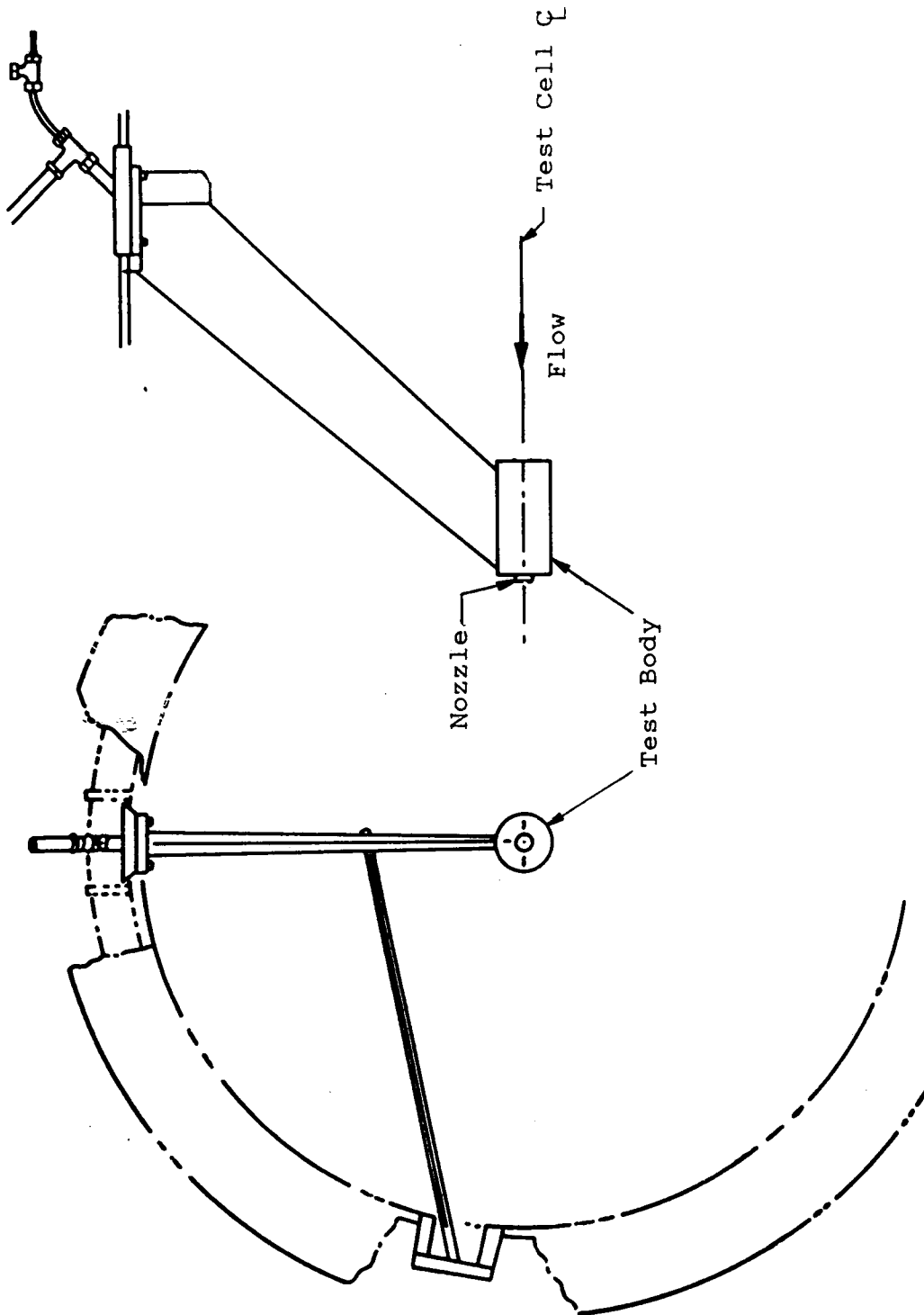


Figure 3. Liquid Injection Strut

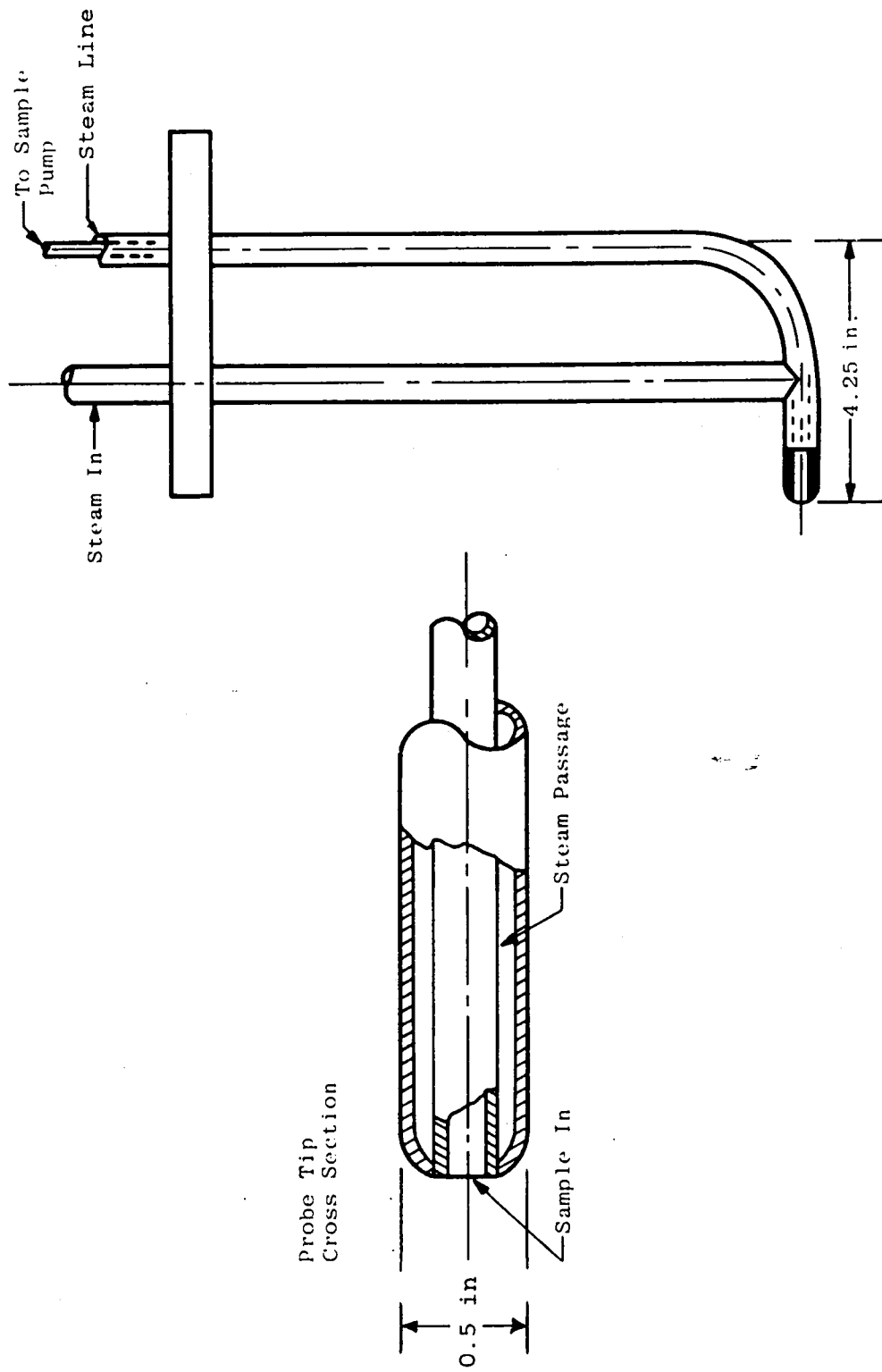


Figure 4. Liquid Mass Sampling Probe

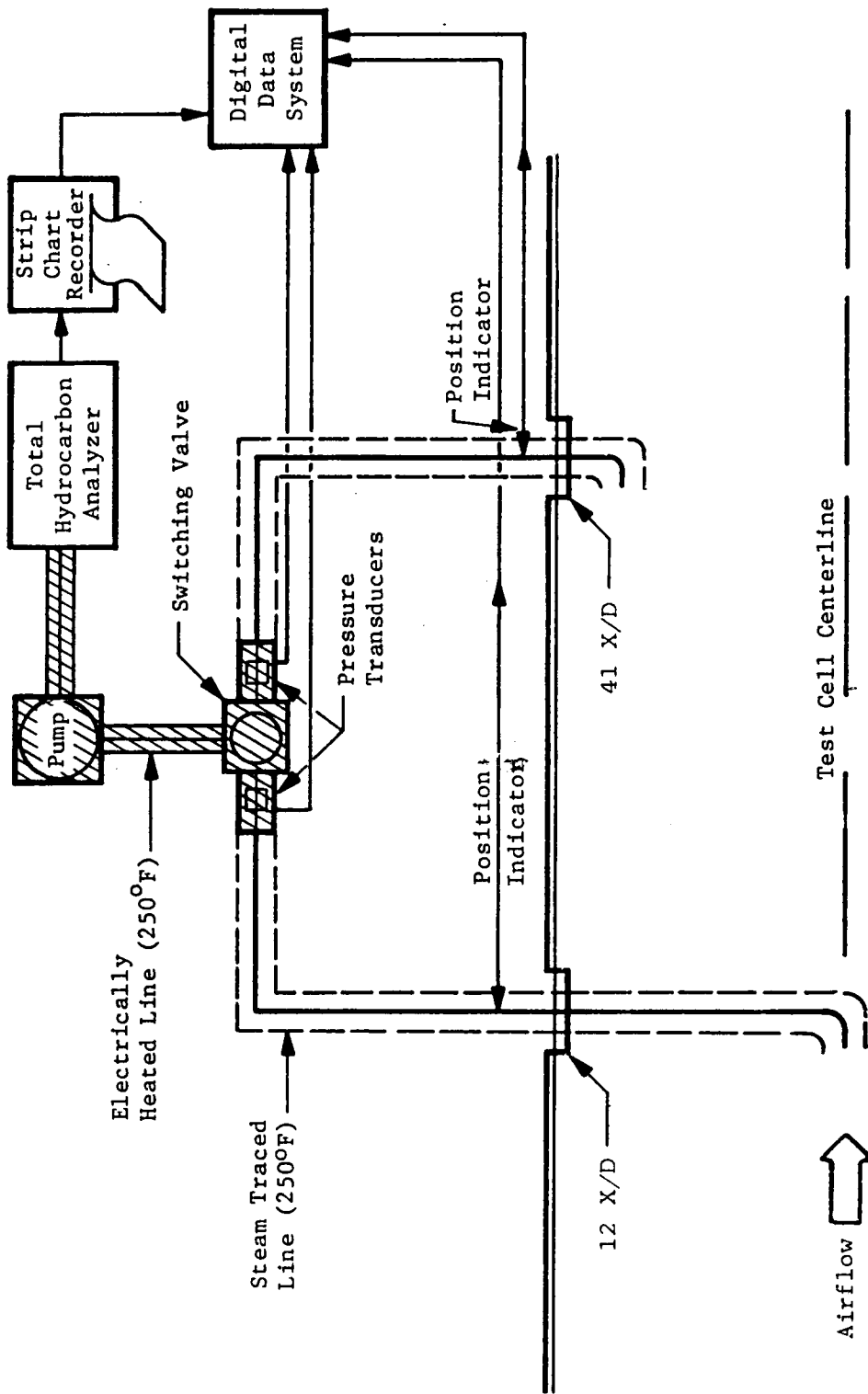


Figure 5. Liquid Mass Sampling System

taking mass samples at 12 and 41 X/D, the probe was traversed radially from the outermost flow boundary to the centerline, stopping at discrete radial locations.

3.1.2 Experimental Data

Mass concentrations of the ejected liquid specie were measured under various tunnel conditions, liquid injection flow rates, and a variety of liquid injection nozzles. Table 1 summarizes the conditions and test article configurations which were used to obtain these data. The probe sample was not isokinetic, but experimental data was analyzed to assure that experimental profiles summed up to give the same total mass of liquid as was injected.

3.2 LIQUID SPRAY AND PARTICLE CHARACTERIZATION

3.2.1 Test Apparatus

Two systems were used to measure and verify the droplet size distribution of the liquid spray. The primary measurement system employed the Forward Scatter Spectrometer Probe (FSSP) built by Particle Measuring Systems, Inc (Fig. 6). The FSSP system is designed to measure droplet size distributions in the diameter range of 0.5 to 48 μm . The design principle is based on measuring the absolute intensity of small forward angle light scattering by single particles. The system utilizes a laser beam light source

TABLE 1. TEST CASE CONDITIONS

Case	Type of Orifice	Orif. Dia., cm	Alt, m	Air Vel., m/sec	Tunnel Mach No., M_∞	T, °K	P_∞ , Pa	Nozzle Mass Flow, kg/sec	Liquid Ejection Velocity, m/sec
1	Standard single-hole	.1143	1494	83.8	0.262	255	84627	.0113	13.6
2	"	"	8778	129.9	0.406	"	31774	.0120	14.4
3	"	.2261	10607	112.8	0.352	"	24074	.0493	15.2
4	"	"	1507	120.4	0.376	"	84475	.0515	15.8
5	"	"	1524	120.0	0.375	"	84323	.0314	9.7
6	Gas atom., single-hole tran ¹	.3175	1554	112.5	0.351	"	83996	.0531	8.3
7	"	"	1524	36.0	0.112	"	84323	.0518	8.1
8	Gas atom., multi-hole tran ²	.0406	1478	36.6	0.114	"	84788	.0214	17.0
9	"	"	1478	38.4	0.120	"	84788	.0491	39.0

¹Gas atomizer, single-hole transverse²Gas atomizer, multi-hole transverse, 12 holes, each of .0406 cm diameter³Fuel Flow Velocity calculated from $V=m/A$, where $=0.810$ gm/cm

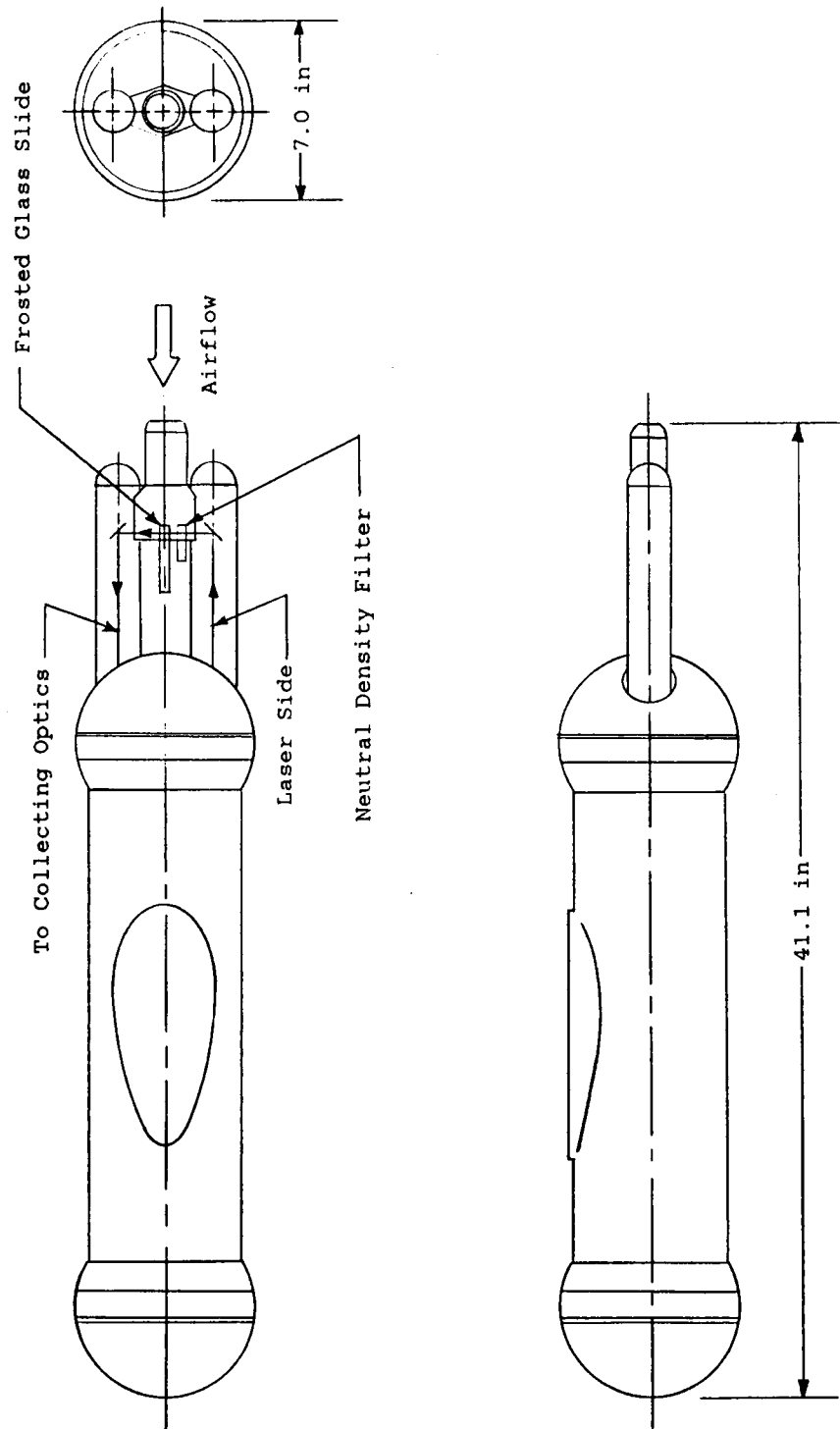


Figure 6. Forward Scatter Spectrometer Probe

whose diameter was much smaller than the droplet diameter so that only one droplet would scatter the light at a time. The system was precalibrated using known droplet diameters prior to its installation in the T-6 test cell. The optics and detector are housed within the probe which was mounted 15 ft. downstream of the cylindrical body in the test cell (Fig. 7).

To obtain a level of confidence in the FSSP measurements, the Fiber Optics System (FOS) developed at AEDC was also used to measure the droplet size distributions of the liquid spray [20]. The FOS system is capable of measuring droplet diameters in the range of 3 to 90 μm . In the technique employed, a magnified shadow image of a particle passing through the laser beam is focused onto a linear array consisting of 32 optical fibers. The passage of a particle image across the array triggers a number of photo-detector modules, corresponding to the number of fibers covered by the shadow, thus recording the relative size of the particle. If either of the end fibers is shadowed, an error signal is generated to indicate the image was not adequately centered or was too large for the array. A schematic of the system is shown in Fig. 8.

The mass mean diameters, d_{30} , presented in this thesis are from distributions recorded by the FSSP droplet sizer.

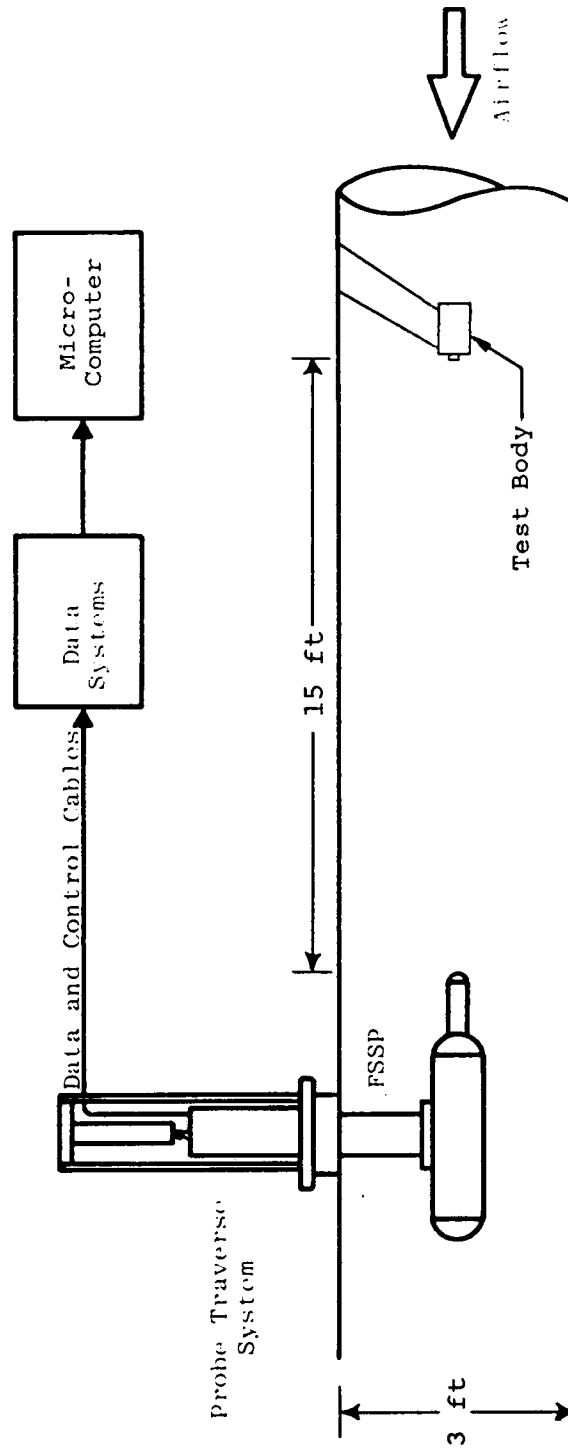


Figure 7. Model FSSP Particle Sizer Installation

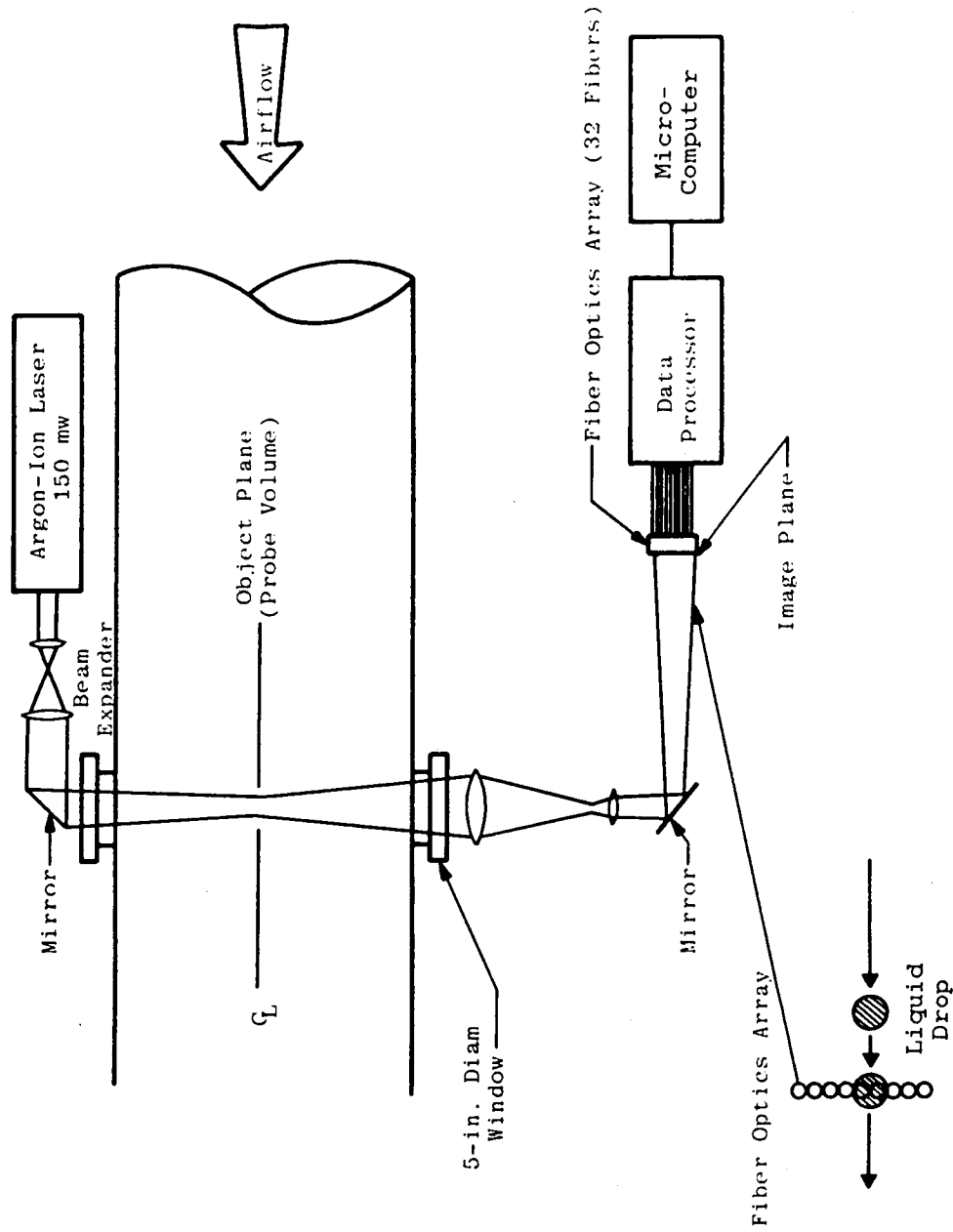


Figure 8. Fiber Optics Particle Sizing System (FOS)

The droplet count size distributions of the FOS particle sizer generally agreed with the FSSP measurements [19].

3.2.2 Experimental Data

When the liquid specie was ejected from the cylindrical body, it broke up into a spray of liquid droplets. Characteristics of the liquid sprays were studied under a range of tunnel air velocities, altitudes, and nozzle parameters such as orifice sizes, liquid injection pressures and flow rates, and atomizing air pressures and flow rates. The volumetric or mass mean diameter d_{30} was used to quantify the size distribution of the liquid droplets. The d_{30} is defined as

$$d_{30} = \frac{\sum d_i^3 N_i}{N}^{\frac{1}{3}} \quad (1)$$

where N_i is the number density of particles with diameters d_i , and N is the sum $N = \sum N_i$.

If the spray had the same total number of droplets, but each droplet had the diameter d_{30} , the spray would contain the same total volume or mass of liquid as does the actual spray; i.e., the arithmetic average mass is contained in a droplet diameter d_{30} .

The data on droplet diameters will be presented in this study, but it is beyond the scope of the study to attempt to

analytically predict the spray and droplet characteristics. Rather, the numerical model was based on the Local Homogeneous Flow (LHF) theory described and discussed in Chapter 4. However, these droplet diameter data were used to better understand the results of the comparisons between the model and experimental data.

3.3 BASE PRESSURE

3.3.1 Test Apparatus

The gas injection nozzle opening on the downstream base of the cylindrical body was refitted to be used as a port to measure the cylindrical body base pressure under conditions of different tunnel air velocities. The cylindrical test body was mounted in a Ground-Level Test Stand (GLTS) low-speed wind tunnel facility as shown in Fig. 9 [18]. The wind tunnel test section was 20 in. in diameter and could produce air velocities from 140 to 320 ft/sec.

3.3.2 Experimental Data

Cylindrical body base pressures were measured on the downstream end of the body for various tunnel air velocities. This was done by attaching the liquid injection nozzle opening to a pressure transducer. Hence, no liquid spray injection took place during the measurement of base pressures. The base pressure coefficient is given by

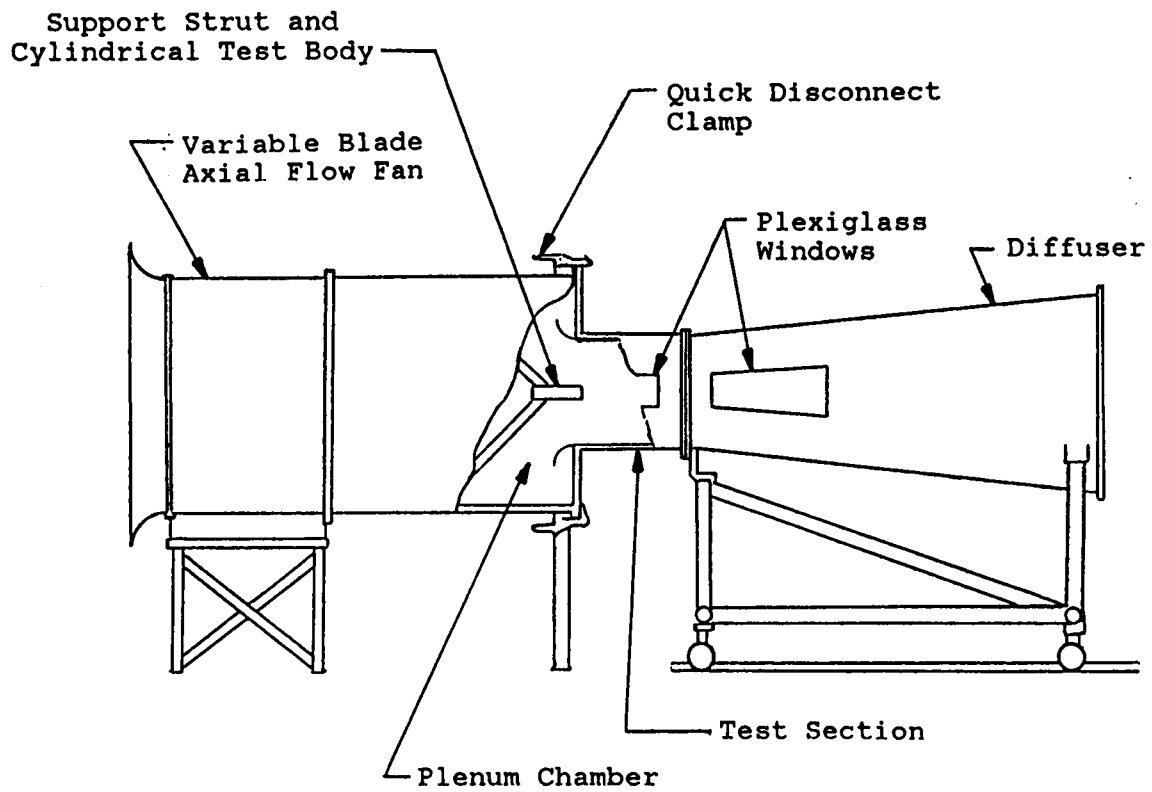


Figure 9. Ground-Level Test Stand (GLTS) Wind Tunnel Facility

$$C_p = \frac{-(P_\infty - P_b)}{q} = \frac{-2(P_\infty - P_b)}{P_\infty \gamma M_\infty^2} \quad (2)$$

where P_∞ and M_∞ are the tunnel flow free-stream pressure and Mach number in the plane of the body, P_b is the base pressure, γ is the ratio of specific heats for air (taken to be 1.4), and q is the air flow dynamic pressure. The base pressure coefficients for the various tunnel flow conditions are tabulated in Table 2 [18].

TABLE 2. BASE PRESSURE COEFFICIENT

Case	Tunnel Air Velocity m/sec	Tunnel Mach No., M_∞	Tunnel Wall Pressure P_∞ , Pa	Cyl Body ¹ Wall Base Pres $P_\infty - P_b$, Pa	EXP ² Base Pressure Coeff	MM ³ Base Pressure Coeff
10	47.50	0.143	96530	86.2	-0.0624	-0.2420
11	62.48	0.187	95841	134.5	-0.0802	-0.2391
12	74.98	0.225	95151	202.7	-0.0601	-0.2402
13	91.74	0.276	93772	321.3	-0.0643	-0.2419
14	97.23	0.292	93083	468.9	-0.0844	-0.2427

¹Cylindrical Body

²Experiment

³Math Model

Since the base pressures given correspond to the cases where there was no liquid being ejected from the base, these data will be compared to numerical calculations of flow over the cylindrical body without base mass ejection. This

permits a level of calibration of the numerical method to be performed.

CHAPTER 4

THEORY

4.1 MODEL DESCRIPTION

The model used in the present study is a Navier-Stokes solver developed for axisymmetric flow fields, with or without swirl. The code provides theoretical predictions of the distributions of velocity (3 components), static and total enthalpy, one-species concentration, temperature, pressure, density, and turbulence kinetic energy with its rate of dissipation. It is based on the Patankar-Spalding Semi-Implicit, Pressure-Linked Equations (SIMPLE) method, the main ideas of which have been embodied into the 1974 Imperial College TEACH (Teaching Elliptic Axisymmetric Characteristics Heuristically) computer program [9]. Advances to the TEACH code have been made elsewhere and applied to other 2-D problems [13-16]. The current code will treat variable density and subsonic, mildly compressible flow, since it is based on a variable density pressure-correction field equation. For compressible flows, the energy equation must be solved in addition to the momentum equations. Details of the way the SIMPLE method preserves continuity while yielding pressure gradient source terms for the momentum equations are provided by Patankar

[12]. Additional information on the numerical solution of 2-D and axisymmetric problems via the primitive pressure-velocity approach is presented in References 10-12.

The code used in the present study originated from the STARPIC code, described in Reference 17, which modeled flow through circular pipes of varying areas, including those shown in Fig. 10. Modifications were made to the STARPIC code prior to this study to simulate a flow with combustion and variable density. It was further modified to simulate flow around a cylindrical body by changing the boundary conditions as necessary. This study then involved further modifications in order to simulate liquid mass ejection at the base of the body. The LHF approximation theory was used to model the liquid jet spray and is discussed in section 4.1.2.

4.1.1 Theoretical Foundation of Model

This code, being based on the Patankar-Spalding SIMPLE algorithm, solves iteratively a set of transport equations for momentum, energy, and species. All transport equations are written in differential form in cylindrical coordinates, that is, in terms of radial distance r and axial distance x as

$$\frac{1}{r} \left[\frac{\partial}{\partial x} (\psi u r \phi) + \frac{\partial}{\partial r} (\psi v r \phi) - \frac{\partial}{\partial x} (r \Gamma_{\phi} \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial r} (r \Gamma_{\phi} \frac{\partial \phi}{\partial r}) \right] = S_{\phi} . \quad (3)$$

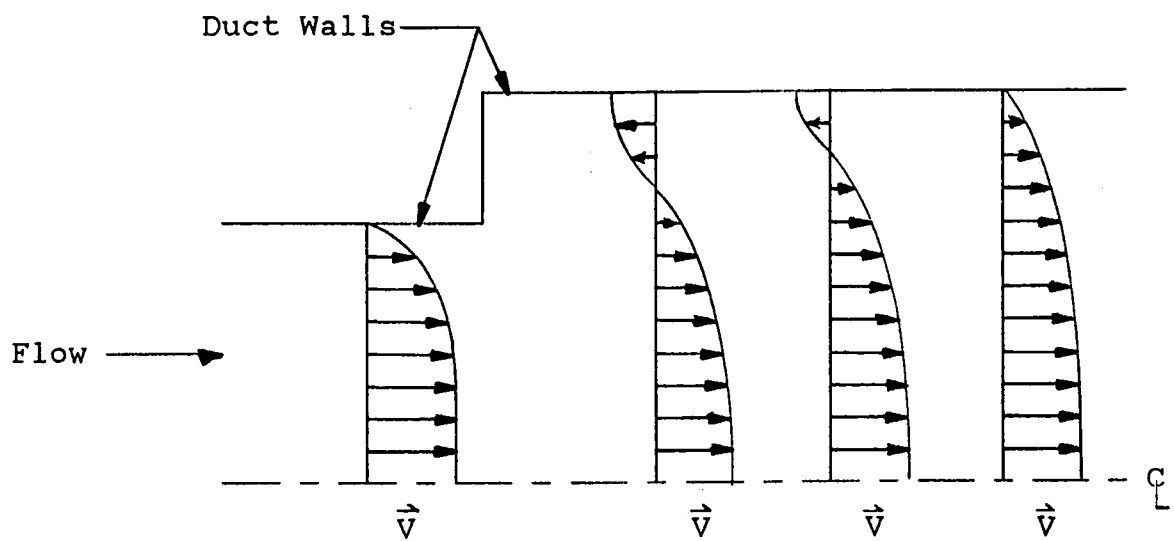


Figure 10. Example of a Flow Field Which the Original Code, STARPIC, was Designed to Simulate

The variable ϕ represents a set of transported scalar quantities. In the present study, ϕ represents the following set of variables:

$$\phi = (u, v, w, H, C, k, \epsilon)$$

These variables are defined in Table 3 where their corresponding transport (Γ_ϕ) and source (S_ϕ) terms are indicated.

In Table 3, μ_t is the total viscosity or effective viscosity, and ϕ_H , ϕ_C , ϕ_k , and ϕ_ϵ are Prandtl numbers or Schmidt numbers appropriate for each variable. The terms S_u , S_v , and G are defined as,

$$S_u = \frac{\partial}{\partial x} (\mu_t \frac{\partial u}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r} (r \mu_t \frac{\partial v}{\partial x}) \quad (4)$$

$$S_v = \frac{\partial}{\partial x} (\mu_t \frac{\partial u}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial r} (r \mu_t \frac{\partial v}{\partial r}) \quad (5)$$

$$G = \mu_t \{ 2 [(\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial r})^2 + (\frac{v}{r})^2] + (\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x})^2 + [r \frac{\partial}{\partial r} (\frac{w}{r})]^2 + (\frac{\partial w}{\partial x})^2 \} \quad (6)$$

The equation for total viscosity is defined by,

$$\mu_t = \frac{C_\mu \psi k^2}{\epsilon} + \mu_L \quad (7)$$

TABLE 3. VARIABLES IN THE MODEL

Transport Variable	Coefficient, Γ_ϕ	Source Term, S_ϕ
u. Axial Velocity	μ_t	$-\partial p / \partial x + S^u$
v. Radial Velocity	μ_t	$-\partial p / \partial r + e w^2 / r - 2\mu_t v / r^2 + S^v$
w. Swirl Velocity	μ_t	$-e v w / r - w / r^2 \partial / \partial r (r \mu_t)$
H. Total Enthalpy	μ_t / σ_H	0
C. Conserved Species	μ_t / σ_C	0
k. Turbulence Kinetic Energy	μ_t / σ_k	$G = C_D e^\epsilon$
ϵ . Turbulence Dissipation Rate	μ_t / σ_ϵ	$C_1 \epsilon G - C_2 \epsilon e^2 / k$

where μ_L is the laminar viscosity given by Sutherland's formula or selected as some convenient reference value, depending on the nature of the problem to be studied numerically. The values of the constants ϕ_H , ϕ_C , ϕ_k , ϕ_e , C_D , C_1 , C_2 , and C_μ used in the present study are listed in Table 4. The density of the gas mixture was calculated from the perfect gas law,

$$\psi = \frac{P}{(R/MW_{\text{mix}}) T} \quad (8)$$

where MW_{mix} is the molecular weight of the mixture. The equation for MW_{mix} is given by

$$\frac{1}{MW_{\text{mix}}} = \frac{MF_{\text{air}}}{MW_{\text{air}}} + \frac{MF_{\text{jet}}}{MW_{\text{jet}}} \quad (9)$$

The theoretical solution procedure for the set of equations of the form given by equation (4) is an iterative finite-difference solution procedure. The differential equations are reduced to linearized algebraic equations in finite-difference quantities by integration of the differential equations over finite volumes that make discrete the space of the physical problem. The linearized algebraic equations are solved by iterative use of a line-by-line, tridiagonal matrix reduction procedure. The linearized algebraic equations are cast in a form containing "residuals". A solution is said to occur by "convergence"

TABLE 4. NUMERICAL VALUE OF CONSTANTS IN THE MODEL

Parameter	Numerical Value
σ_H	0.9
σ_C	0.9
σ_k	1.0
σ_ϵ	$K^2 / [(C_2 - C_1) \sqrt{C_\mu}]$
C_D	1.0
C_1	1.44
C_2	1.92
C_μ	0.09
K	0.4187 (von Karman's Constant)

of the set of algebraic equations when the maximum of the residuals is reduced to some arbitrary, small numerical value that, in the present study, was 0.005. Details of the discretion procedure, the linearization scheme, and the tridiagonal matrix solver are presented in general terms in Patankar's book [12]. Further discussion of the simulation and solution of swirling flows in practical applications can be found in Reference 21.

The standard, single-phase, high-turbulence-Reynolds number version of the k - ϵ turbulence model, based on two transport equations, one for k and one for ϵ , was employed in this code to calculate the distributions of turbulence kinetic energy, k , and its isotropic rate of dissipation, ϵ . With k and ϵ computed at each point of the field, the turbulent viscosity was given by equation (7). The values of the coefficients and constants used in the k and ϵ transport equations are presented in Table 4, and are typical for steady, turbulent flows with recirculation. This k - ϵ turbulence model is commonly accepted as representing a reasonable compromise between complexity and realism for single-phase recirculating flow fields [17]. In the present study, the sprays created by the liquid injection were very dilute-phase, since the amount of mass injected was so small compared to the air flow rate. Thus, the

single-phase k - ϵ model was deemed adequate. Dense-phase spray flows require additional k - ϵ modeling.

Further details on the simulation and solution of numerical computations for turbulent flow is discussed in references 22 and 23. Since the turbulence model is the main mechanism for the mixing rates between the liquid spray and external air flow, this study will provide a level of calibration of this turbulence model for dilute-phase flows with recirculation such as those which exist in the base recirculation zone.

4.1.2 Description of LHF Approximation Theory

The LHF modeling technique, as described by Faeth in Reference 1, assumes that the interphase transport rates between the phases of two-phase flow are infinitely fast. Therefore, both phases have the same velocity and are in thermodynamic equilibrium at each point in the flow. This implies that the liquid spray is actually treated as a fully atomized spray where the particle sizes are infinitely small. This being the case, the initial drop size and velocity distributions of the jet spray play no role in the computations. The spray is then treated as a perfect gas as described below.

4.2 MODELING OF THE INITIAL FLOW FIELDS

4.2.1 Initial Density of the Jet Spray

The application of the LHF modeling technique was used to model the spray particles being ejected from the base of the cylindrical body in an external subsonic flow field. In accordance with the LHF theory, the spray was assumed to be a vaporized single-phase gas where the perfect gas law was applicable. It was also assumed that the pressure and temperature of the spray were equal to the free-stream pressure and temperature of the external flow. The entire flow field was assumed to be adiabatic and isothermal (constant total enthalpy). These assumptions allowed for the spray density to be calculated using the perfect gas law,

$$\psi_{\text{jet}} = \frac{P}{(R/MW_{\text{jet}}) T} \quad (10)$$

where MW_{jet} is the molecular weight of the jet spray of n-butyl alcohol, C_4H_{10} .

The mass flow rate of the jet spray in the computational model was set equal to that in the experimental data.

4.2.2 Initial Velocity Profile of the Jet Spray

4.2.2.1 Power Law Velocity Profiles

In accordance with the LHF approximation theory, the ejector characteristics were not modeled. Therefore, the initial jet spray radius and velocity profile used in the model were treated as variables. After an initial jet spray radius was chosen, the jet spray mean velocity was then determined from the conservation of mass equation,

$$U_{\text{mean}} = \frac{\dot{m}_{\text{jet}}}{\psi_{\text{jet}} \int_{r=0}^{r=R_{\text{jet}}} 2\pi r_i dr_i} \quad (11)$$

where U_{mean} is the jet spray mean velocity, and $\dot{m}_{\text{jet}}$ is the jet spray mass flow rate as measured from the experimental data. For the power law velocity distributions of the jet spray, the maximum velocity was related to the mean velocity and the power n by,

$$U_{\text{max}} = U_{\text{mean}} / \frac{2n^2}{(n+1)(2n+1)} \quad (12)$$

where n is the power of the velocity power law profile, and U_{max} is the maximum jet velocity of the jet spray. Finally, the local velocity U was related to the maximum velocity by the power law relation,

$$\frac{U(r)}{U_{\max}} = \left(\frac{y'}{R_{\text{jet}}} \right)^{\frac{1}{n}} \quad (13)$$

Fig. 11 shows the coordinate axis for y' defined for the jet spray. The power law exponent could be varied from 2 for a laminar type spray profile to 12 or greater for a fully turbulent velocity profile.

4.2.2.2 Spherical Cap Velocity Profiles

Spherical cap velocity profiles were also evaluated for the jet spray. First, the maximum spray angle, $\theta_{\max}$, was chosen. In Fig. 12, $\theta_{\max}$ is shown schematically as the angle at which the spherical cap intersects the body base. The velocity V is fixed by the mass flow rate of the jet spray and the $\theta_{\max}$ chosen. The velocity V was determined by iterating until the mass flow rate equalled that of the experimental data,

$$\dot{m}_{\text{jet}} = \psi_{\text{jet}} \int_{r=0}^{r=R_{\text{jet}}} 2\pi r_i dr_i U(r) \quad (14)$$

where the local axial velocity $U(r)$ was calculated from,

$$U(r) = V \cos\left(\sigma_{\max} \frac{r}{R_{\text{jet}}}\right) \quad (15)$$

Once the iteration process yielded the correct mass flow of the jet spray, the radial velocity was then calculated from

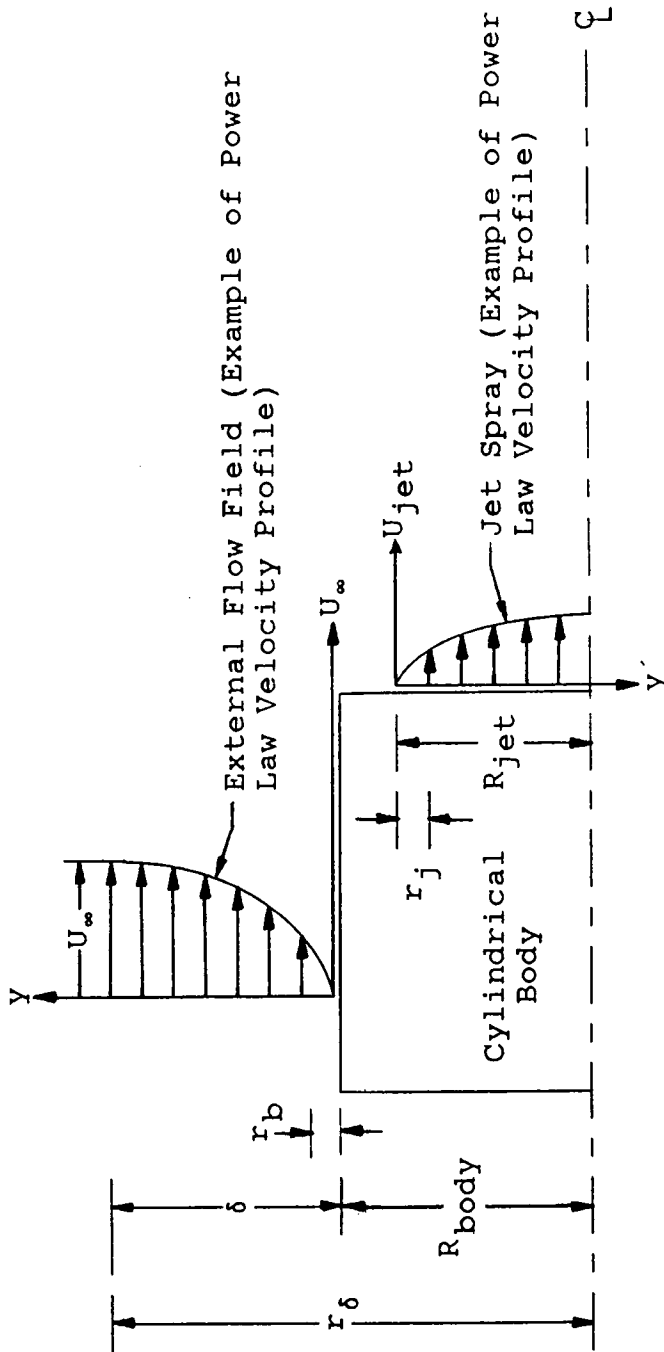


Figure 11. Coordinate Axis for y and y' Defined for the Initial Profiles of the External Flow Field or Jet Spray, Respectively

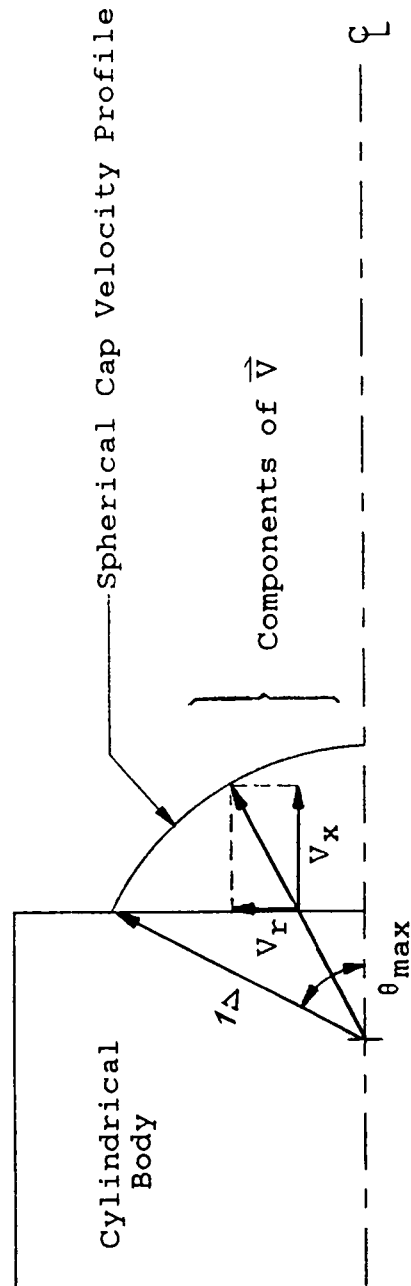


Figure 12. Spherical Cap Velocity Profiles for the Jet Spray

$$V(r) = V \sin(\sigma_{\max} \frac{r}{R_{\text{jet}}}) \quad . \quad (16)$$

4.2.3 Initial Velocity Profile of the Body Boundary Layer

4.2.3.1 Power Law Velocity Profiles

For the free-stream air flow along the body surface, the boundary layer thickness was related to the body radius since it is physically dependent on the displacement effect of the body. The mass which is displaced by the body is given by,

$$\psi_{\infty} U_{\infty} A_{\infty} = 2\pi \int_0^{R_{\delta}} \psi U r dr \quad (17)$$

where R_{δ} is the radial distance to the top of the boundary layer (Fig. 11). From the power law relation,

$$\frac{U}{U_{\infty}} = \left(\frac{r - R_{\text{body}}}{\delta} \right)^{\frac{1}{n}} \quad \text{for } r \geq R_{\text{body}} \quad (18)$$

one can solve for U and then substitute into equation (17) to obtain

$$\int_{R_{\text{body}}}^{R_{\delta}} \psi U_{\infty} \left(\frac{r - R_{\text{body}}}{\delta} \right)^{\frac{1}{n}} = \frac{1}{2} \psi_{\infty} U_{\infty} R_{\text{body}} \quad . \quad (19)$$

Assuming incompressible flow and integrating, one obtains the quadratic equation,

$$\delta^2 + \left(\frac{2n+1}{n+1}\right) R_{\text{body}} \delta - \left(\frac{2n+1}{2n}\right) R_{\text{body}}^2 = 0 \quad . \quad (20)$$

Solving the quadratic equation,

$$\delta = \frac{R_{\text{body}}}{2} \left(\frac{2n+1}{n+1}\right) \left[-1 \pm \sqrt{1 + \frac{2(n+1)^2}{n(2n+1)}}\right] \quad . \quad (21)$$

Since $y=r-R_{\text{body}}$, equation (21) only applies on the body between $r=R_{\text{body}}$ and $r=R_{\text{body}} + \delta$. In this form, δ is completely parameterized by n , for a given value of R_{body} , resulting in Table 5 which relates n to δ/R_{body} .

TABLE 5. POWER LAW BOUNDARY LAYER RELATIONSHIPS

n	δ/R_{body}
2	0.56
3	0.52
7	0.46
12	0.44
∞	0.41

The local velocities in the boundary layer were then calculated by,

$$\frac{u(y)}{U_{\infty}} = \left(\frac{y}{\delta}\right)^{\frac{1}{n}} \quad (22)$$

where Fig. 11 shows the coordinate axis for y defined for the body boundary layer.

4.2.3.2 Wake Velocity Profiles

A similar derivation for wake-type profiles can also be done to relate the boundary layer thickness to the body radius. The derivation begins with equation (17), that is,

$$2\pi \int_0^{R_\delta} \psi U r dr = \psi_\infty U_\infty \pi R_{\text{body}}^2 \quad . \quad (23)$$

For incompressible flow, the equation can be reduced to

$$\int_0^\delta U r dr = U_\infty R_{\text{body}}^2 / 2 \quad . \quad (24)$$

The wake profiles used were assumed to be of the form

$$U = U_\infty \left[\frac{1}{2} - \frac{1}{2} \cos \left(\pi \frac{r - R_{\text{body}}}{\delta} \right) \right] \quad \text{for } r \geq R_{\text{body}} \quad , \quad (25)$$

$$U = 0 \quad \text{for } r < R_{\text{body}} \quad . \quad (26)$$

By substituting equation (25) into (24) the integral becomes,

$$\int_{R_{\text{body}}}^{R_\delta} \left[\frac{1}{2} - \frac{1}{2} \cos \left(\pi \frac{r - R_{\text{body}}}{\delta} \right) \right] r dr = R_{\text{body}}^2 / 2 \quad . \quad (27)$$

By substituting $\delta = R_\delta - R_{\text{body}}$ into equation (27) and then performing the integration, a quadratic expression for δ results,

$$\left(\frac{1}{4} + \frac{1}{\pi^2}\right)\delta^2 + \left(\frac{R_{\text{body}}}{2}\right)\delta = R_{\text{body}}^2 / 2 \quad . \quad (28)$$

Solving the quadratic for δ results in a single value,

$$\delta = 0.667 R_{\text{body}} \quad . \quad (29)$$

4.2.4 Initial Turbulence Kinetic Energy, Viscosity, and Turbulence Energy Dissipation of the Jet Spray and External Flow Field

The initial profiles for the remaining parameters are presented below for both the jet spray and the external flow field. These parameters include the turbulent kinetic energy and its rate of dissipation, and the turbulent viscosity.

Since the flow fields over the cylindrical body and in the body base recirculation zone were not determined in the experiment, the Prandtl mixing lengths (PML) for circular pipes were therefore utilized to calculate the initial profiles for the turbulence kinetic energy and the turbulence energy dissipation. These assumptions were utilized due to the similarity of the geometry involved to serve as substitutions for experimental data. The PML's are defined as,

$$\frac{PML}{\delta} = 0.14 - 0.08 \left(1 - \frac{Y}{\delta}\right)^2 - 0.06 \left(1 - \frac{Y}{\delta}\right)^4 \quad (30)$$

for the body B.L.,

$$\frac{PML}{R_{jet}} = 0.14 - 0.08 \left(1 - \frac{Y}{\delta}\right)^2 - 0.06 \left(1 - \frac{Y}{\delta}\right)^4 \quad (31)$$

for the jet spray,

where δ is the boundary layer thickness on the surface of the body, and R_{jet} is the jet spray radius. Fig. 11 illustrates the coordinate axis y and y' if referring to the external flow field or the jet spray, respectively. The derivation of the PML and its application in deriving the turbulence kinetic energy, dissipation energy, and viscosity is discussed by Schlichting [24]. The profiles for the turbulence kinetic energy were calculated by,

$$k(y) = \frac{PML^2(y)U^2(y)}{y^{2n^2}} \quad \text{for the body B.L.,} \quad (32)$$

$$k(y') = \frac{PML^2(y')U^2(y')}{y'^{2n^2}} \quad \text{for the jet spray,} \quad (33)$$

where U is the local velocity and n is the order used in the power law velocity profile.

Since k may be singular when y or y' equals zero, this special case was taken into account by:

For $y = 0$ or $r = R_{\text{body}}$, set $k(R_{\text{body}}) = k(R_{\text{body}} + \Delta r_b)$
for the body B.L., (34)

For $y' = 0$ or $r = R_{\text{jet}}$, set $k(R_{\text{jet}}) = k(R_{\text{jet}} - \Delta r_j)$
for the jet spray, (35)

where Δr_b and Δr_j are one grid spacing closest to the body or the edge of the jet, respectively; see Fig. 11.

The turbulent viscosity could then be calculated by,

$$\mu_t(y) = 0.09 \psi(y) \sqrt{k(y)} \text{PML}(y) \quad \text{for the body B.L.,} \quad (36)$$

$$\mu_t(y) = 0.09 \psi(y') \sqrt{k(y')} \text{PML}(y') \quad \text{for the jet spray.} \quad (37)$$

Also, the turbulence energy dissipation was calculated by,

$$\epsilon(y) = \frac{0.09 \psi(y) k^2(y)}{\mu_t(y)} \quad \text{for the body B.L.,} \quad (38)$$

$$\epsilon(y') = \frac{0.09 \psi(y') k^2(y')}{\mu_t(y')} \quad \text{for the jet spray.} \quad (39)$$

For the external flow field in the free-stream outside the body boundary layer, all variables were set equal to those at the boundary layer edge where $U(y) = U_\infty$. Of course, all variables in the body base where $R_{\text{jet}} < r < R_{\text{body}}$ were initialized to zero.

4.3 OUTPUTS FROM THE ANALYTICAL MODEL

The main outputs in the model are axial velocity, radial velocity, pressure, turbulence kinetic energy, turbulence energy dissipation, viscosity, density, the gas constant, temperature, "liquid" mass fraction, enthalpy, and mass flow rates of the liquid and air.

4.4 DESCRIPTION OF MESH

The grid geometries used model planar and axisymmetric (cylindrical) flows. The construction of the grid is arbitrary, and is typically rectangular but with nonuniform spacing between nodes. A cylindrical polar coordinate system was used. This system, shown fitted to the cylindrical body, is illustrated in Fig. 13. An explanation of how variables are stored and calculated at each grid node of this mesh is presented in Reference 17, and details of the special merits of this staggered grid system have been reported previously [9,13].

The initial velocity profiles of the external flow field were assigned across a vertical mesh line at an arbitrarily chosen finite distance upstream of the base of the body. This is shown in Fig. 14 along with the general dimensions of the computational domain. Along this first mesh line, the axial and radial velocities, the pressure, temperature and density, and the turbulence kinetic energy

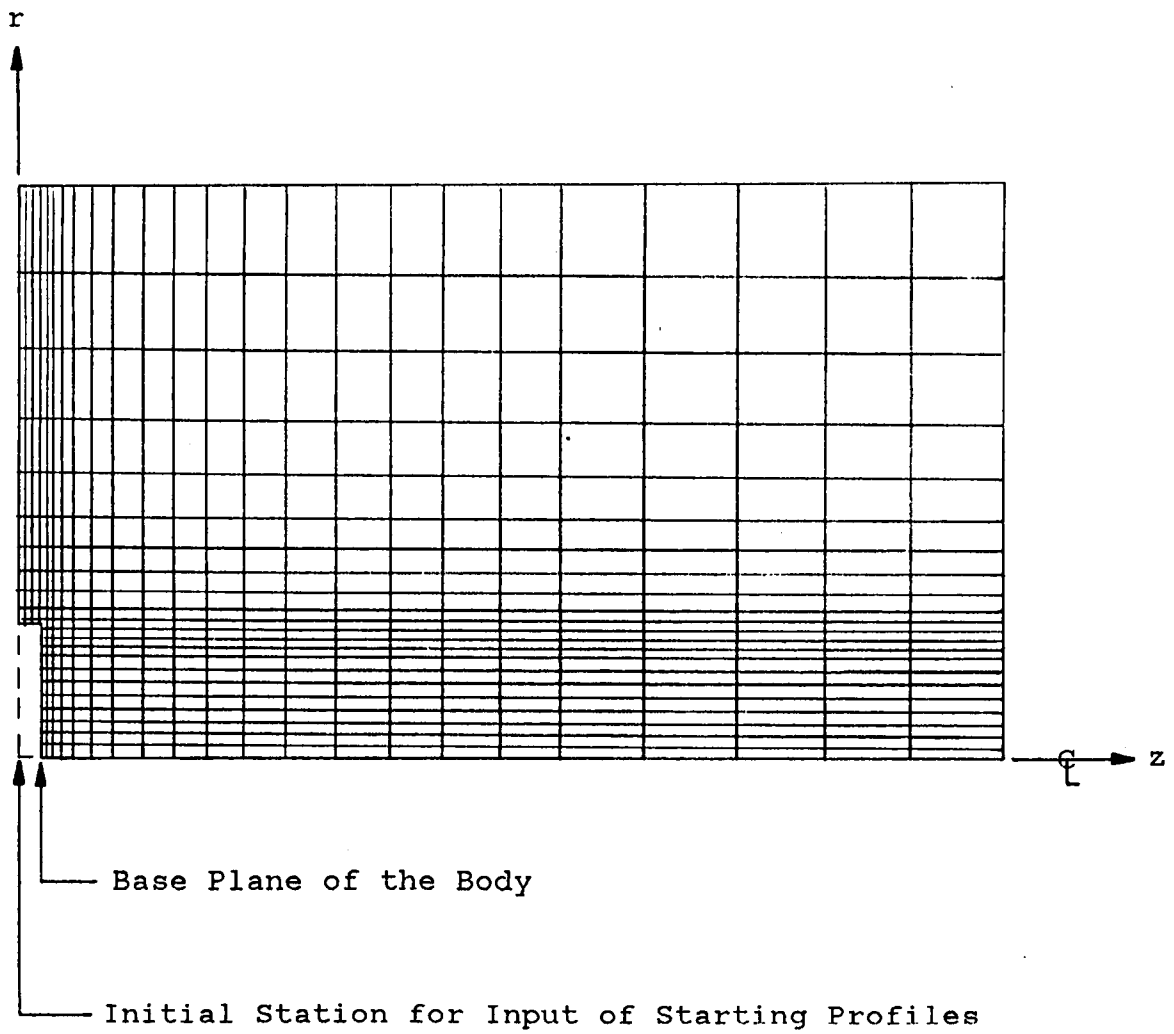
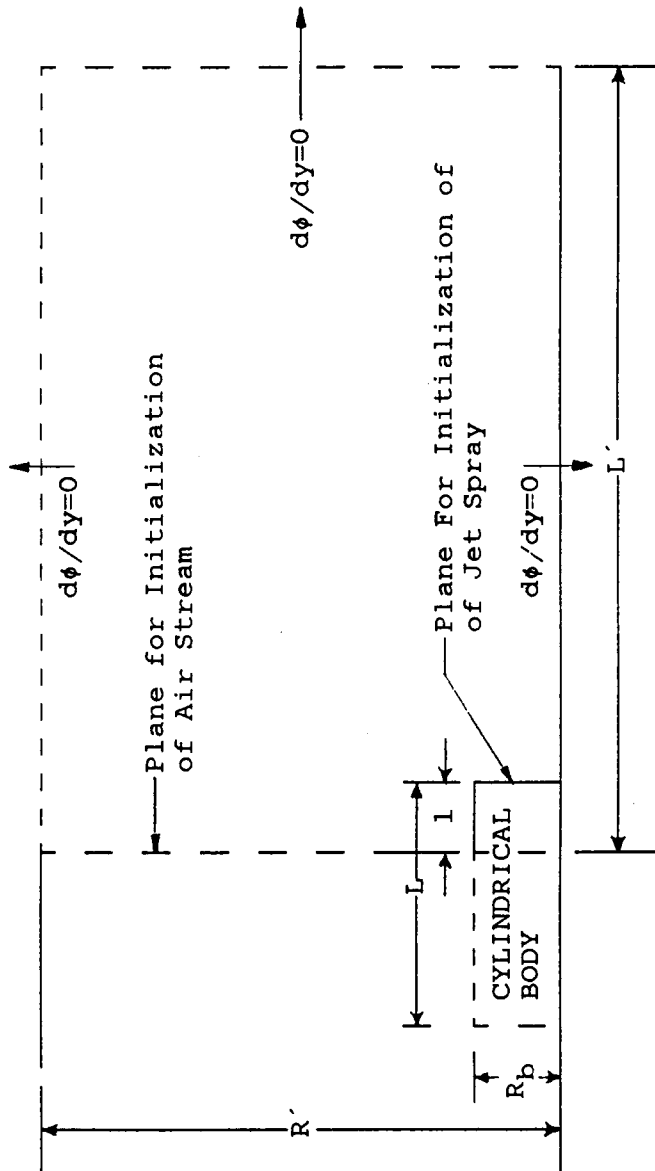


Figure 13. Schematic of Numerical Coordinate System Used in the Model



Characteristic Dimensions of the Computation

l	$= 0.0359$ m	Distance from Base to Starting Velocity Profile
L	$= 0.127$ m	Length of Body
L'	$= 4.00$ m	Length of Computational Domain
R_b	$= 0.03175$ m	Radius of Body
R'	$= 0.99$ m	Radius of Computational Domain Outer Boundary
ϕ	$= (u, v, w, H, C, k, \epsilon)$	

Figure 14. Dimensions of the Body and its Computational Domain

with its rate of dissipation were defined for the external flow field. Grid geometry refers to the axial length and radial width of the entire grid mesh, and the grid densities in the axial and radial directions. This rectangular grid was well suited to fit the contour of the cylindrical body. Axial and radial nodes were packed at the base of the body to achieve high resolution in this complex flow regime where most of the flow mixing and recirculation occurs. The minimum number of grid lines required to achieve a converged solution was determined and the results of these investigations are presented in Appendix A.

4.5 MASS CONSERVATION

The mass conservation of the numerical algorithm was checked by calculating the mass flow rates of the liquid and air at each axial grid line by,

$$\dot{m}_{\text{air}} = \sum (\psi U)_i \text{MF}_{A_i} 2\pi r_i dr_i \quad (40)$$

$$\dot{m}_{\text{air}} = \sum (\psi U)_i \text{MF}_{L_i} 2\pi r_i dr_i \quad (41)$$

$$\dot{m}_{\text{total}} = \sum (\psi U)_i 2\pi r_i dr_i \quad (42)$$

where MF_A and MF_L are the mass fractions of the air and liquid, respectively, and $2\pi r_i dr_i$ is the annulus strip area

perpendicular to the axial flow for the i th cell in an axisymmetric mesh system (Fig. 15). The results are presented in section 5.1.1.

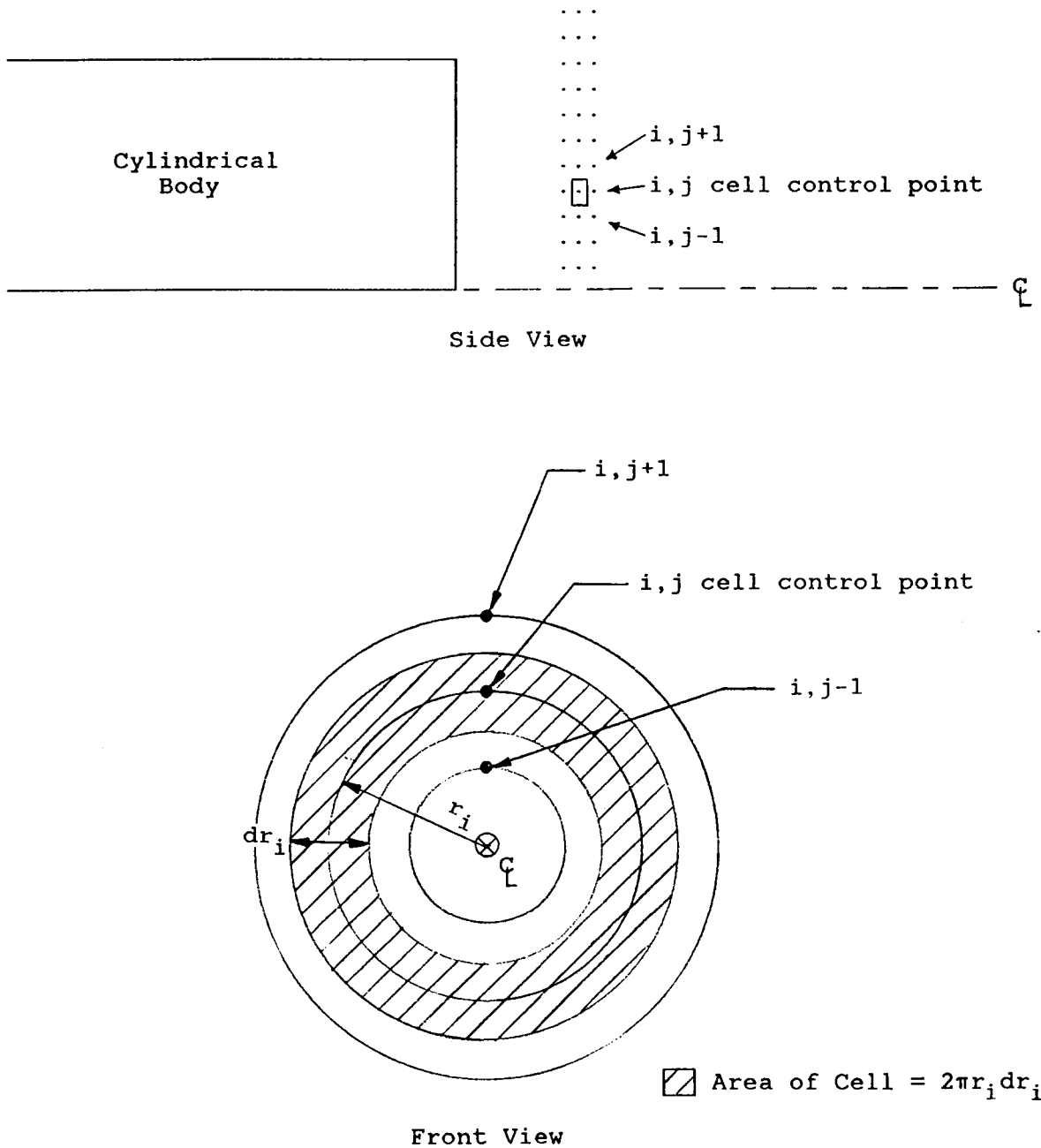


Figure 15. Differential Area Used for the Computation of Mass Flow Rate at Each Axial Grid Line

CHAPTER 5

RESULTS

5.1 INJECTION MODELING PROCESS

The computational flow model was evaluated by randomly choosing one experimental test condition and analyzing the ability of the model to predict this test data. The boundary conditions and initial flow profiles were varied until the best prediction of the test data for this one condition was obtained. These optimum initial flow profiles were then used without change to run the model for all the remaining experimental test cases and the final evaluation of the model's utility and physical adequacy was determined. The initial profiles which were varied in the model included the jet spray radius, the jet spray velocity profile, and the initial velocity profiles for the external flow field and boundary layer on the body. The test condition which was randomly chosen for the initial model comparisons was called Case 1. However, before the initial profiles were varied in the model, the mass flows of the liquid and air at each axial grid line were checked to assure that the masses were being conserved.

5.1.1 Mass Conservation

The mass conservation investigation was conducted by running the model for Test Case 1 with the jet spray radius arbitrarily set equal to that of the body radius. The results revealed that the mass of the liquid being ejected from the base of the body would increase as the model calculations were carried out further downstream of the body. At several meters downstream, the calculated liquid mass flow rate had increased by 97%. The changes in the overall total mass flow rate and the air mass flow rate were negligible (Fig. 16). In a way this means that the liquid spray mass flow was a tiny percent of the surrounding air flow rate, so that large errors in liquid flow rate had essentially no effect on total flow rate. An effort was made to isolate the cause for the growth of the liquid mass as the calculations progressed downstream of the body base. The following variables of the code were investigated: the boundary conditions at the top of the flow field, the boundary conditions at the centerline (symmetry axis), and the liquid mass ejection velocity. But before all this was done, one final grid test was made specifically designed to assure that the grid was not the cause of this particular problem. The entire number of grid lines were doubled from 62 X 38 to 124 X 76. Although the model run using a 124 X 76 mesh did not fully converge due to the CPU time limit

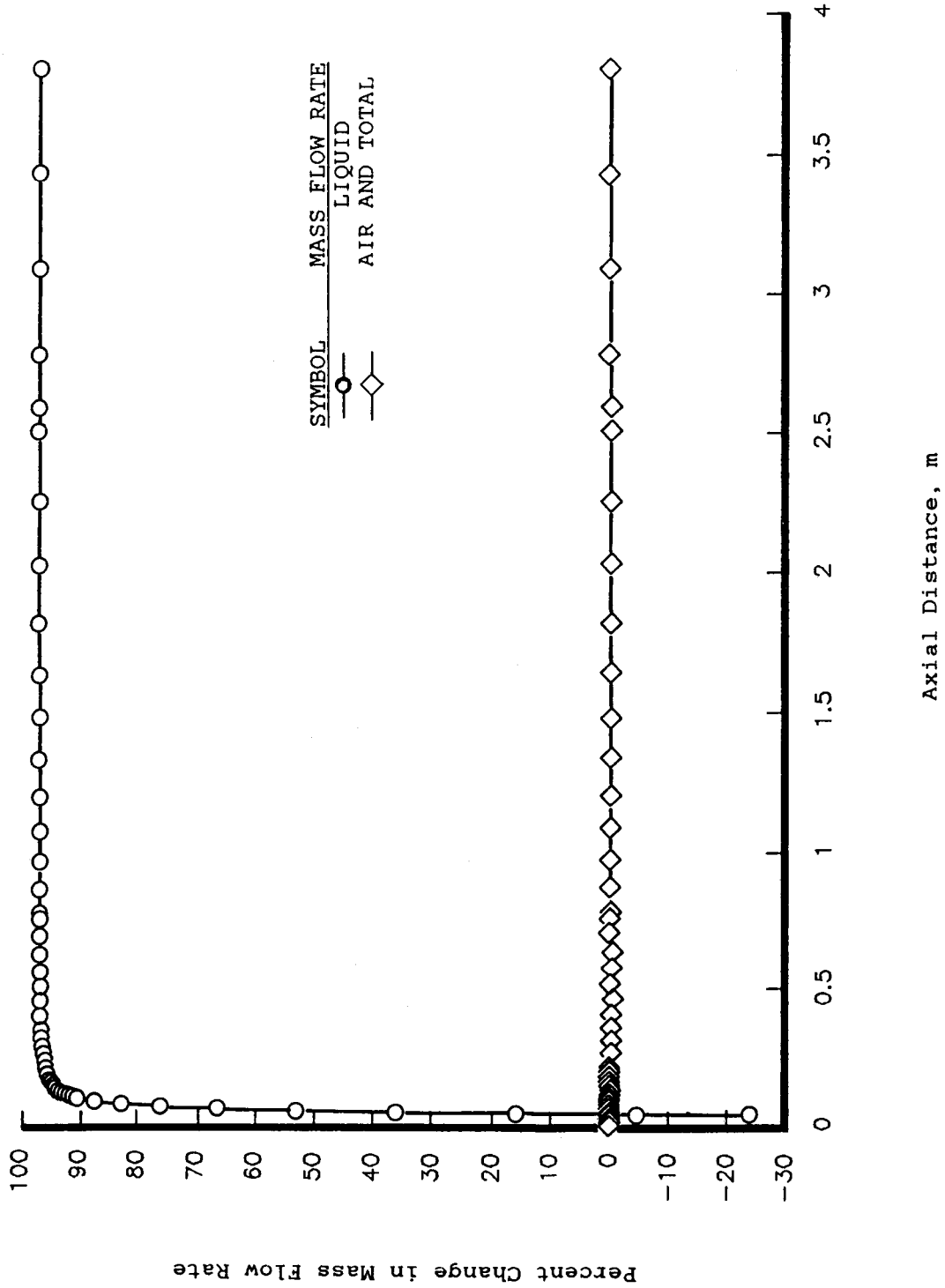


Figure 16. Mass Conservation of Liquid and Air for Test Case 1 with R_{jet} equal to R_{body}

set, the mass concentrations downstream of the body did converge beyond the point where the change in the liquid mass occurred. The growth in the liquid mass were similar for both grids (Fig. 17). Since no improvement in the liquid mass conservation resulted, it was concluded that the mass conservation problem is not related to the grid. Also it can be concluded that the same problem cannot be attributed to erroneous source terms in any of the subroutines, otherwise the change in liquid mass flow rate would be proportional to the increase in the number of axial or radial nodes added.

The boundary conditions at the top of the flow field were tested to assure that no mass flow was entering the flow field by the free-boundary conditions. This test was made by changing the top boundary condition from a free-boundary to a slip wall. The results in the growth of the liquid mass were identical, indicating there is no problem with the top boundary conditions. The boundary conditions at the symmetry axis were investigated next. The original boundary condition set all derivatives at the centerline equal to zero ($\delta\phi/\delta y=0$). Boundary conditions thought to be more realistic were tried. The Lagrangian extrapolation method was used subject to the constraint that the derivatives at the centerline were set to zero. This involved forcing the mass fractions for the first three

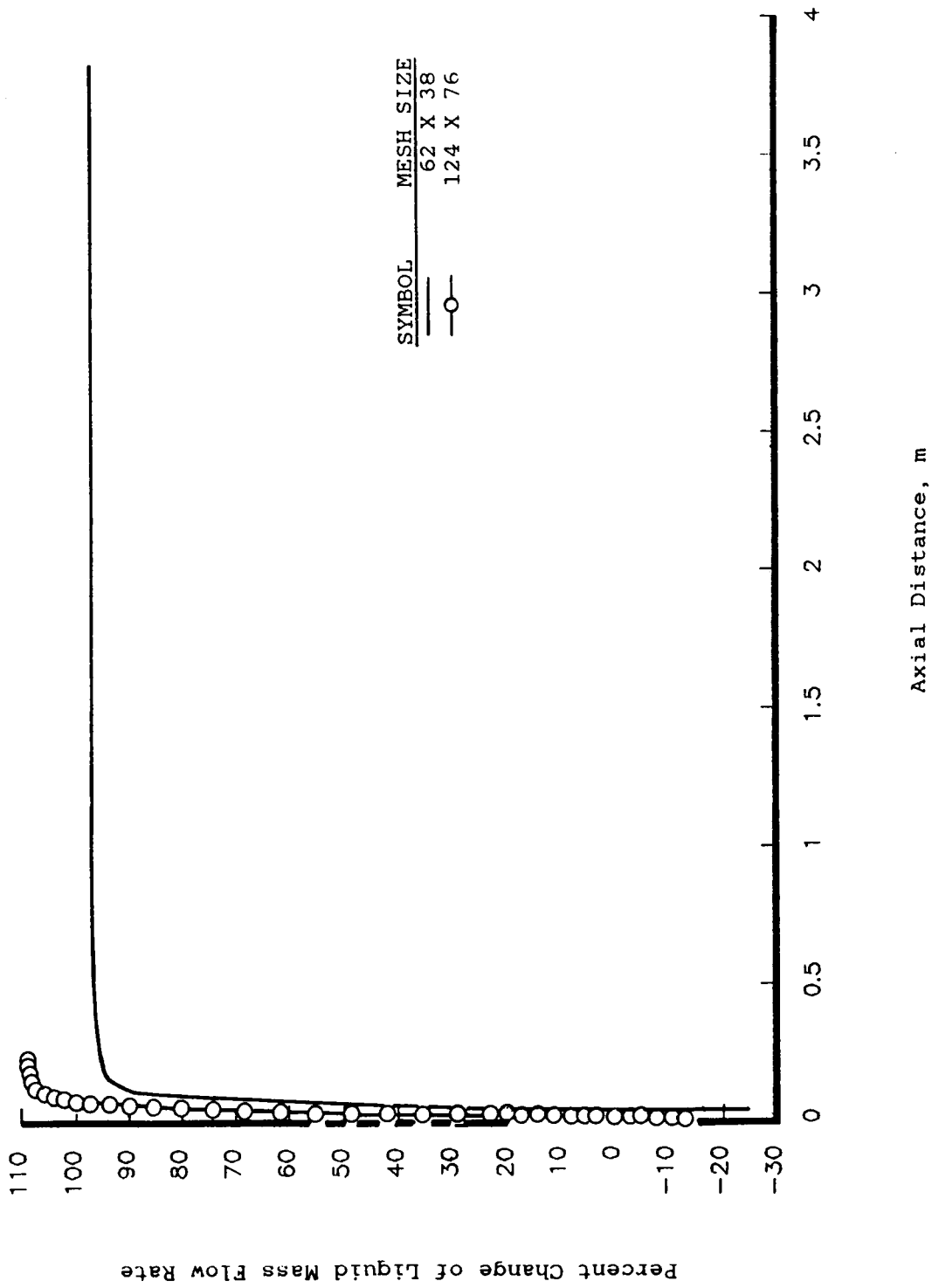


Figure 17. Liquid Mass Conservation for Various Grid Sizes

radial nodes away from the centerline to form a parabolic behavior while still maintaining that the partials at the centerline be equal to zero $(\delta\phi/\delta y)=0$. This required that

$$\frac{MF_{L_2} - MF_{L_1}}{MF_{L_3} - MF_{L_1}} = \frac{(y_2 - y_1)^2}{(y_3 - y_1)^2} \quad (43)$$

where MF_L is the liquid mass fractions at the indicated radial J nodes. The results in the growth of the liquid mass fractions were identical as before, indicating that the problem did not exist with the boundary conditions at the symmetry axis.

To better understand the mass growth phenomenon, the liquid mass ejection velocity was perturbed to determine the extent it had on the growth in the liquid mass flow rate. As a baseline case, the velocity and density of the liquid jet were set equal to that of the external airstream so very little mixing and no recirculation took place. Then, holding the density constant, the jet velocity was gradually decreased from the air velocity to the actual jet spray velocity for a jet spray radius equal to one body radius. The results of these velocity perturbations as well as all the test cases run for this thesis are presented in Table 6 and plotted in Fig. 18. These results show that when the jet velocity to free-stream velocity ratio was less than

TABLE 6. CONSERVATION OF LIQUID MASS FLOW RATE

Test Case	U_{jet}/U_{∞}	% CHANGE OF LIQUID MASS
-	0.6181	0
-	0.3091	0
-	0.1539	0
-	0.0618	13
-	0.0144	97
-	0.0226	64
-	0.0402	28
-	0.0904	-2
-	0.3616	-8
-	1.4439	-10
1	0.0905	-1
2	0.1700	-7
3	1.0531	-5
4	0.2958	-7
5	0.1807	-7
6	0.3286	-7
7	1.0000	-5
8	0.4044	-6
9	0.8646	-5

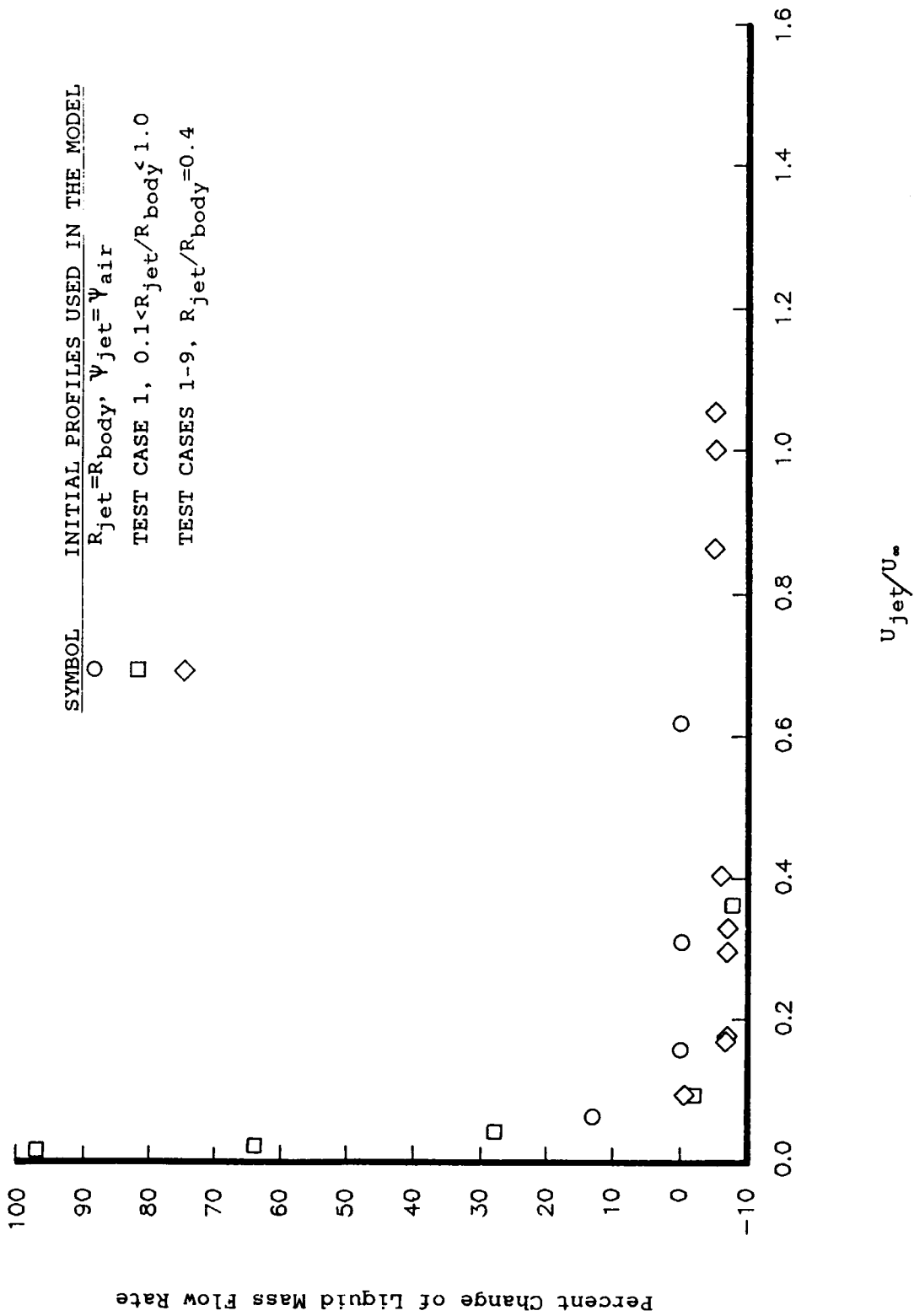


Figure 18. Effect of Jet to Free-Stream Velocity Ratio on the Conservation of Liquid Mass

0.08, the mass growth became very significant. When this ratio was greater than 0.08, no significant change in the liquid mass flow rate resulted.

Based on the changes of the behavior of the model due to the jet velocity perturbations, and the results showing that the model is not grid dependent and no problems exist with the source terms or boundary conditions, it was concluded that the solution for the model computation for Case 1 with the jet spray radius equal to that of the body radius surpasses the numerical accuracy of this model. Specifically, the resolution of the calculations required for this specific model run surpassed the numerical accuracy of the computed convective fluxes of transported scalar quantities in the numerical algorithm. Spray radii were then assumed and tested between 0.2 and 1.0 times that of the body radius to determine the optimum spray radius at which no mass growth would occur. The results show that as the spray radius decreased, the growth in the liquid mass flow rate decreased dramatically (Fig. 19). This is plausible because as the jet spray radius is decreased, the initial spray velocity must increase to permit the numerically modeled mass injection to equal the experimental values. This decreased the difference between the jet spray and air flow velocities. Also, as the spray radius decreases, much of the mixing takes place in the

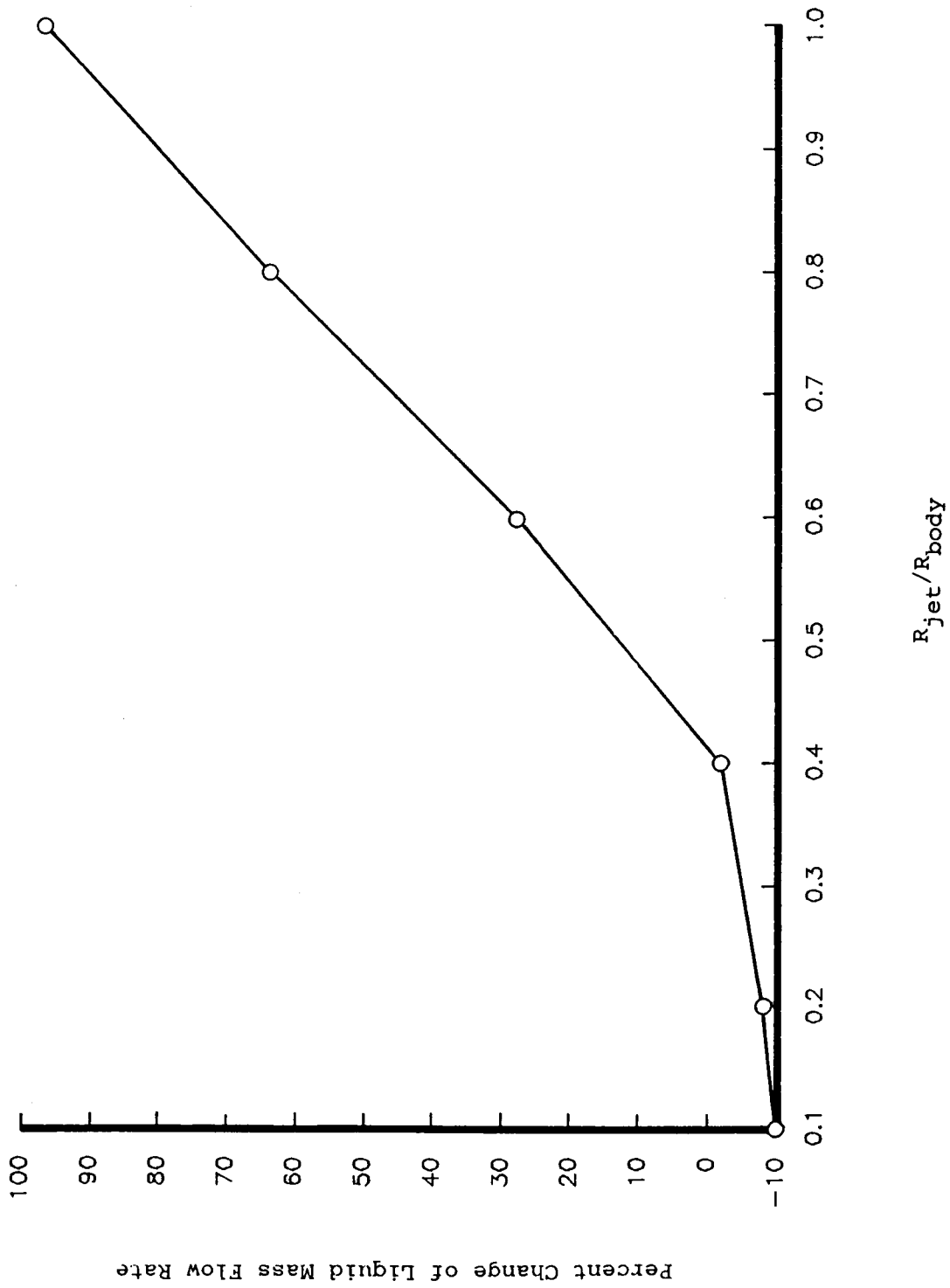


Figure 19. Effect of Jet Radius on the Liquid Mass Conservation for Test Case 1

recirculation zone where the air velocity is lower than it is at the body surface, further decreasing the velocity difference between the two flows where mixing occurs. Almost no growth in the liquid mass flow rate occurred when the jet spray radius was 0.4 times the body radius. Therefore, a jet spray radius of 0.4 times the body radius was used for all remaining model predictions. This spray radius resulted in no more than a 7% change in mass flow rate for Test Cases 1 through 9 as shown in Table 6.

5.1.2 Initial Velocity Profiles

5.1.2.1 Effect of the Initial Velocity Profile of the External Flow Field on the Model Predictions

The effect of the body boundary layer velocity profiles on the predicted spray profiles were investigated. Power Laws of $n=2, 3, 7, 12$, and infinity were analyzed with the corresponding boundary layer thicknesses of $\delta/R_{\text{body}} = .56, .52, .46, .44$, and $.41$, respectively. No significant effect on the model predictions resulted at $12 X/D$ (Fig. 20) or $41 X/D$ (Fig. 21). Wake profiles for the body boundary layer were also tested in the model. Although it was shown in section 4.2.3.2 that δ/R_{body} for wake flows was equal to 0.667 , a range of boundary layer thicknesses were analyzed where δ/R_{body} was set equal to $1.2, 1.0, 0.8, 0.5$, and 0.2 to understand the effect of these profiles on the model

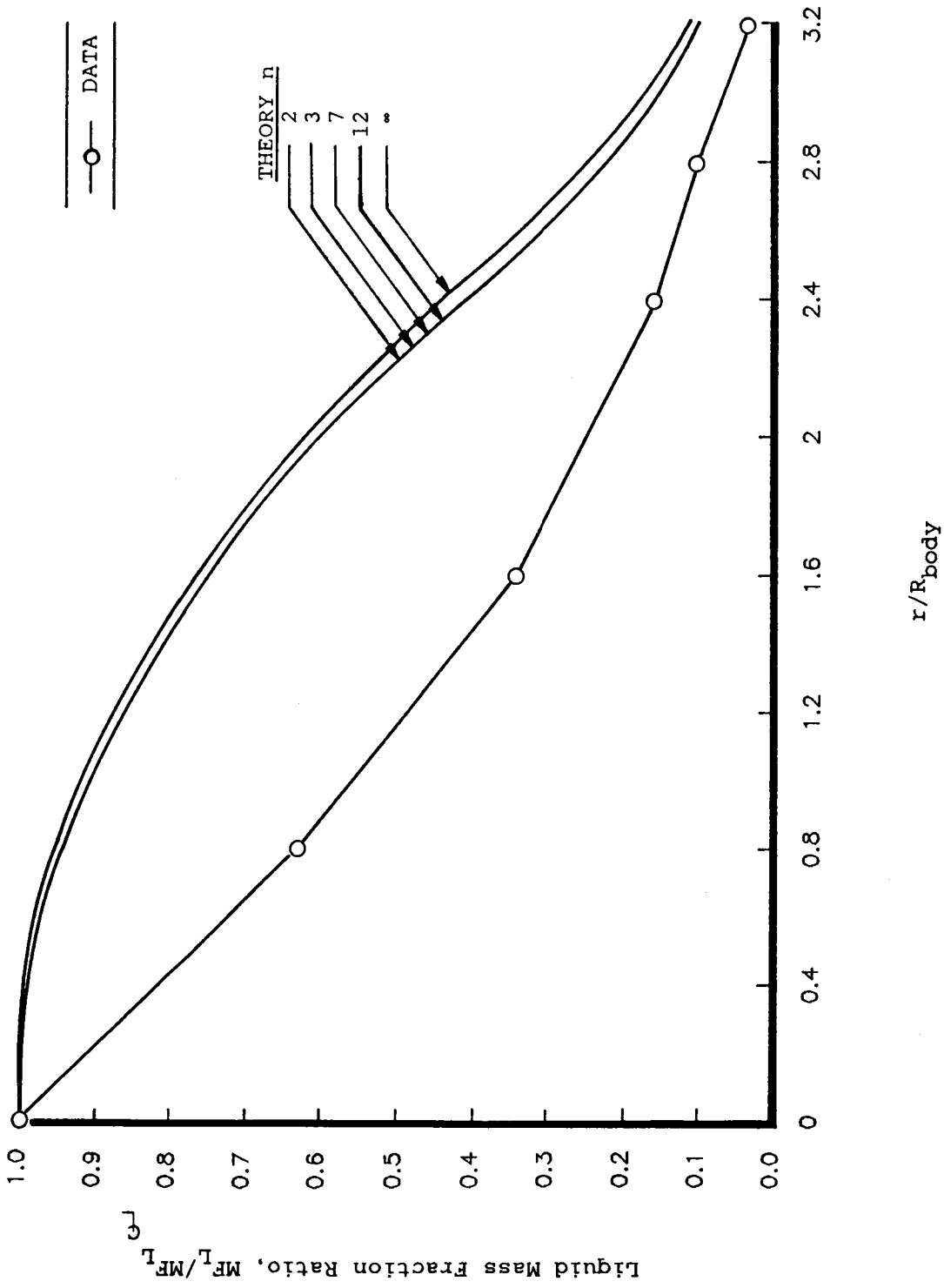


Figure 20. Effect of Body Boundary Layer Power Law Velocity Profiles on Model Predictions at 12 X/D

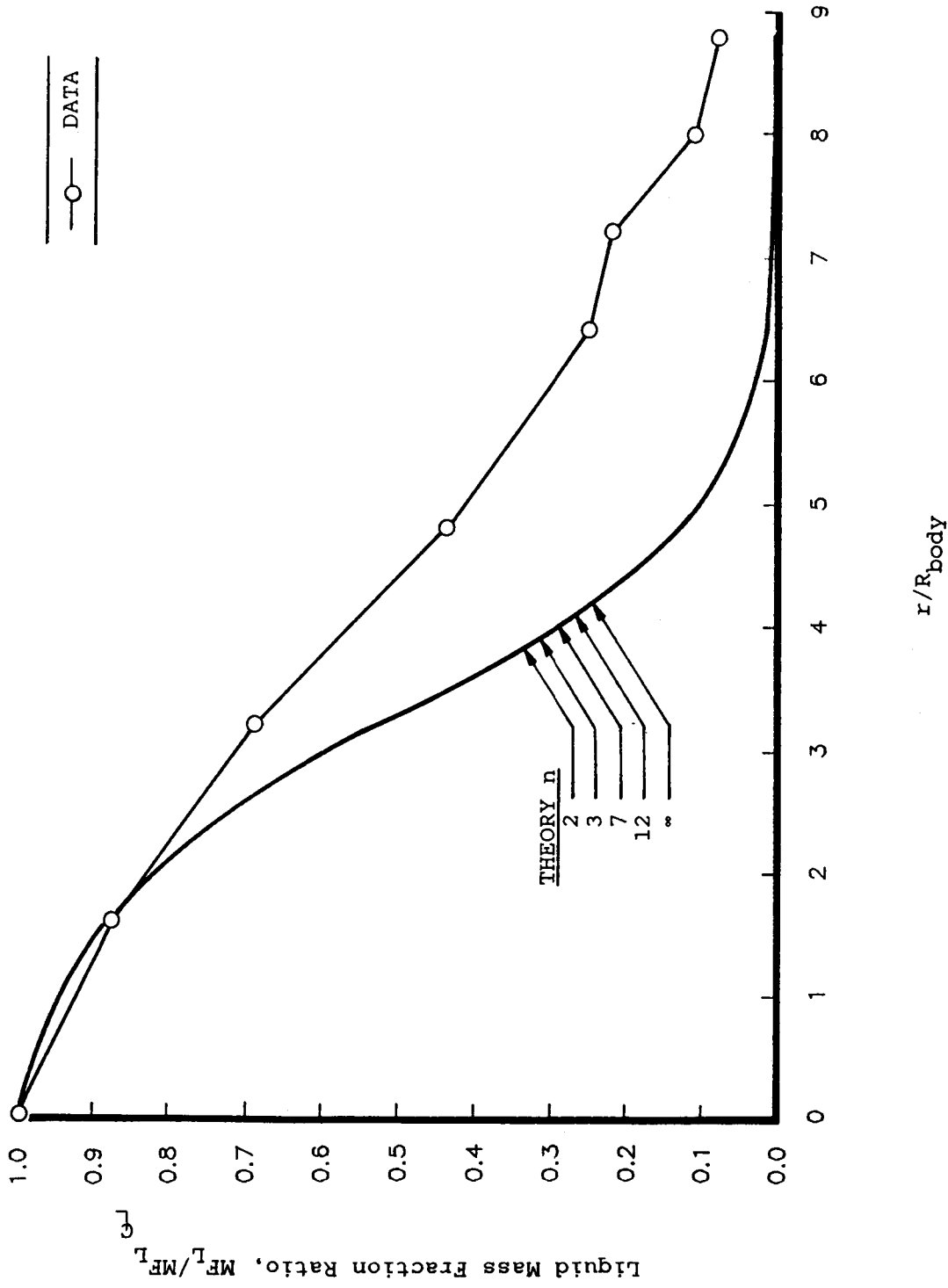


Figure 21. Effect of Body Boundary Layer Power Law Velocity Profiles on Model Predictions at 41 X/D

predictions. The mass concentrations predicted by the model show slightly better results at 12 X/D with $\delta/R_{\text{body}}=0.2$ (Fig. 22), but at 41 X/D the best results were obtained with $\delta/R_{\text{body}}=1.2$ (Fig. 23). Therefore, no overall improvement of model performance was obtained for various wake profiles in the body boundary layer.

5.1.2.2 Effect of the Initial Velocity Profile of the Jet Spray on the Model Predictions

The effect of the velocity profiles of the jet spray on the predicted spray profiles were then investigated. Power laws of $n=2, 3, 7$, and 12 , were analyzed with a corresponding boundary layer thickness of $\delta/R_{\text{jet}}=.56, .52, .46$, and $.44$, respectively. The model predictions for 12 and 41 X/D were not significantly influenced by this range of power law profiles (Figures 24 and 25).

Imparting a radial velocity to the jet spray was then investigated. Spherical cap velocity profiles were utilized for this purpose as described in section 4.2.2.2. The maximum spherical cap angles, θ_{max} , analyzed were $15^\circ, 30^\circ, 45^\circ$, and 60° . The results show a negligible change in the model predictions for different spherical cap velocity profiles at 12 and 41 X/D (Figures 26 and 27).

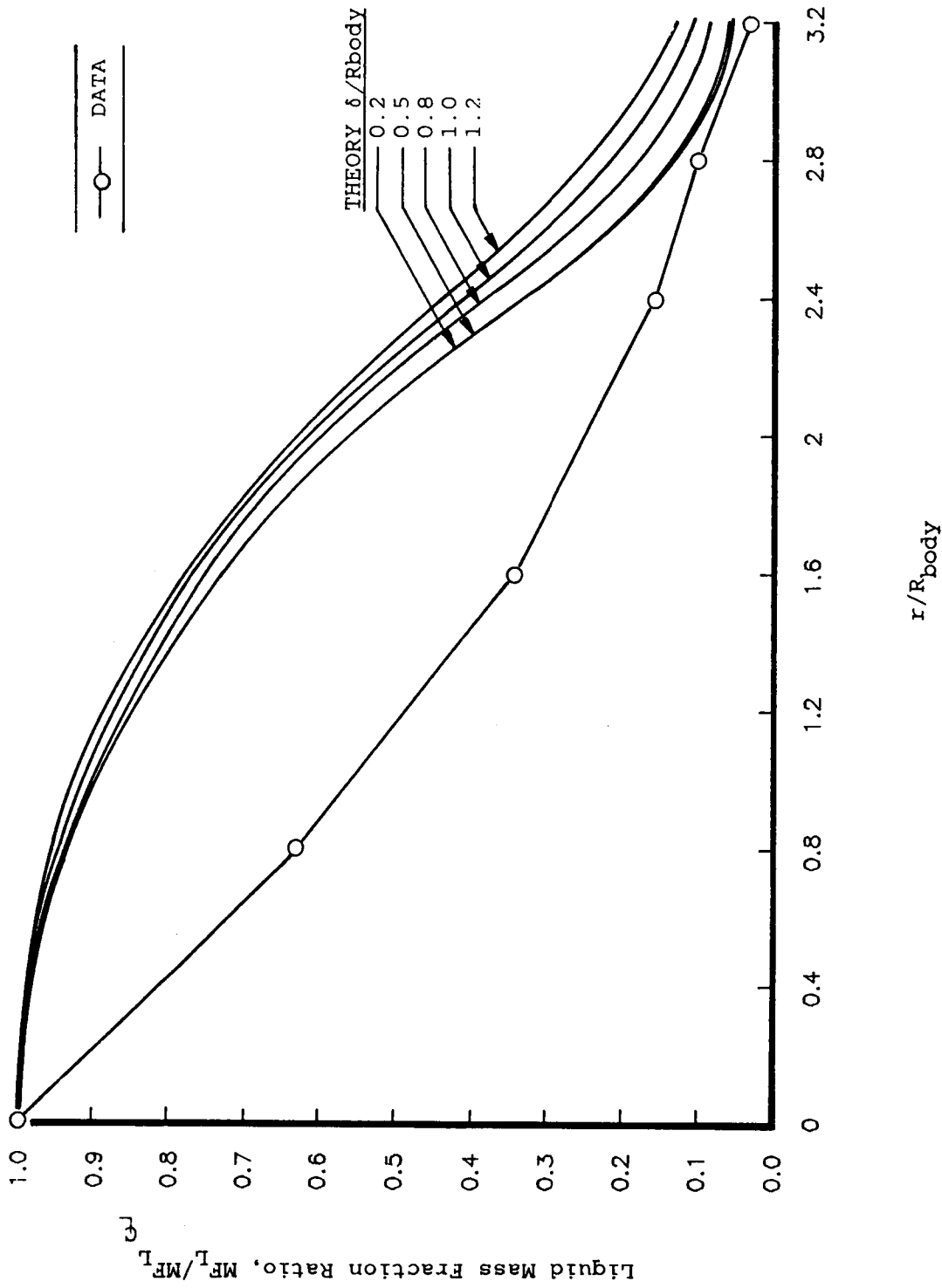


Figure 22. Effect of Body Boundary Layer Wake Velocity Profiles on Model Predictions at 12 X/D

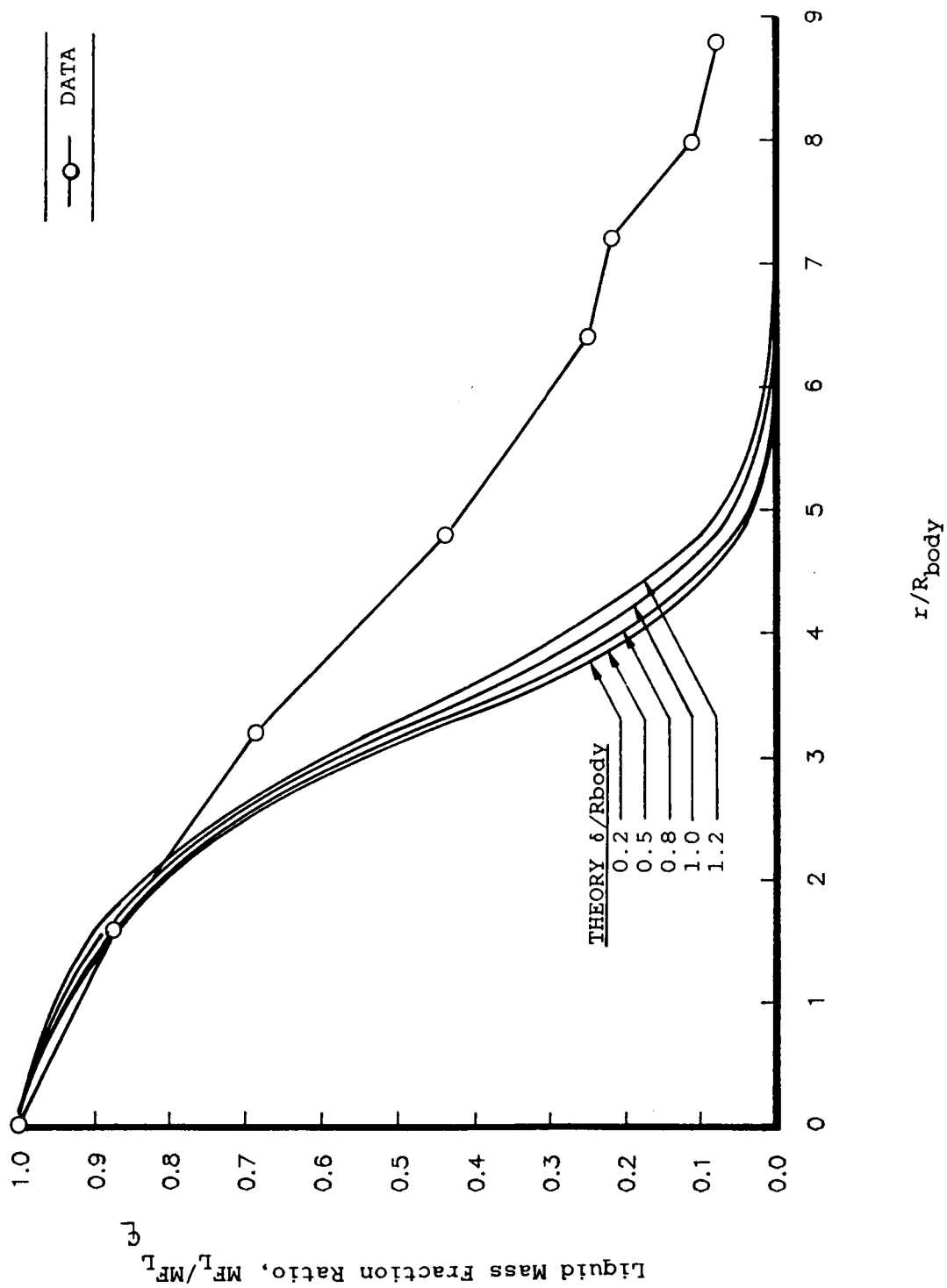


Figure 23. Effect of Body Boundary Layer Wake Velocity Profiles on Model Predictions at 41 X/D

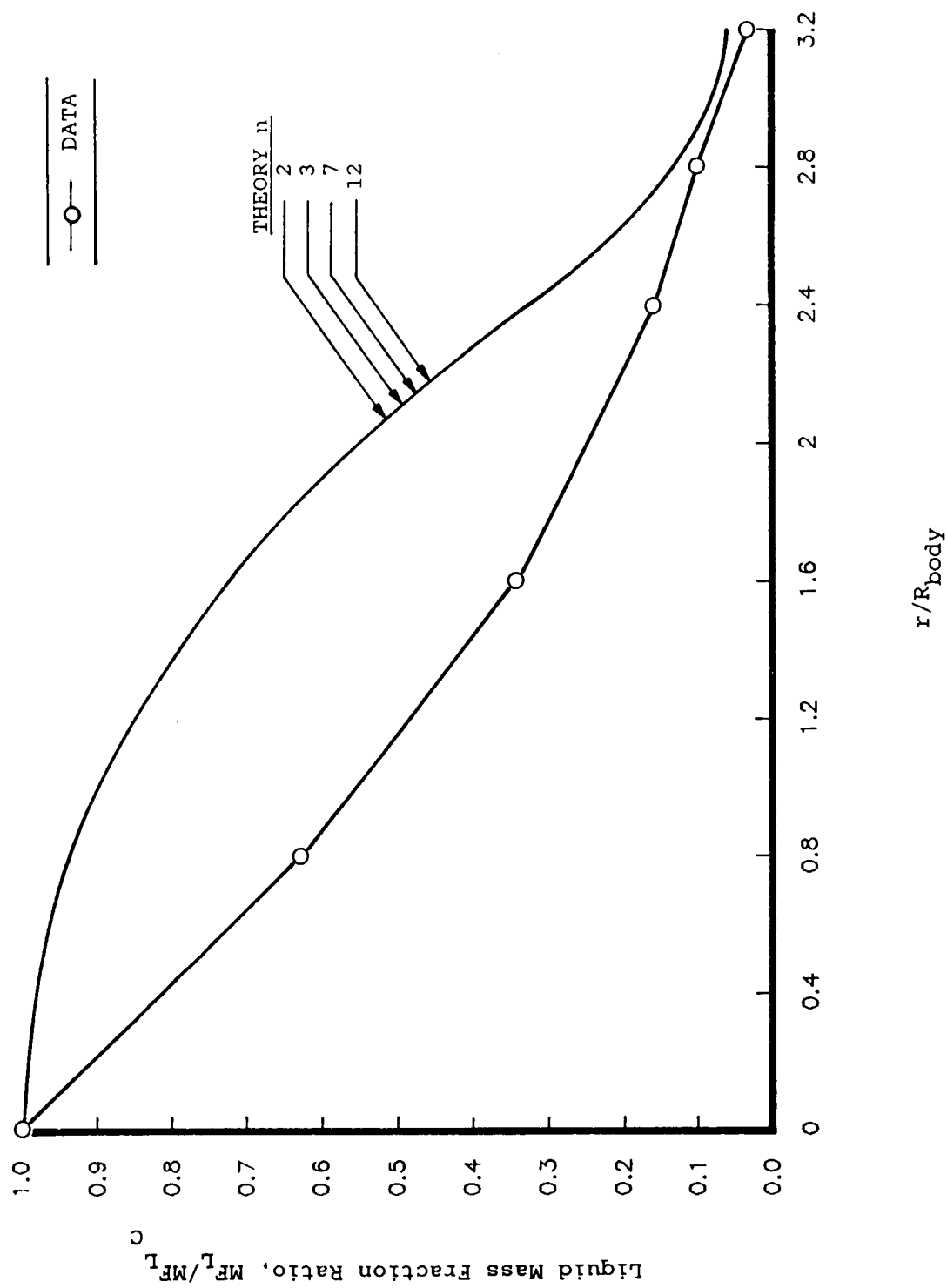


Figure 24. Effect of Jet Power Law Velocity Profiles on Model Predictions at $12 X/D$

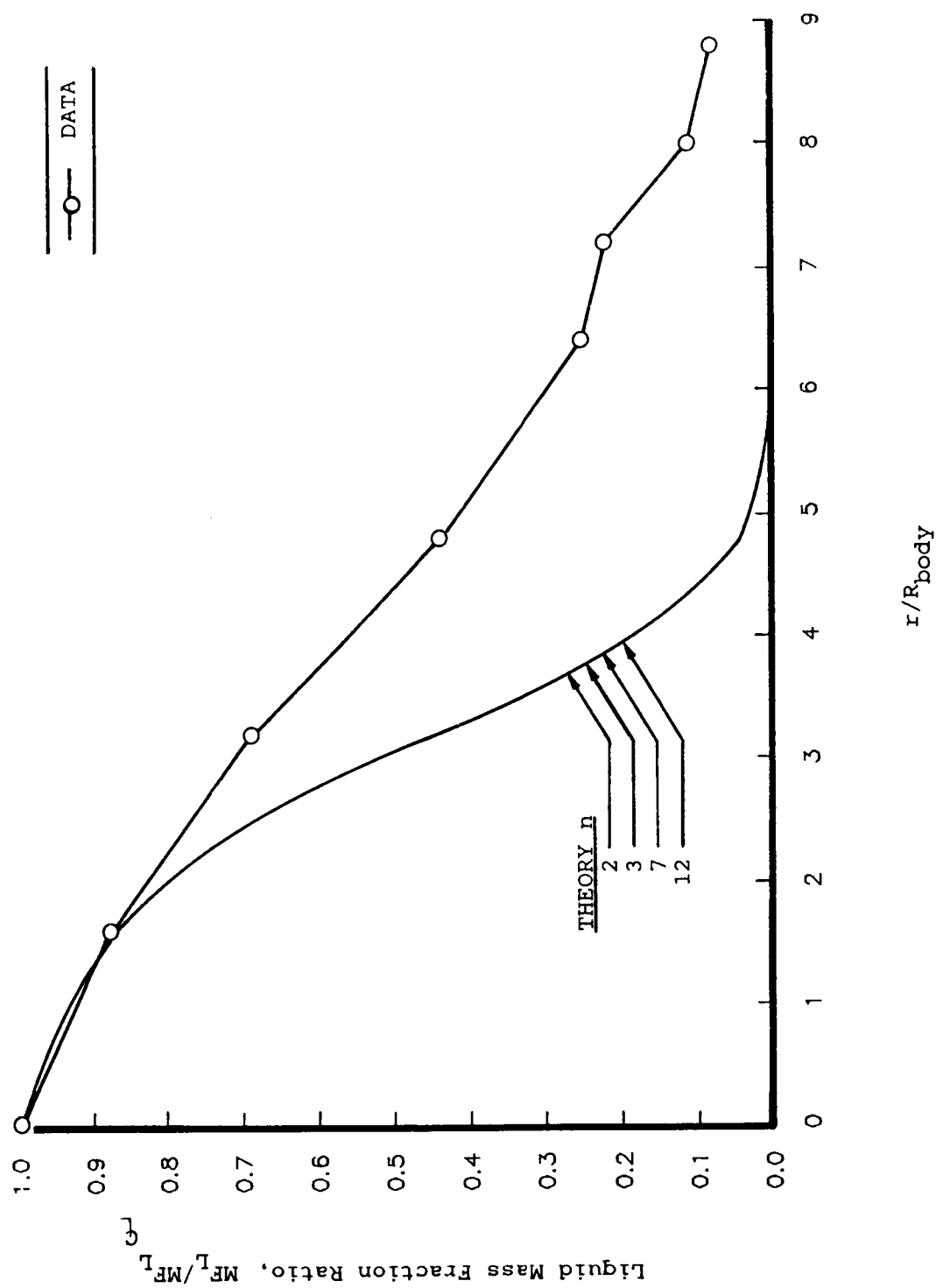


Figure 25. Effect of Jet Power Law Velocity Profiles on Model Predictions at 41 X/D

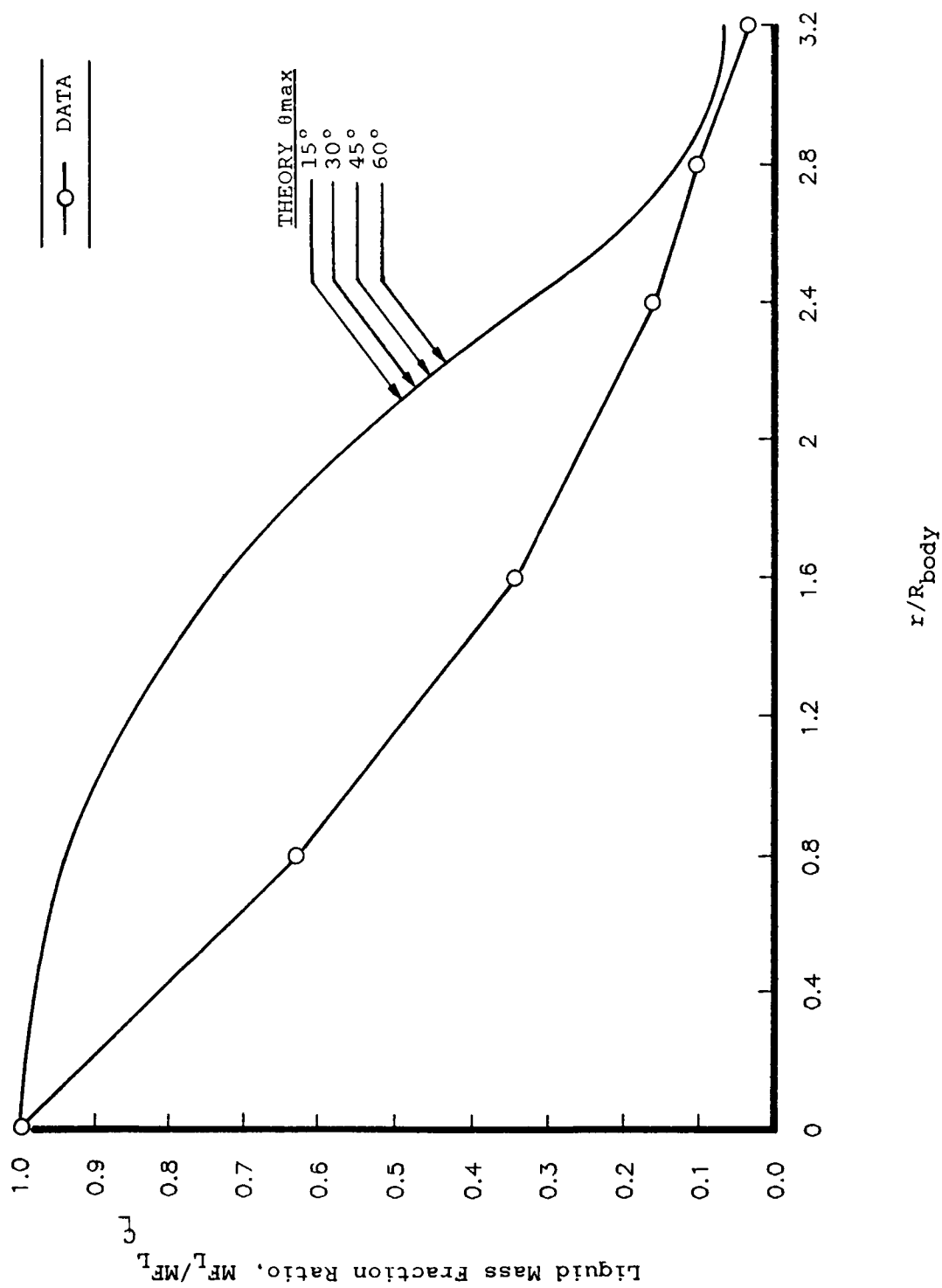


Figure 26. Effect of Jet Spherical Cap Velocity Profiles on Model Predictions at 12 X/D

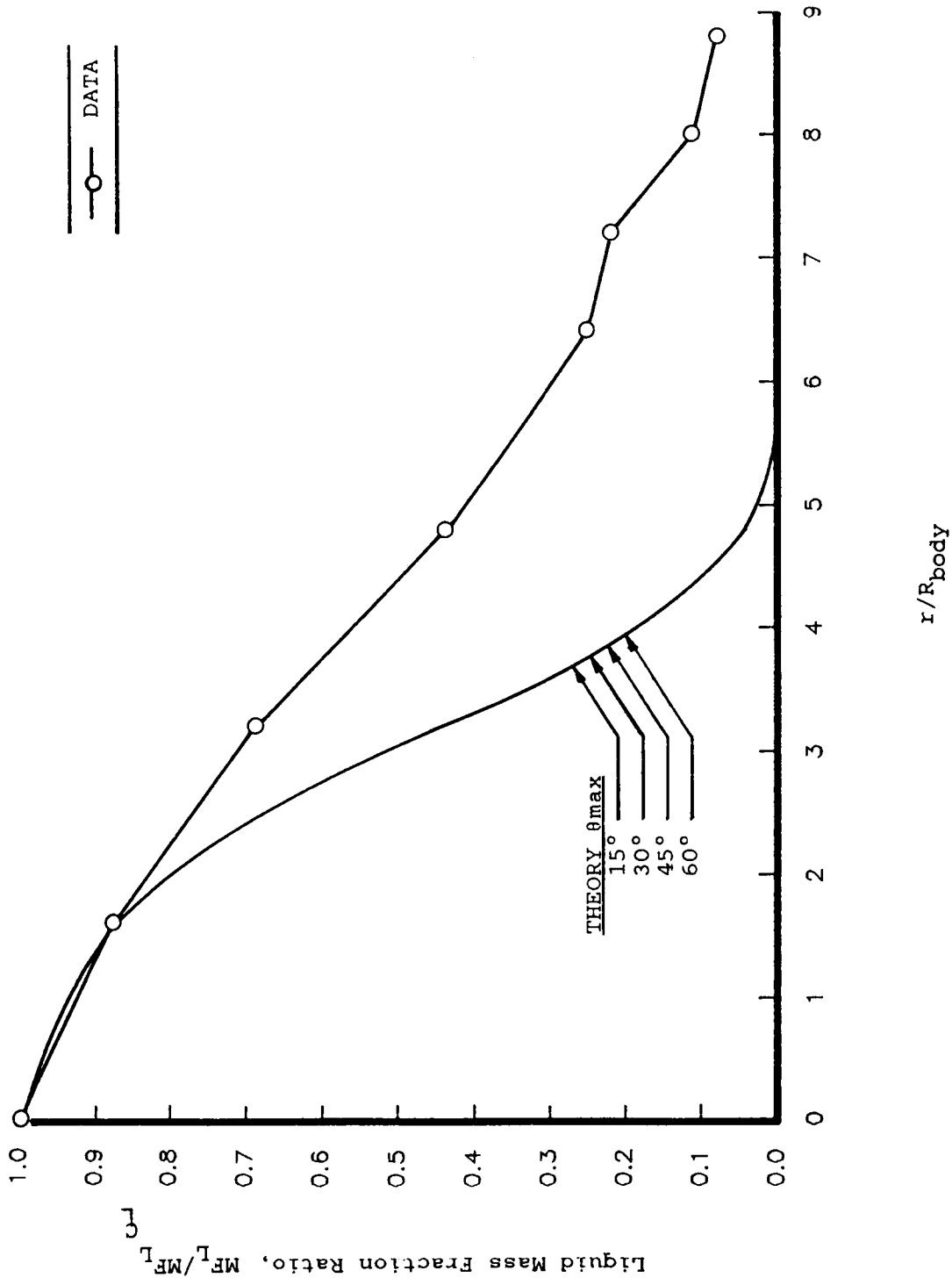


Figure 27. Effect of Jet Spherical Cap Velocity Profiles on Model Predictions at 41 X/D

5.2 PRESENTATION OF TEST CASES

The best results of all the different types of profiles were plotted together to determine which one would give the optimum model predictions for Test Case 1. As can be seen from Figures 28 and 29, the influence of the initial velocity profiles on the model predictions were small. Also, a profile that best predicted the test data at 12 X/D performed worse at 41 X/D, indicating that no profile gave significantly better results overall. Therefore, the most simplistic flow profiles were chosen to initialize the flow fields for the remaining model computations of Test Cases 2 through 9. These profiles consisted of using a slug flow for the jet spray and a standard power law profile where n equals 7 in the body boundary layer.

The adequacy of the model in predicting the experimental data is presented below. The results were divided into five categories so that the behavior of the model at various test conditions and injector nozzle configurations could be established. These five categories included altitude variation, tunnel air velocity variation, liquid ejection flow rate variation, injector nozzle configurations such as single-hole and multi-hole nozzles, and nozzles with and without atomization air. The results of the predictions for Cases 1 through 9 are presented in the figures which follow, and are summarized in Tables 7 and 8. The spray diameter

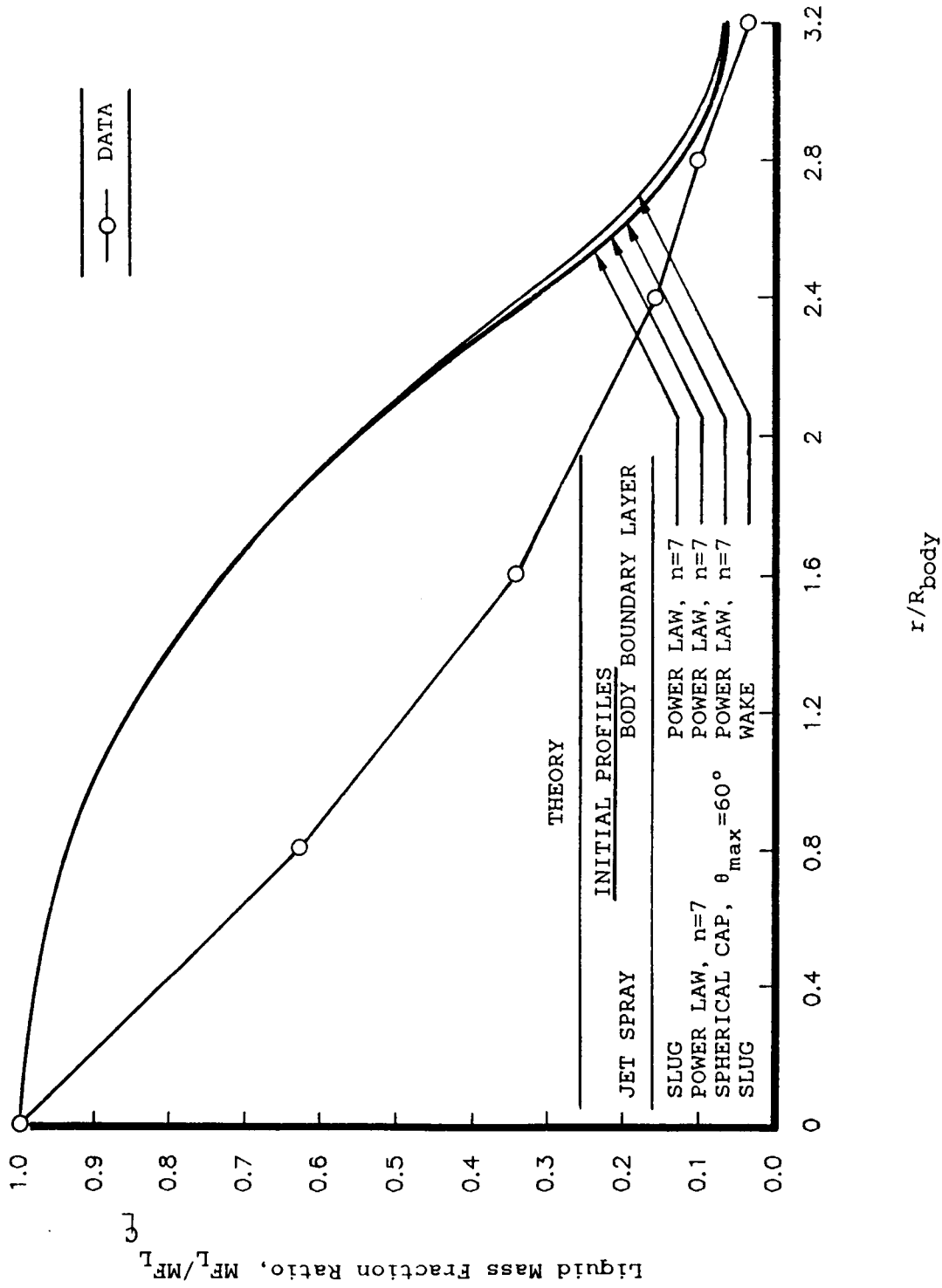


Figure 28. Comparison of All Types of Initial Velocity Profiles on Model Predictions at $12 X/D$

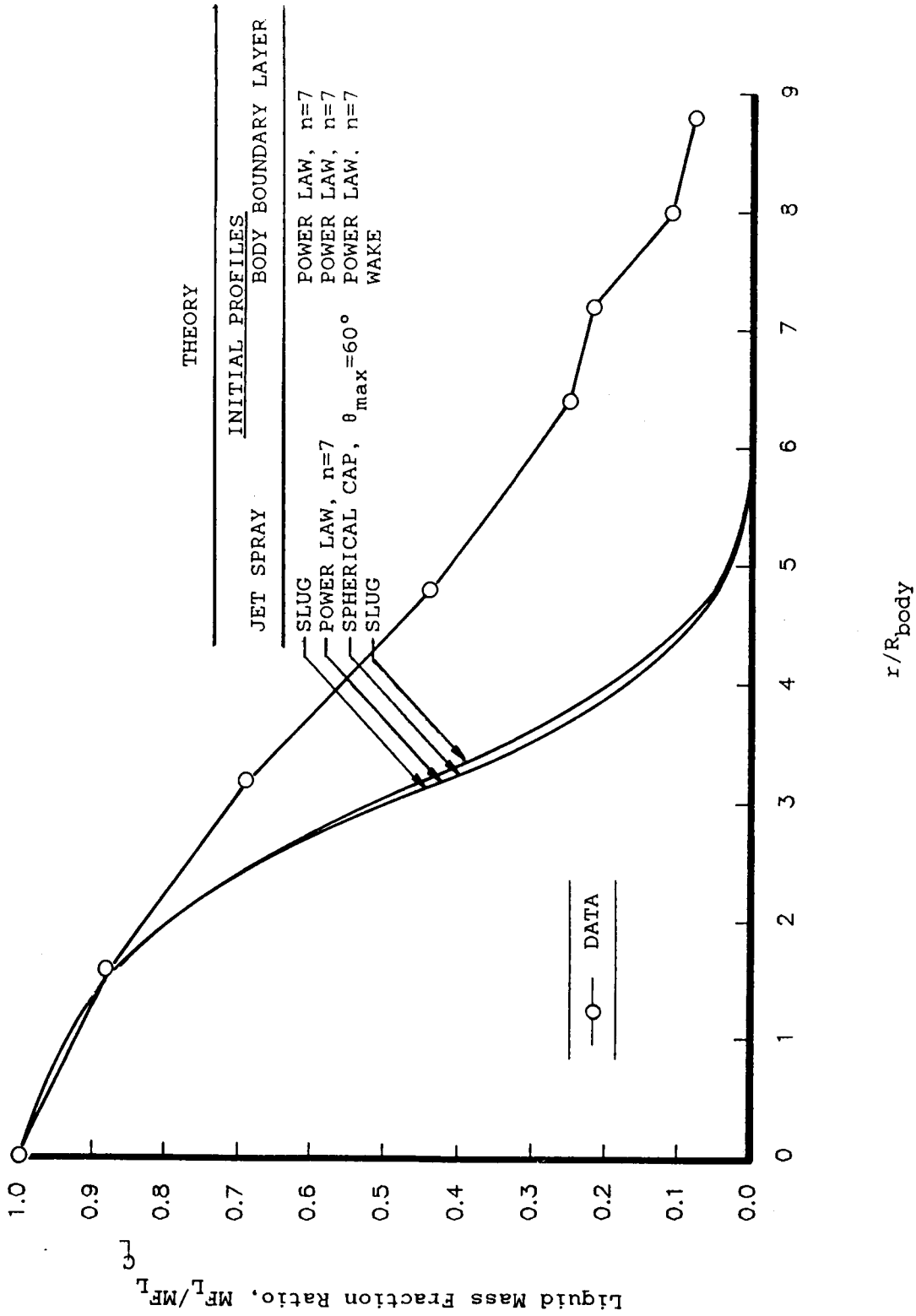


Figure 29. Comparison of All Types of Initial Velocity Profiles on Model Predictions at 41 X/D

TABLE 7. LIQUID MASS FRACTION AT THE CENTERLINE

Test Case	MM % Error		Mass Mean Dia. $d_{30}, \mu\text{m}$	$(U_{\text{jet}})_{\text{mm}}$ $(U_{\text{jet}})_{\text{exp}}$
	12 X/D	41 X/D		
1	-44	39	13.9	0.55
2	-56	9	11.5	1.53
3	55	12	13.0	7.81
4	-36	12	---	2.25
5	-44	28	10.9	2.23
6	-28	14	11.5	4.45
7	66	112	16.5	4.44
8	5	155	15.0	0.87
9	49	29	14.9	0.85

TABLE 8. LIQUID SPRAY DIAMETERS, r/R_{body}^*

Test Case	LIQUID SPRAY DIAMETERS				MM % Error		Mass Mean Dia., d ₃₀	(U _{jet}) _{mm} (U _{jet}) _{exp}
	12 X/D		41 X/D		12 X/D	41 X/D		
	Exp	MM	Exp	MM				
1	1.14	2.08	4.40	3.00	82	-32	13.9	0.55
2	0.85	2.15	3.50	3.10	153	-11	11.5	1.53
3	1.80	2.25	2.80	3.30	25	18	13.0	7.81
4	1.95	2.10	5.00	2.90	8	-42	---	2.25
5	1.75	2.10	5.30	2.90	20	-45	10.9	2.23
6	1.95	2.05	4.00	2.95	5	-26	11.5	4.45
7	1.80	2.20	4.20	3.25	22	-23	16.5	4.44
8	1.25	2.10	5.00	3.20	68	-36	15.0	0.87
9	1.50	2.20	3.40	3.20	47	-6	14.9	0.85

*The spray diameter was arbitrarily defined as the radial distance from the centerline where the mass concentration was equal to one half that at the centerline.

presented in the following tables was arbitrarily defined as the radial distance where the mass concentration was equal to one half that at the centerline. These results are discussed in further detail in the following sections.

5.2.1 Altitude Variation

For the influence of altitude variation on the model results, two different comparisons can be made. Test Case 2 simulated an altitude six times as great as Test Case 1 with all other variables remaining constant. The results of the spray profiles predicted by the model at 12 and 41 X/D for Test Case 1 (Figures 30 and 31) and Test Case 2 (Figures 32 and 33) are summarized in Table 9.

TABLE 9. Altitude Variation

TEST CASE	ALTITUDE,m	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
1	1494	82	-32	-44	39
2	8778	153	-11	-56	9

There is no apparent trend of model accuracy versus altitude when the results of these two test cases are compared.

Another comparison can be made between Test Cases 3 and 4, where the altitude of Case 3 was seven times as great as that of Case 4. The results for Case 3 (Figures 34 and 35)

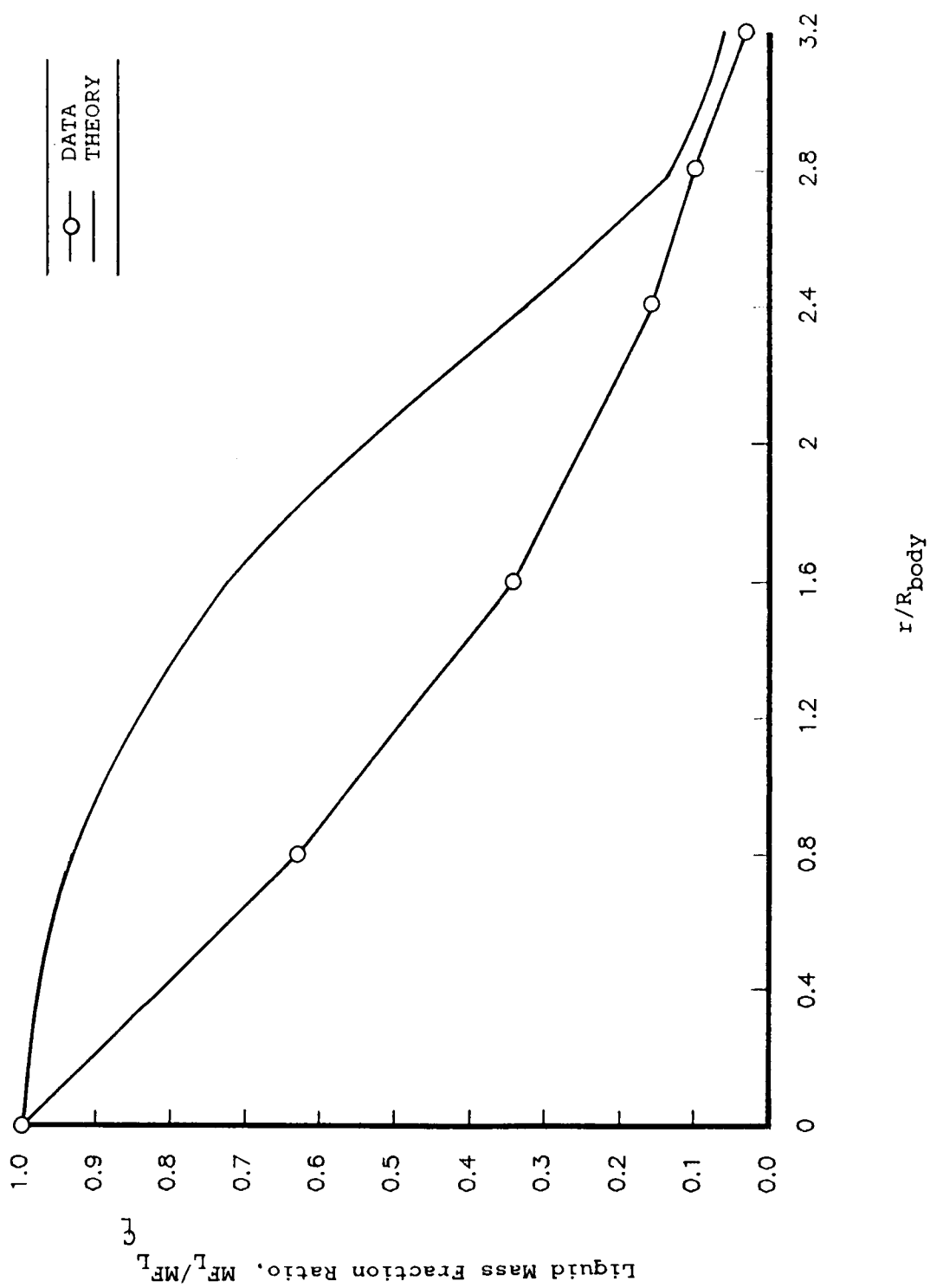


Figure 30. Model Predictions for Test Case 1 at 12 X/D

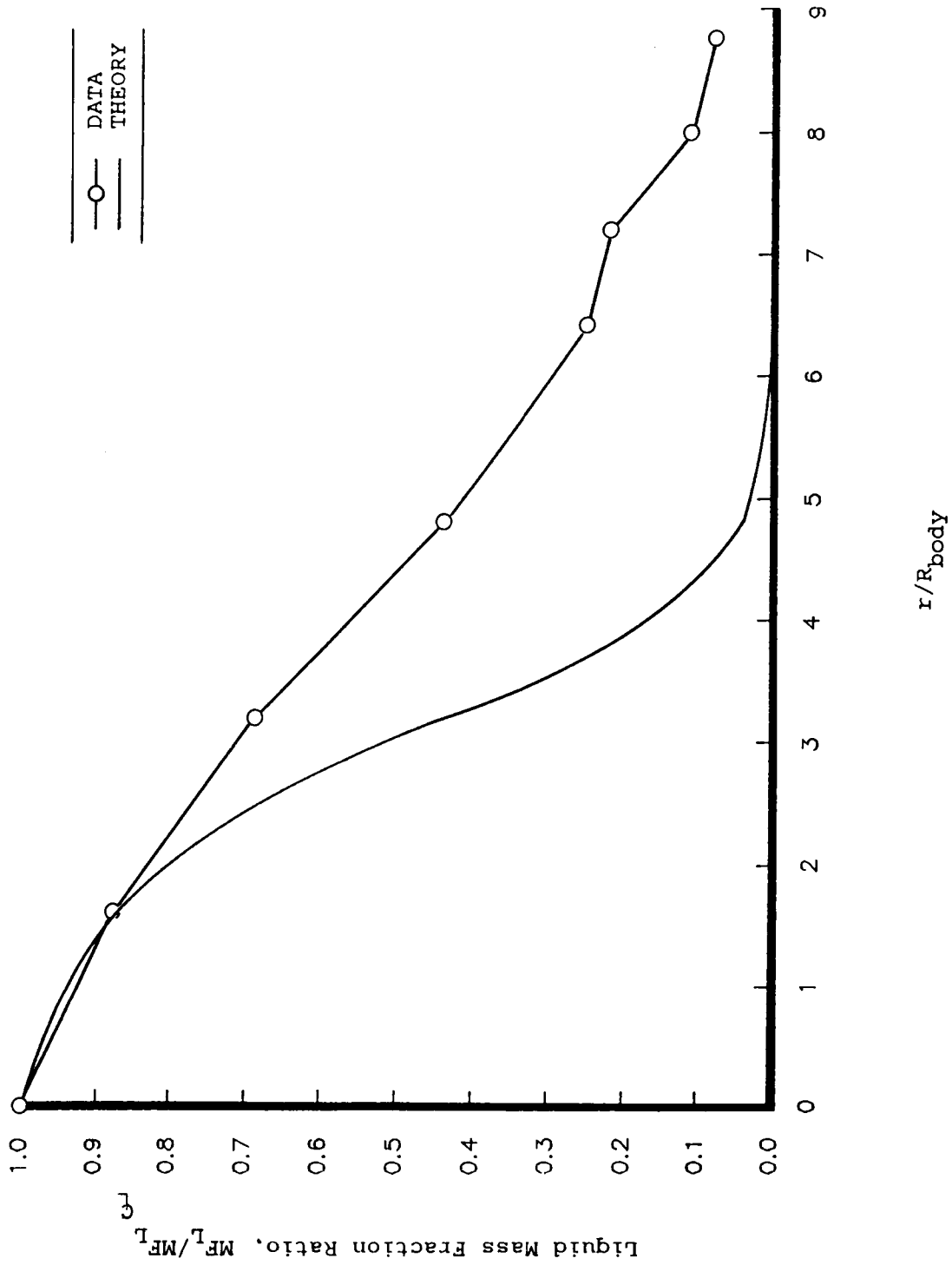


Figure 31. Model Predictions for Test Case 1 at 41 X/D

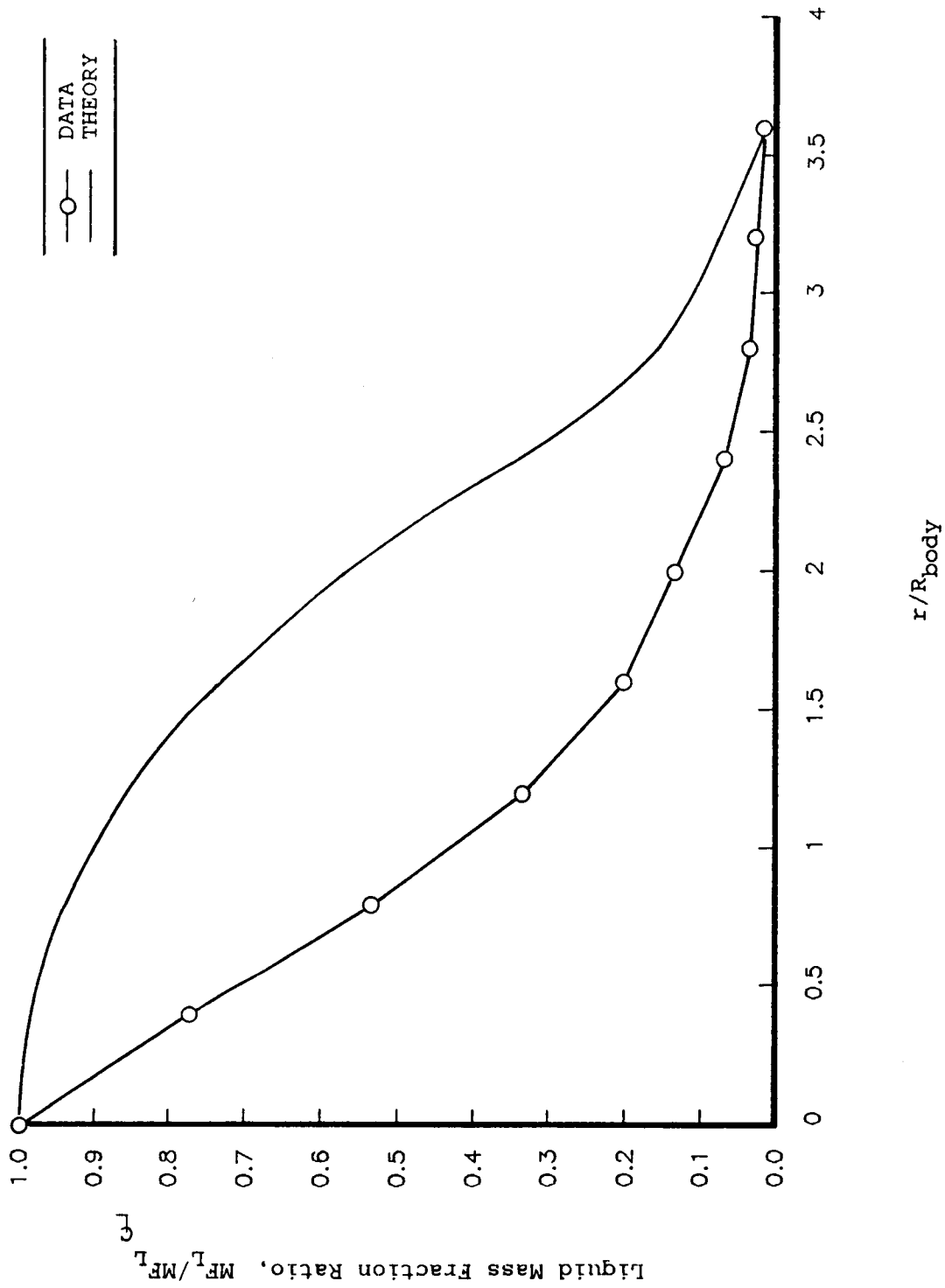


Figure 32. Model Predictions for Test Case 2 at 12 X/D

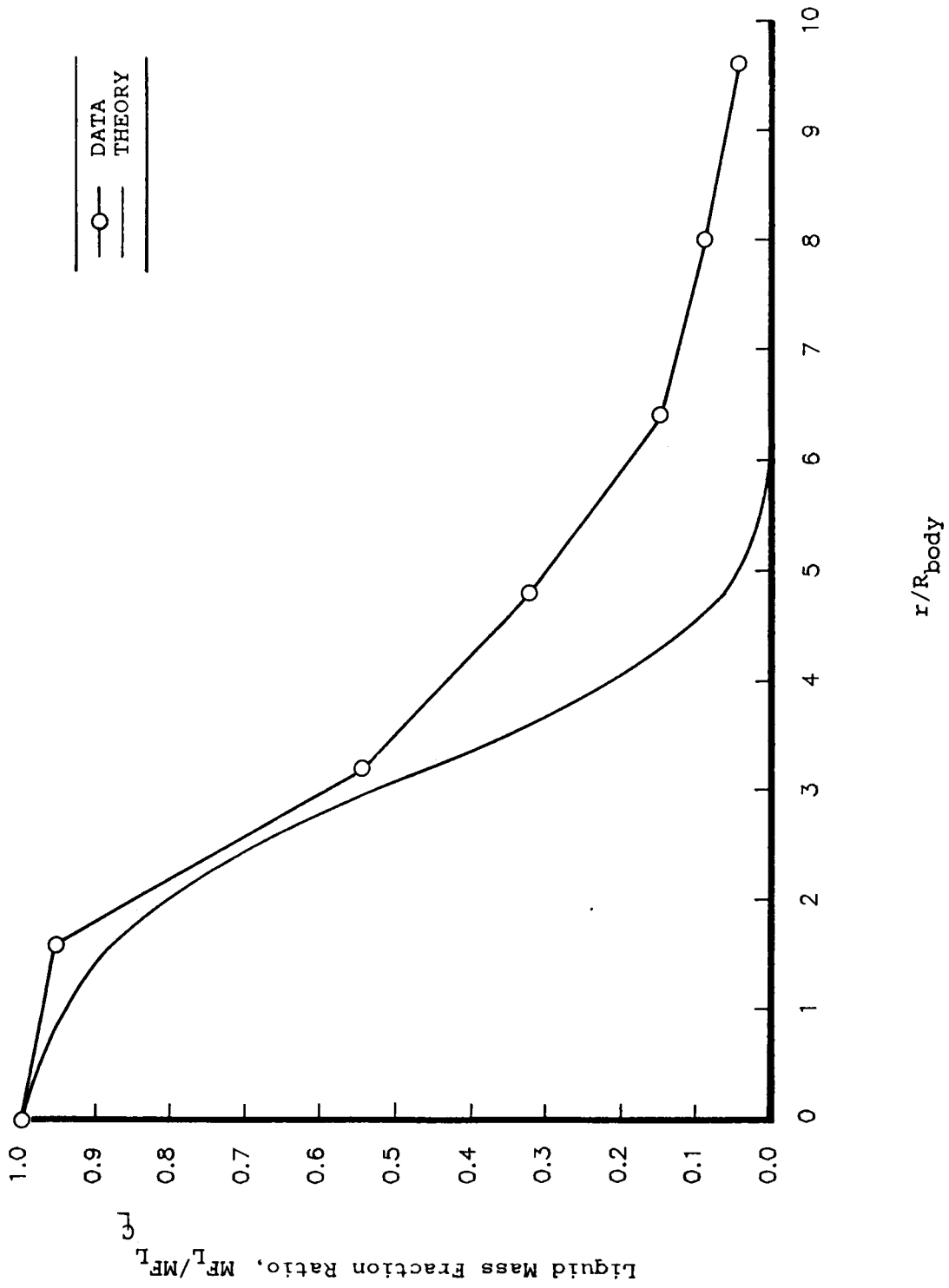


Figure 33. Model Predictions for Test Case 2 at 41 X/D

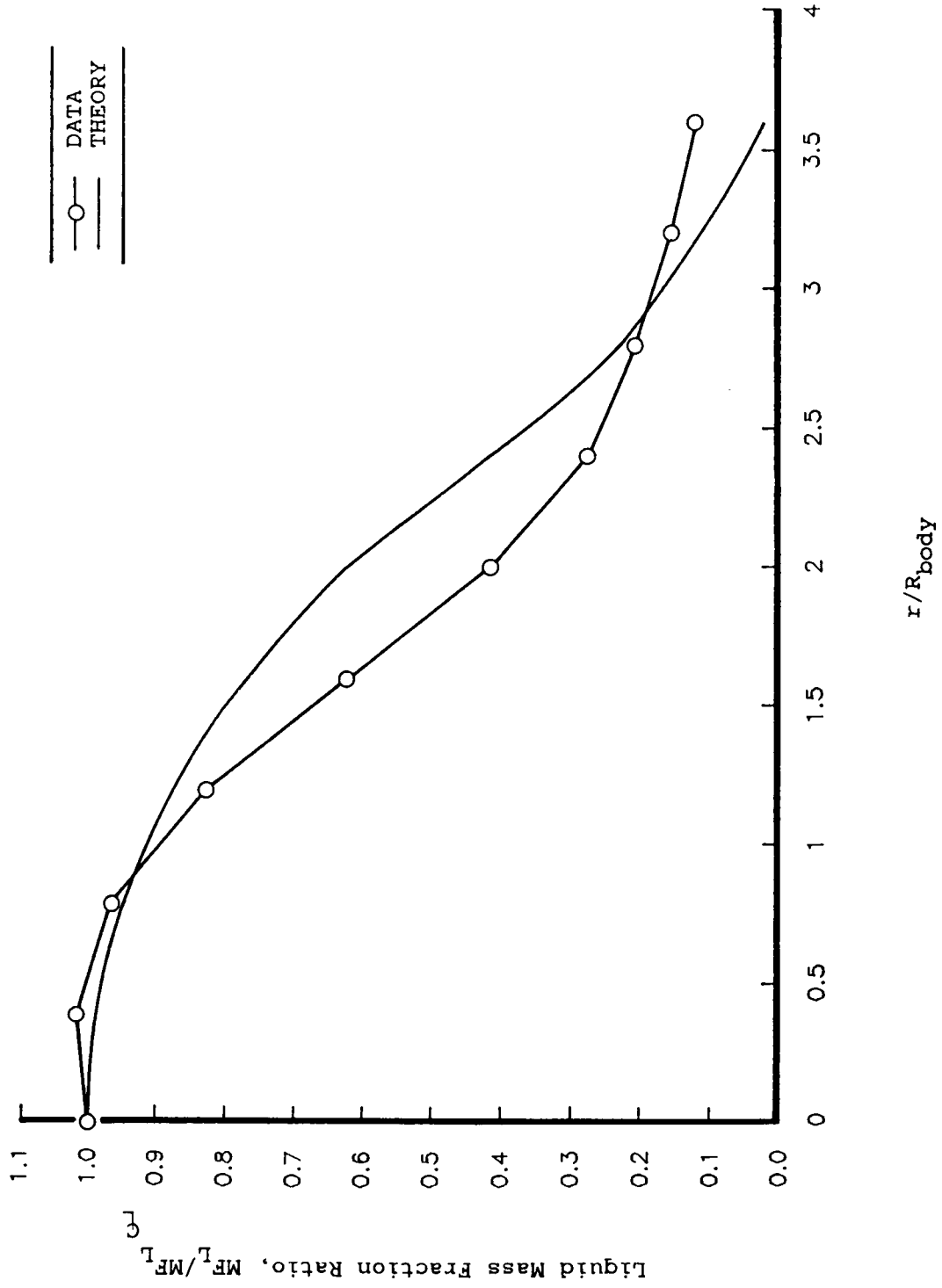


Figure 34. Model Predictions for Test Case 3 at 12 X/D

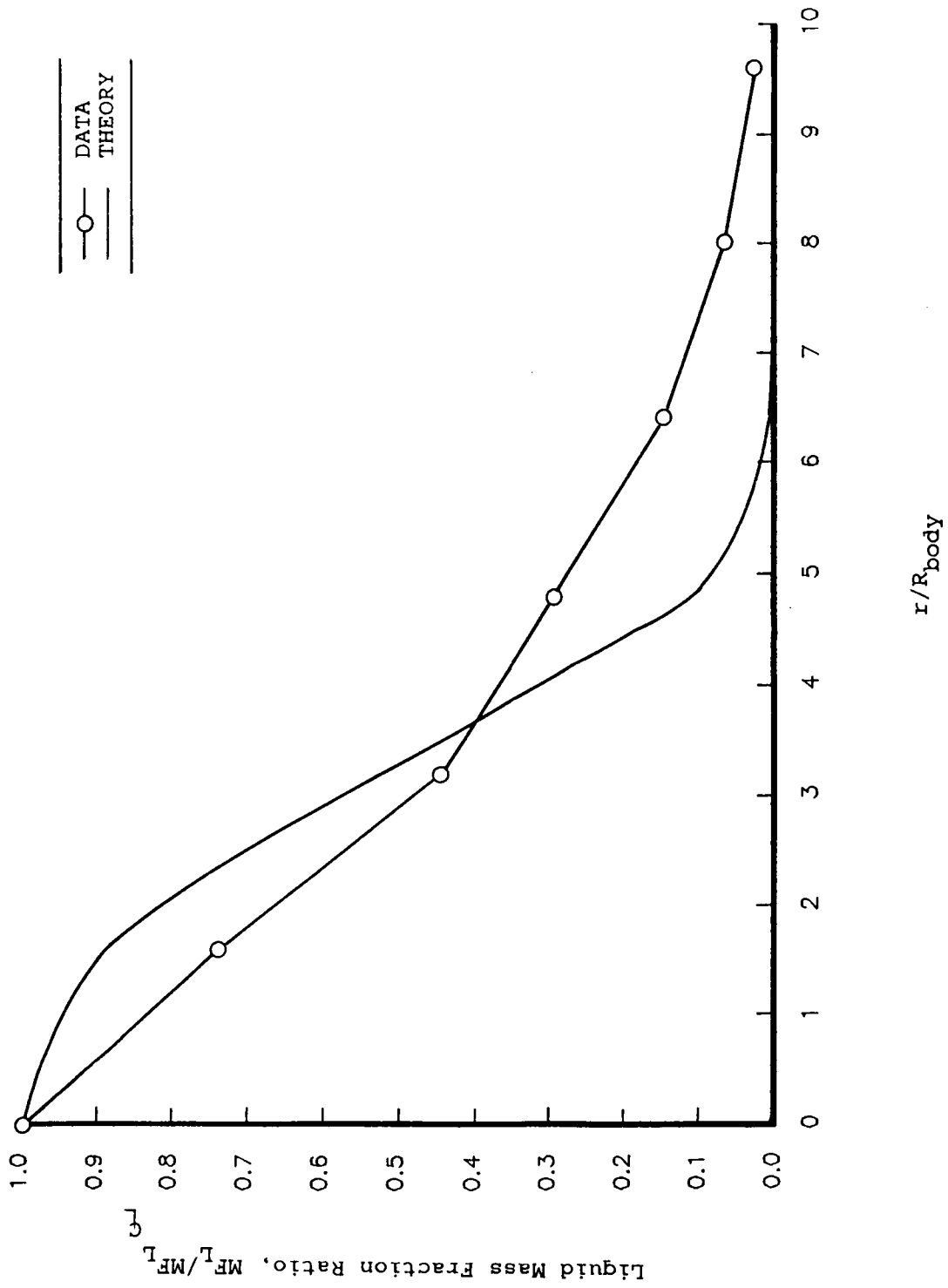


Figure 35. Model Predictions for Test Case 3 at 41 X/D

and Case 4 (Figures 36 and 37) are summarized in Table 10.

TABLE 10. Altitude Variation

TEST CASE	ALTITUDE,m	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
3	10607	25	18	55	12
4	1507	8	-42	-56	12

These results also indicate that no trend of model accuracy versus altitude exists.

The comparisons between Test Cases 1 and 2 and those between Test Cases 3 and 4 show that the accuracy of the predictions is not sensitive to altitude since the results did not show any significant difference in model performance (either improvement or worsening) despite large altitude variations.

5.2.2 Tunnel Air Velocity Variation

For the influence of the tunnel air velocity on the accuracy of the predictions, Cases 6 and 7 were compared. The tunnel air velocity for Case 6 was approximately 3 times as great as that for Case 7 with all other variables remaining constant. The results of the predictions for Case 6 (Figures 40 and 41) and Case 7 (Figures 42 and 43) are summarized in Table 11.

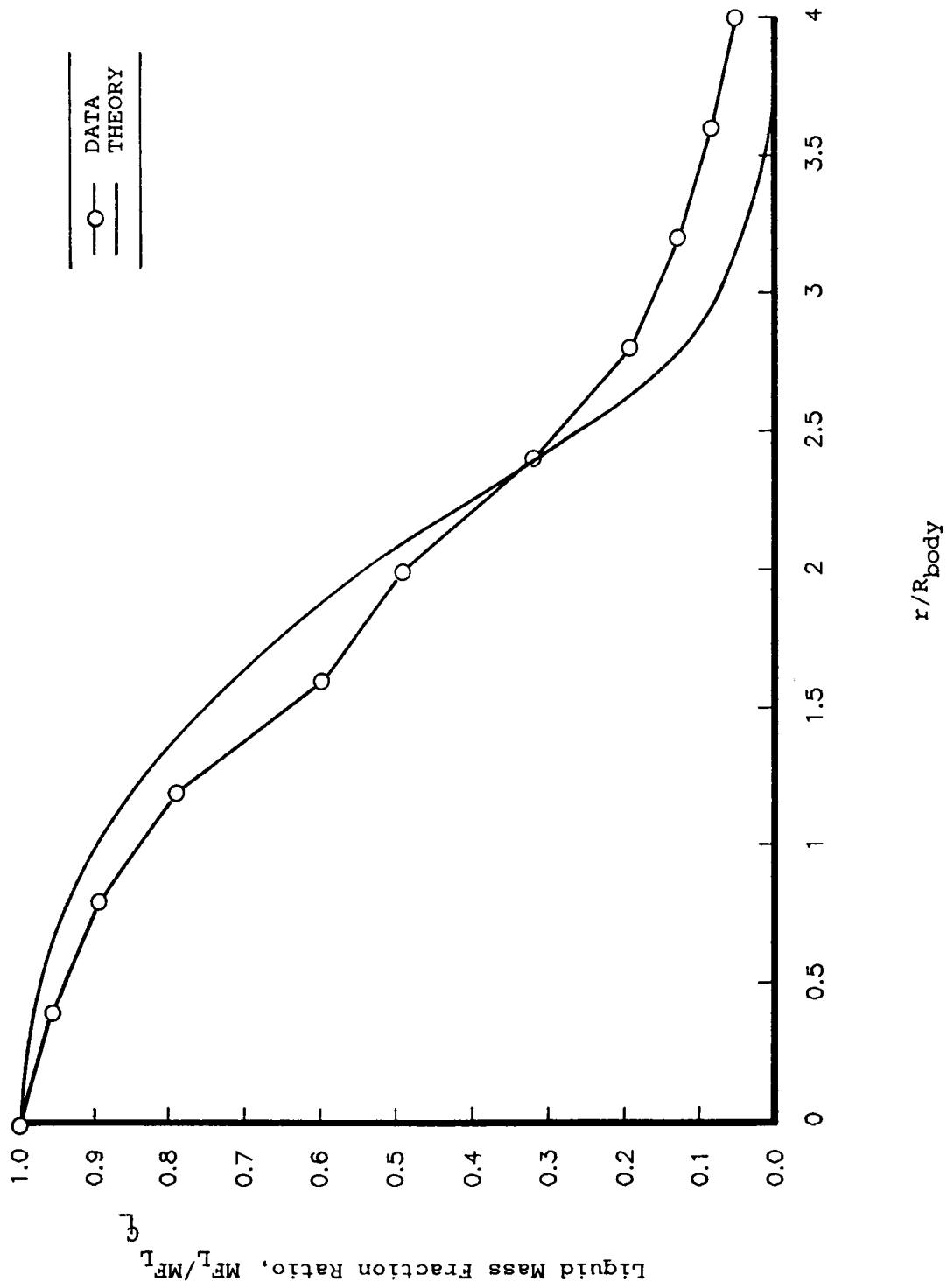


Figure 36. Model Predictions for Test Case 4 at 12 X/D

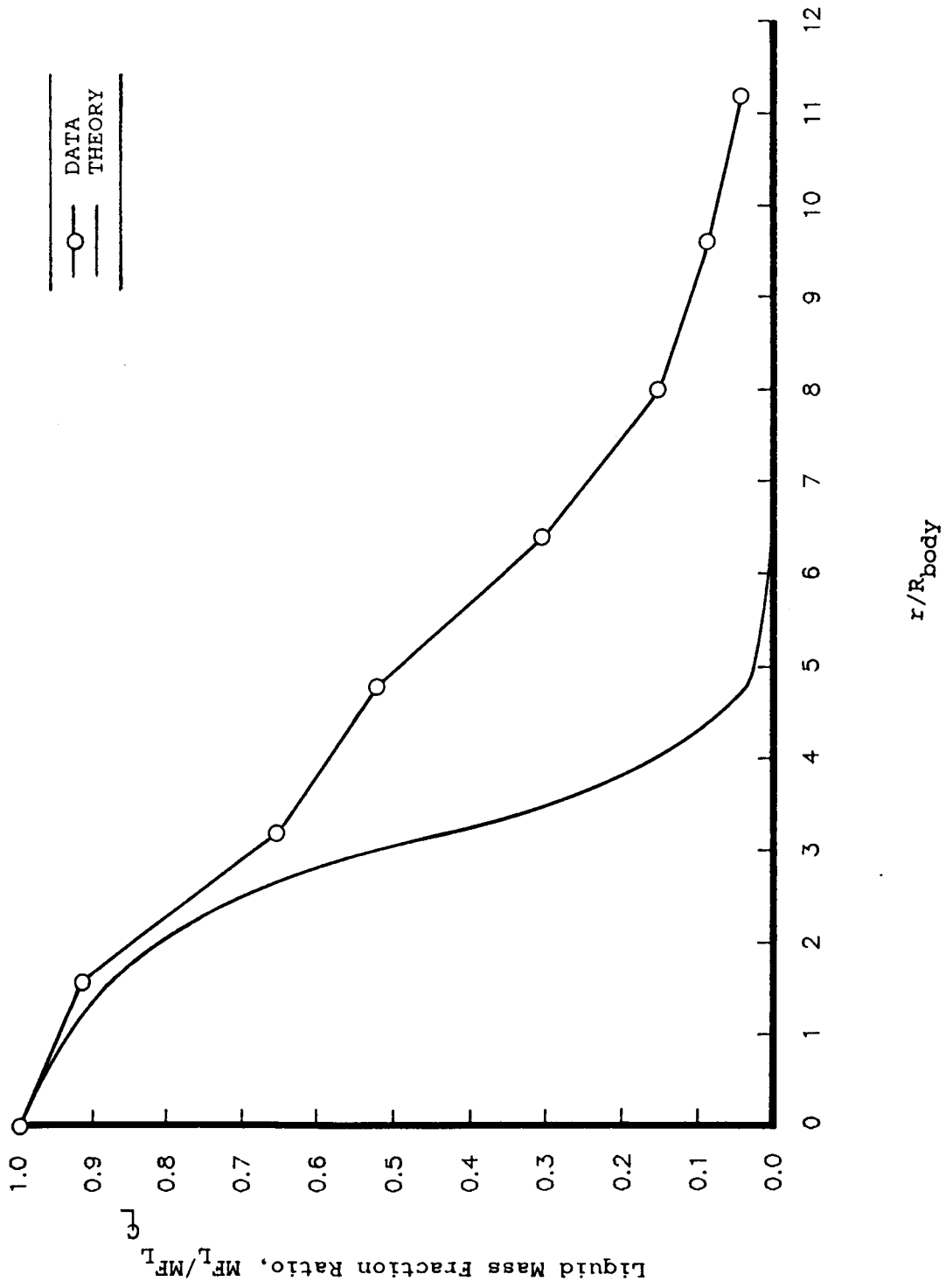


Figure 37. Model Predictions for Test Case 4 at 41 X/D

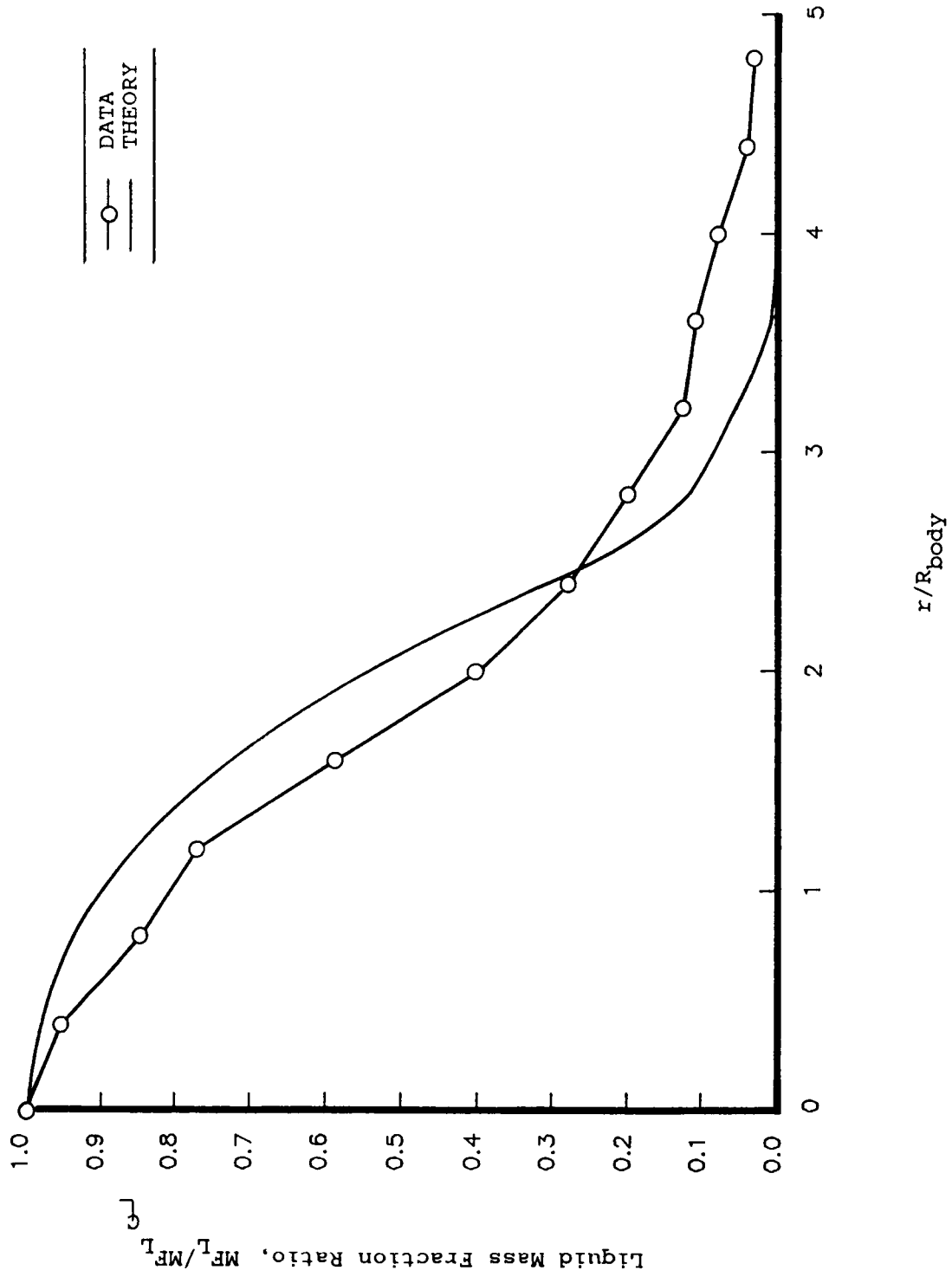


Figure 38. Model Predictions for Test Case 5 at 12 X/D

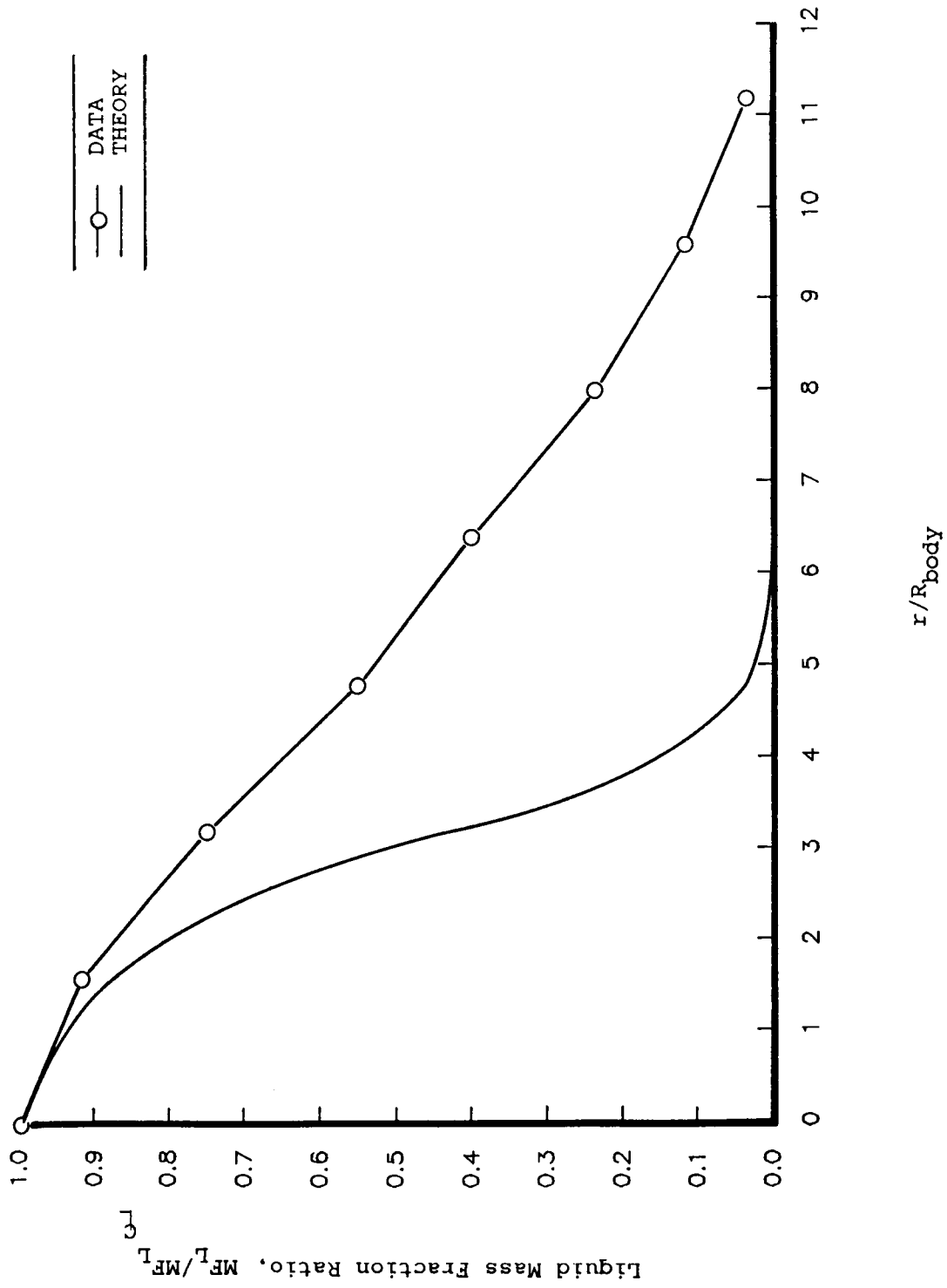


Figure 39. Model Predictions for Test Case 5 at 41 X/D

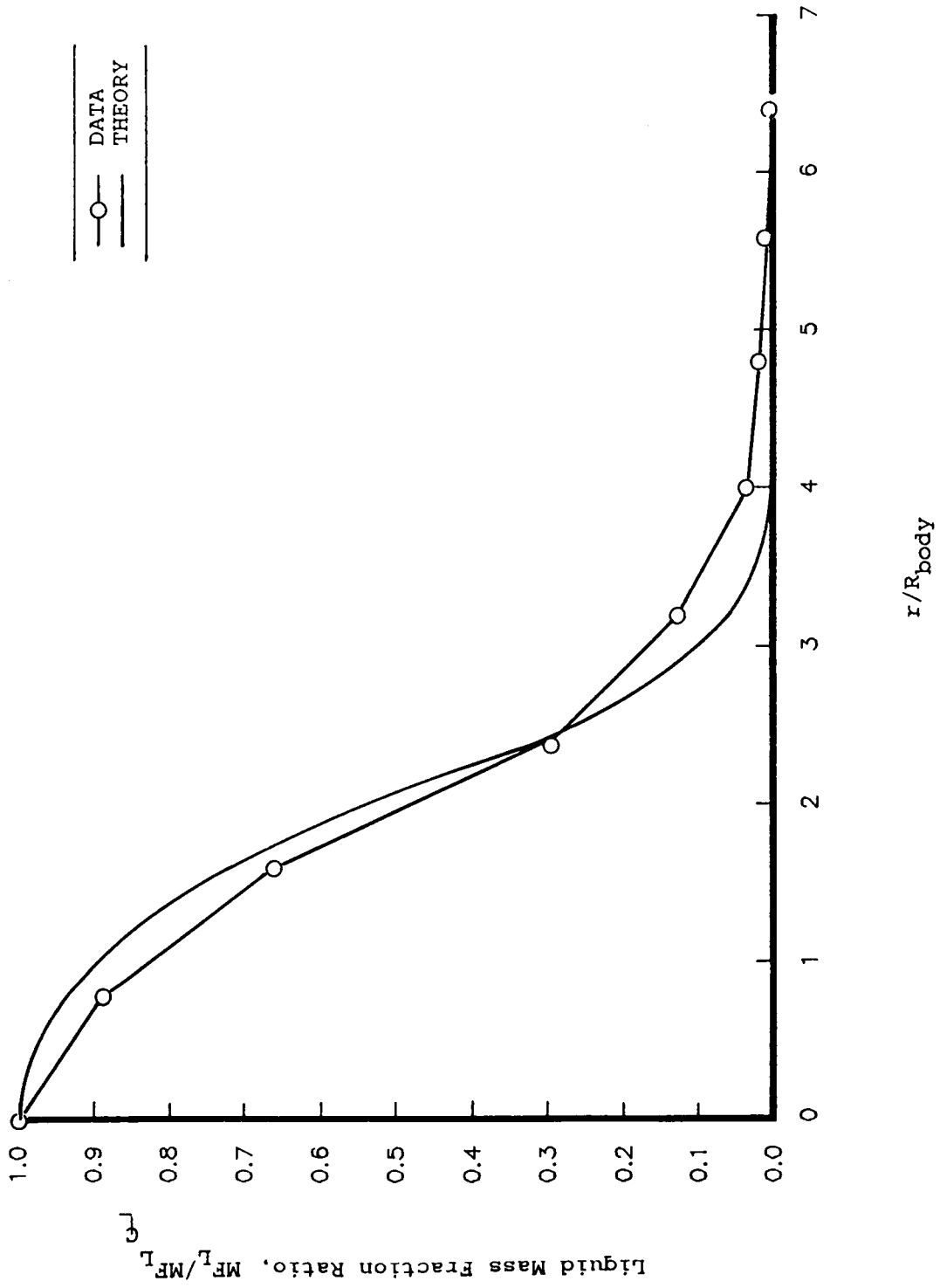


Figure 40. Model Predictions for Test Case 6 at 12 X/D

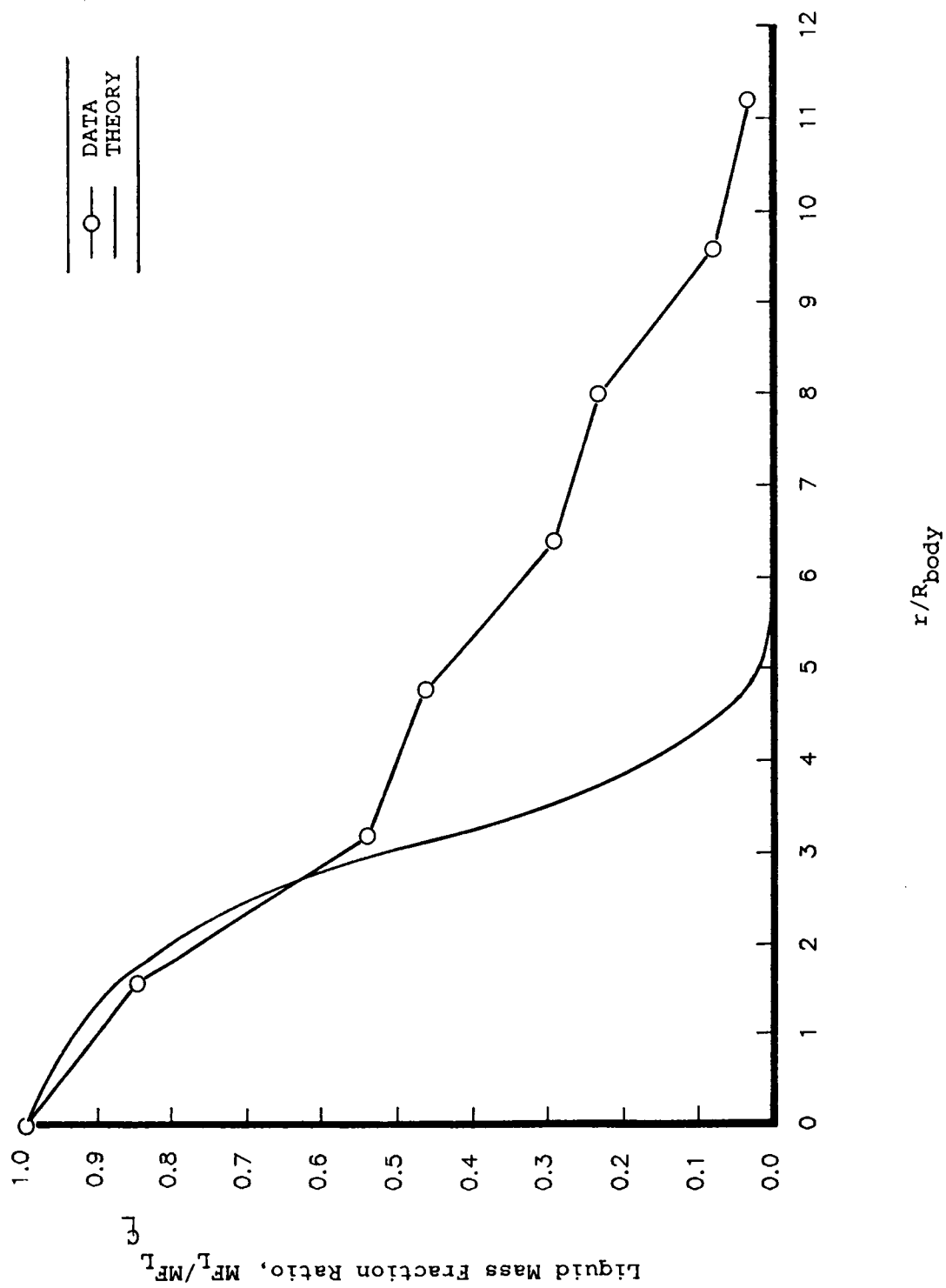


Figure 41. Model Predictions for Test Case 6 at 41 X/D

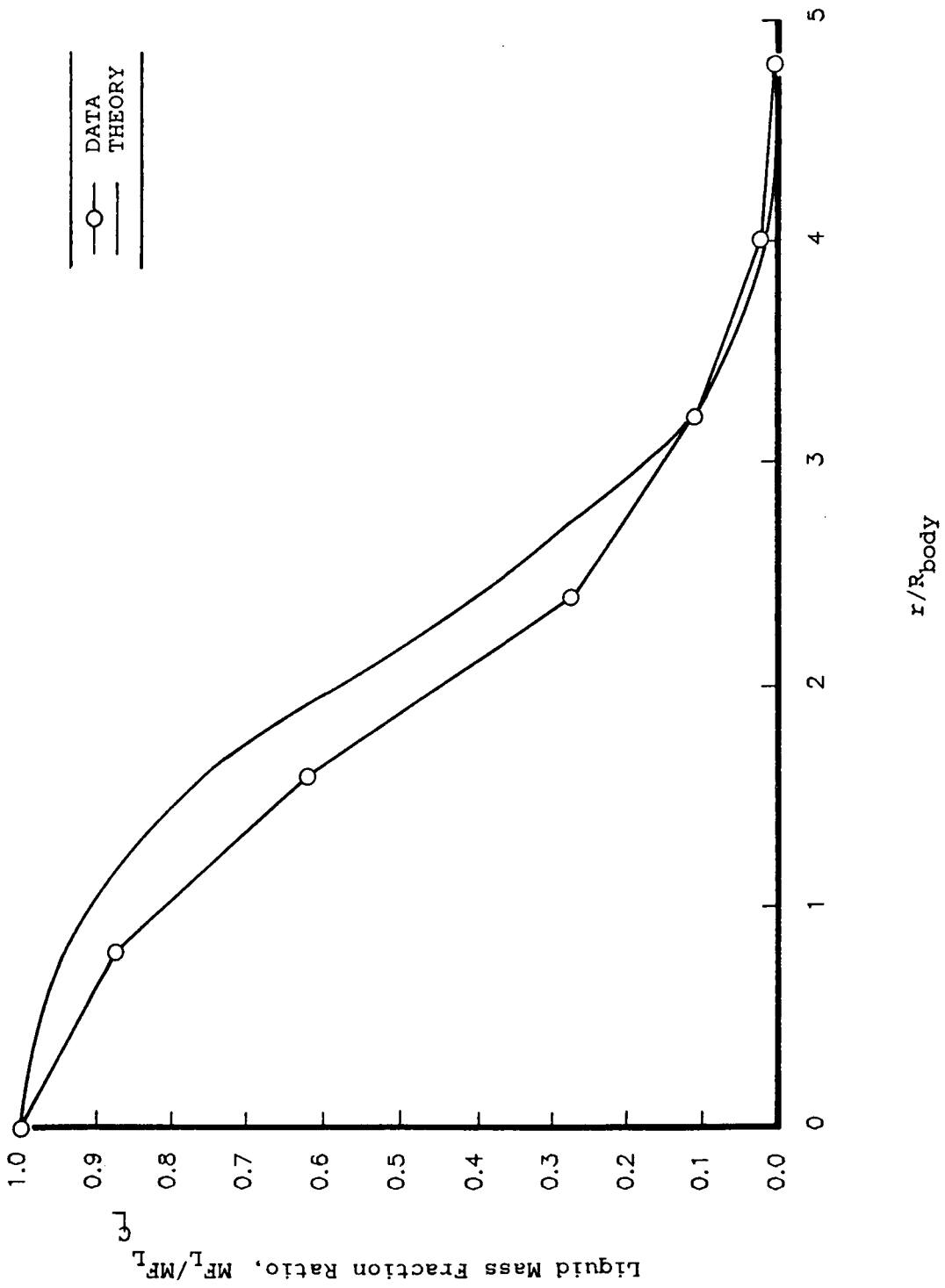


Figure 42. Model Predictions for Test Case 7 at 12 X/D

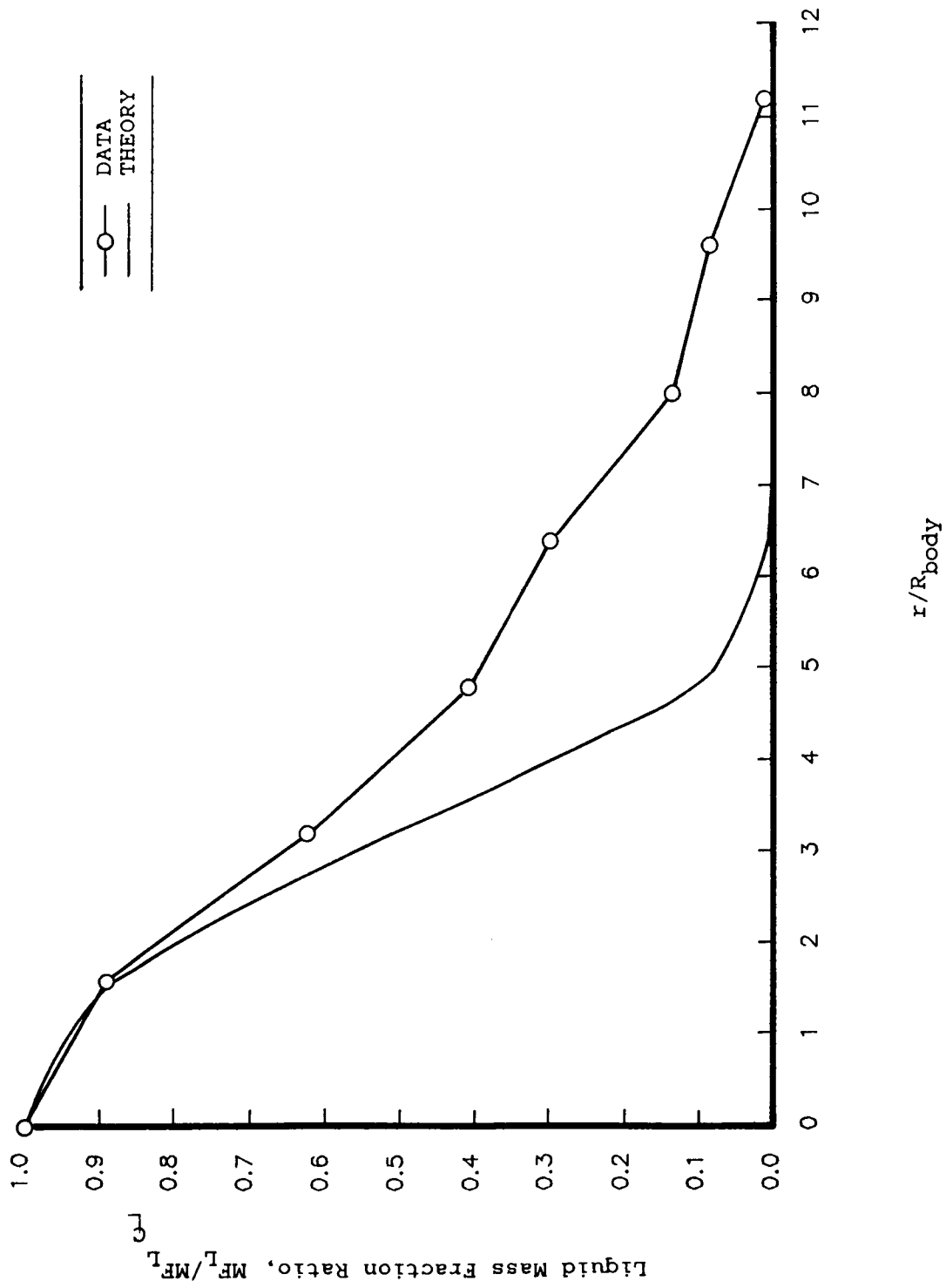


Figure 43. Model Predictions for Test Case 7 at 41 X/D

TABLE 11. Tunnel Air Velocity Variation

TEST CASE	TUNNEL AIR VELOCITY, m/sec	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
6	112.5	5	-26	-28	14
7	36.0	22	-23	66	112

It is apparent that the model performed better for the higher tunnel air velocities of Case 6. These higher velocities probably created higher turbulence levels in the body base recirculation zone, thereby better atomizing the liquid spray in the actual tests. This is supported by the smaller droplet diameters measured for Case 6 versus Case 7, which were $11.5\ \mu\text{m}$ versus $16.5\ \mu\text{m}$, respectively. Hence, the LHF approximations more closely resembled the actual spray in Case 6 than it did for Case 7.

Generally speaking, it appears that the higher the velocity of the free-stream air flow, the more accurate the model predictions will be. This is discussed fully in section 5.3.

5.2.3 Liquid Ejection Flow Rate Variation

To evaluate whether the model better predicted the test data as a function of the liquid ejection flow rates, Cases 4 and 5 were used for one direct comparison, and Cases 8 and 9 for another. Case 4 used a liquid flow rate approximately

70% greater than that of Case 5. The results for Case 4 (Figures 36 and 37) and Case 5 (Figures 38 and 39) are summarized in Table 12.

TABLE 12. Liquid Ejection Flow Rate Variation

TEST CASE	LIQUID EJECTION FLOW RATE, kg/sec	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
4	0.0515	8	-42	-36	12
5	0.0314	20	-45	-44	28

The accuracy of the predictions at 12 and 41 X/D are fairly similar for both cases, but the model was slightly more accurate as the liquid mass flow rate increased. It is interesting to note that the spray profiles for the experimental data are very similar when the two cases are compared. The same holds true for the math model data of the two cases. This indicates that the liquid spray velocity in the model or in the experiments has only a small amount of influence on the spray diameters of the jet spray downstream of the body.

A comparison of Test Cases 8 and 9 can also be made. Case 9 used a liquid flow rate approximately 150% greater than that of Case 8. The results for Case 8 (Figures 44 and

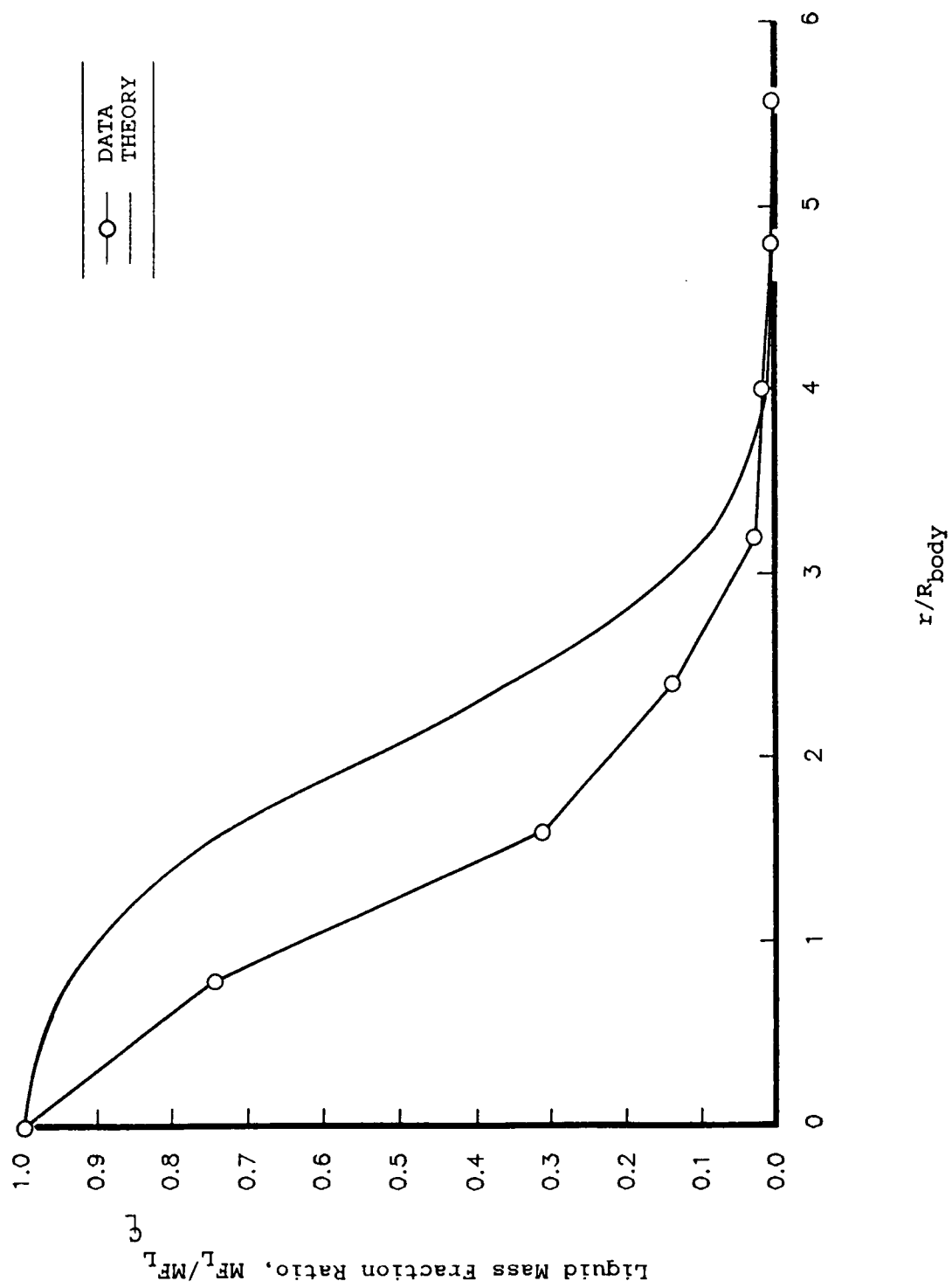


Figure 44. Model Predictions for Test Case 8 at 12 X/D

45) and Case 9 (Figures 46 and 47) are summarized in Table 13.

TABLE 13. Liquid Ejection Flow Rate Variation

TEST CASE	LIQUID EJECTION FLOW RATE, kg/sec	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
8	0.0214	68	-36	5	155
9	0.0491	47	-6	49	29

The comparisons of Cases 8 and 9, as well as those of Cases 4 and 5, show that the model consistently predicted the spray diameters more accurately for the higher liquid mass flow rate. This was generally the case for the mass concentrations at the centerline with the exception of Case 8 at 12 X/D. The droplet diameters were almost identical in both cases.

The effect of the liquid ejection velocity calculated in the model was also investigated since it is based on the actual liquid ejection flow rate. However, since the velocity in the model is related to the jet spray vapor density and an arbitrarily chosen spray radius, the jet velocity calculated in the model has no relationship to that in the actual experiment. As shown in Fig. 48, there is no correlation between the accuracy of the predicted mass

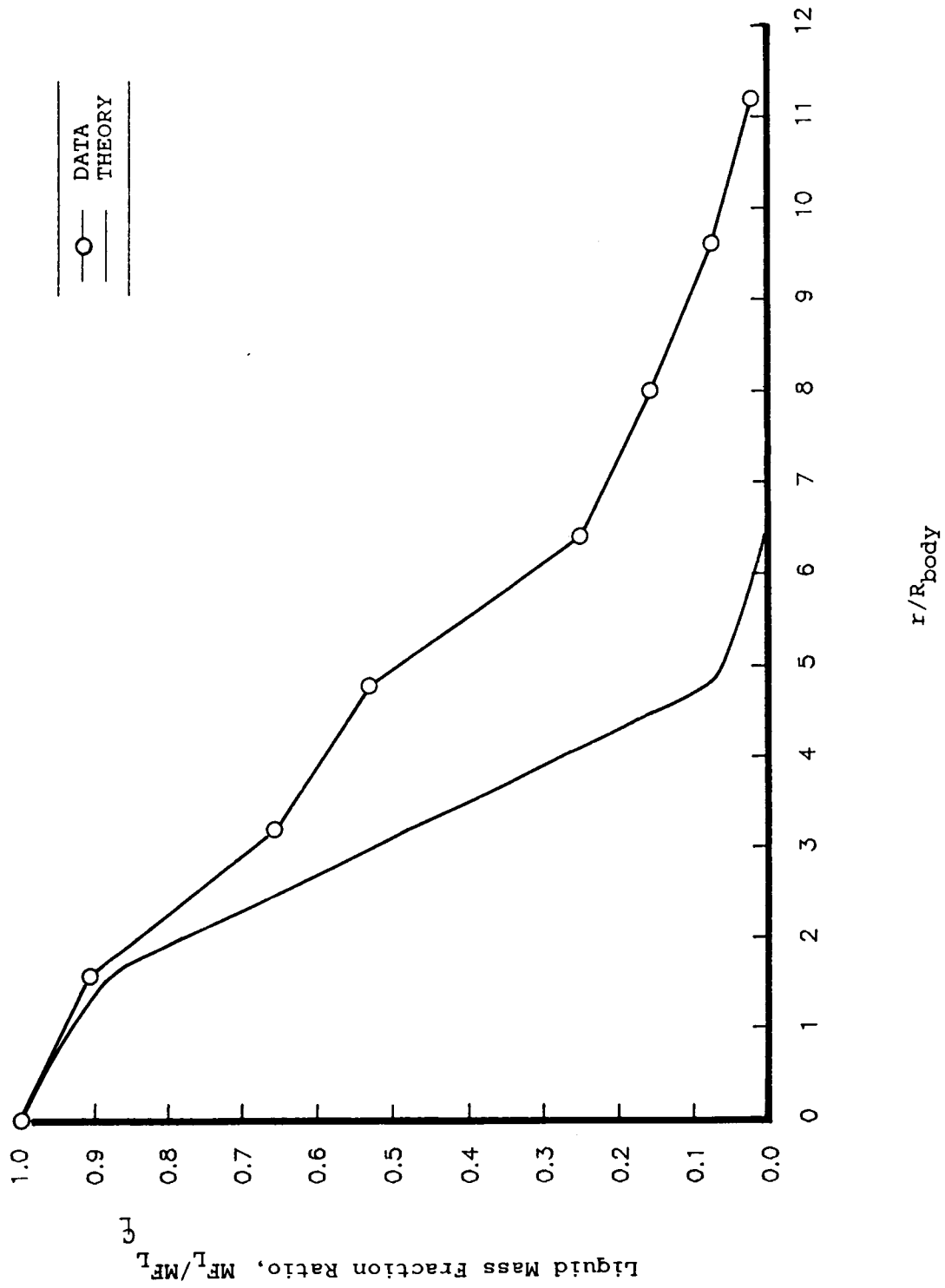


Figure 45. Model Predictions for Test Case 8 at 41 X/D

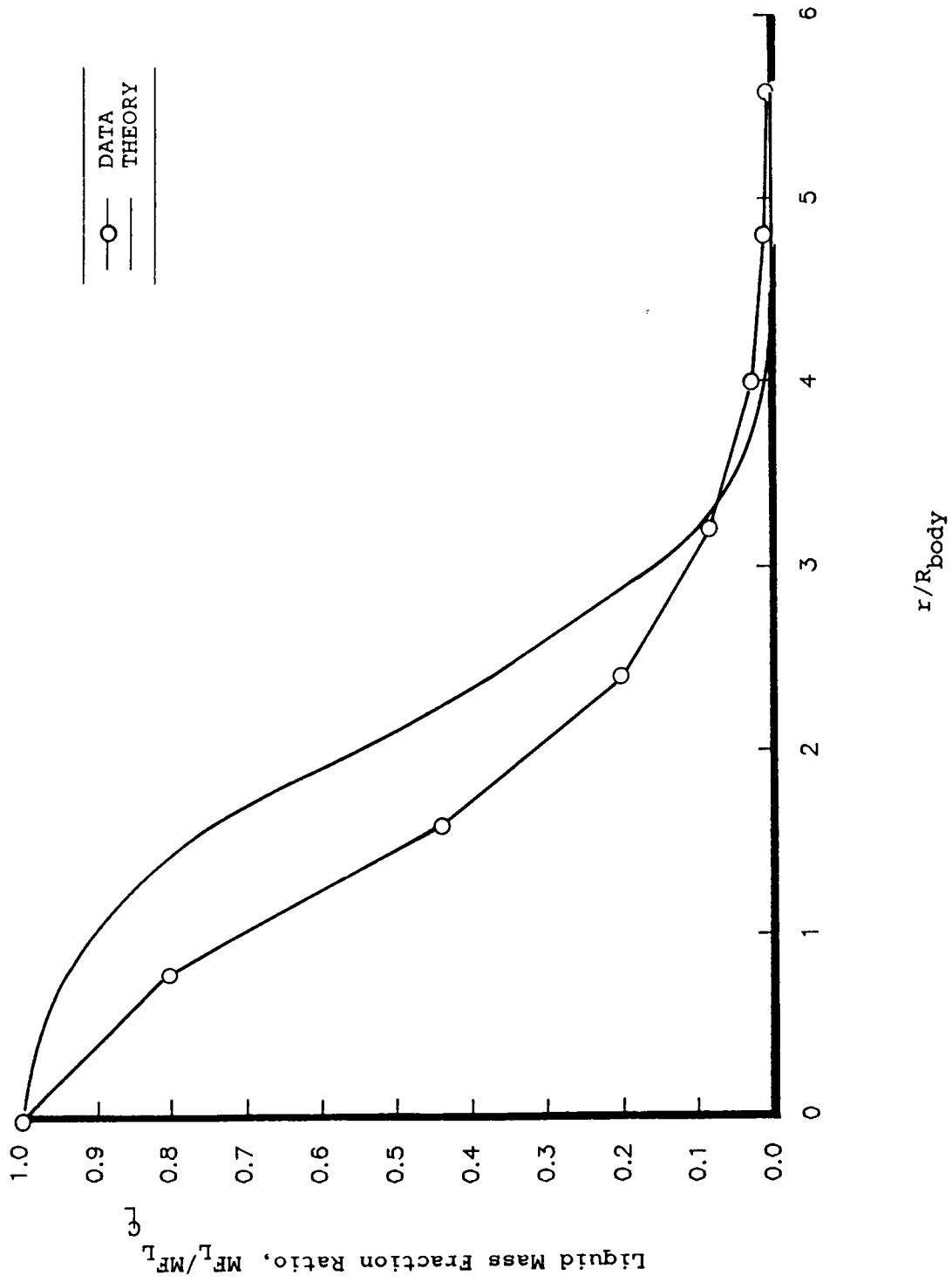


Figure 46. Model Predictions for Test Case 9 at 12 X/D

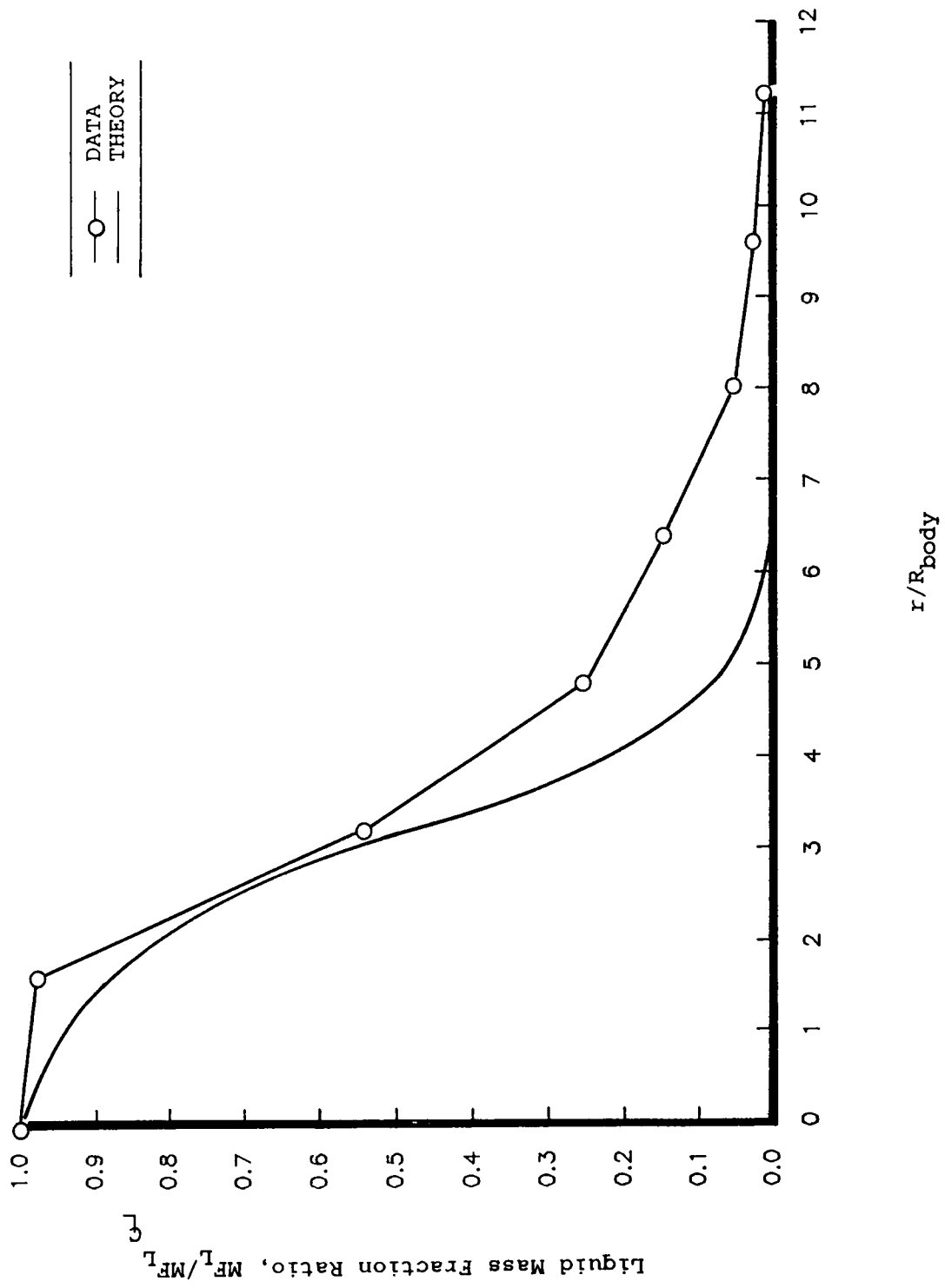


Figure 47. Model Predictions for Test Case 9 at 41 X/D

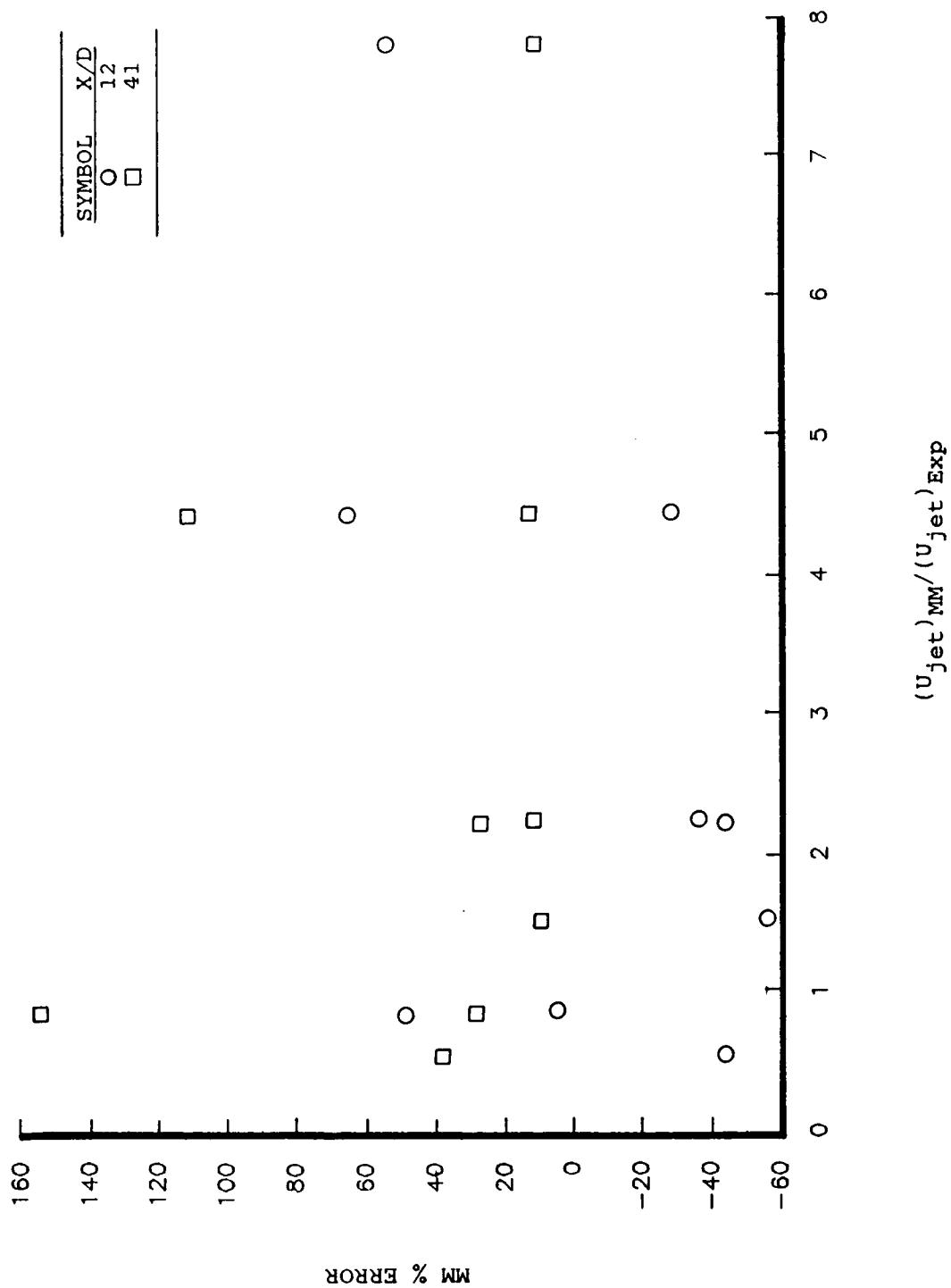


Figure 48. Correlation of the Spray Ejection Velocity Ratio of the Model and Experiment with Model Accuracy of Predicted Mass Concentrations

concentrations at the centerline and the ratio of the jet velocities of the model and experiment. There is also no correlation in the predicted spray diameters and this velocity ratio, as shown in Fig. 49. Therefore, the difference in the jet velocity calculated in the model and the actual jet velocity in the experiments did not have a dominating effect on the accuracy of the predictions.

5.2.4 Single-Hole Versus Multi-Hole Nozzles

One would expect the model to do a better job predicting the test data which used the multi-hole nozzle than the single-hole nozzle since the multi-hole nozzle would result in a more diffused spray pattern. A direct comparison of the results for Case 7 (Figures 42 and 43) which used the single-hole nozzle and Case 9 (Figures 46 and 47) which used the multi-hole nozzle can be made. The results, summarized in Table 14, show that the model performed better for the multi-hole nozzle of Case 9 than for the single-hole nozzle of Case 7.

TABLE 14. Single-Hole versus Multi-Hole Nozzles

TEST CASE	NOZZLE TYPE	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
7	Single-Hole	22	-23	66	112
9	Multi-Hole	47	-6	49	29

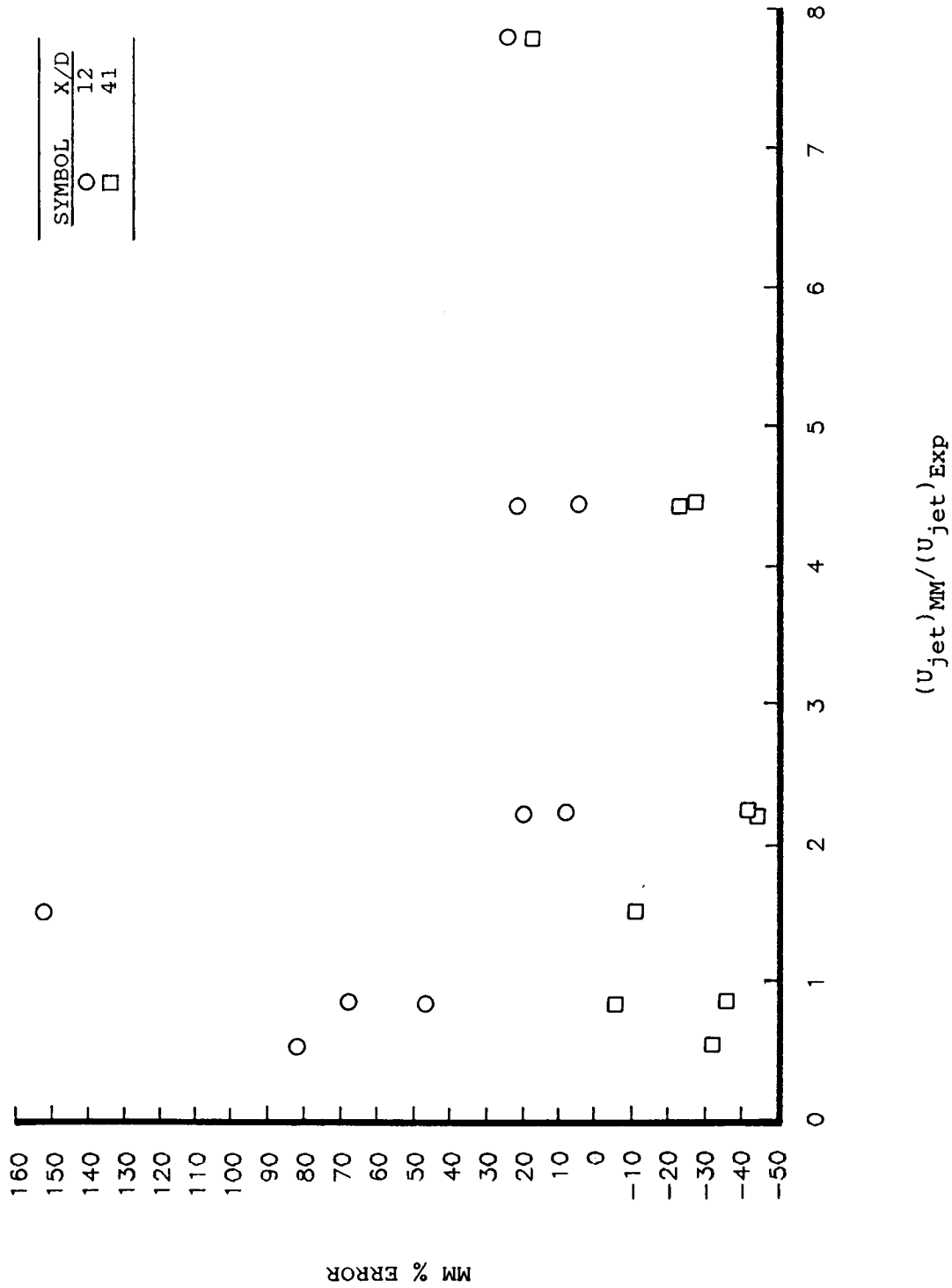


Figure 49. Correlation of the Spray Ejection Velocity Ratio of the Model and Experiment with Model Accuracy of Predicted Spray Diameters

These results may be attributed to the better atomization of the liquid spray which occurred for Case 9 as proved by the smaller droplet diameters measured, i.e., 14.9 μm for Case 9 versus 16.5 μm for Case 7.

5.2.5 Nozzles With and Without Atomization Air

Theoretically, the more atomized the jet spray is in the experimental data, the better the model should predict the results. A comparison of Case 4 and Case 6 verifies this to be true. Both cases used a single-hole nozzle, but Case 4 did not use atomization air where Case 6 did. The results for Case 4 (Figures 36 and 37) and Case 6 (Figures 40 and 41) are summarized in Table 15.

TABLE 15. Nozzles With and Without Atomization Air

TEST CASE	NOZZLE TYPE	MM % ERROR Spray Diameter		MM % ERROR Mass Conc. @ C_L	
		12 X/D	41 X/D	12 X/D	41 X/D
4	Single-Hole	8	-42	-36	12
6	Single-Hole, Gas Atomized	5	-26	-28	14

These results show that the predictions did improve as the actual sprays became increasingly atomized.

5.3 MODEL ACCURACY VERSUS DROPLET SIZE

One would expect the accuracy of the predictions to generally depend on the amount of atomization of the spray in the actual test cases since the model assumes a vaporized jet spray. The results of the two direct comparisons made for nozzle types in sections 5.2.4 and 5.2.5 showed this to be true. A broader look at model accuracy versus drop size was made which included all nine of the test cases. Fig. 50 shows that there is no real trend between the accuracy of the predicted mass concentrations at the centerline and the droplet diameter at both 12 and 41 X/D. Also, Fig. 51 reveals that no trend exists for the predicted spray diameters versus drop size at 12 and 41 X/D. On the other hand, when the model results are plotted against the free-stream pressure, the mass concentrations (Fig. 52) and the spray diameters (Fig. 53) indicate that overall model results improved as the free-stream pressure increased. More specifically, the error in the predicted mass fractions at 41 X/D show a tendency to improve as the free-stream pressure increased. A slight improvement, if any, is seen at 12 X/D. Unlike the results versus droplet diameters, the predicted spray diameters at 12 X/D improve as free-stream pressure increases. Therefore one can conclude that the model accuracy in predicting both the mass concentrations and the spray diameters generally improve as the free-stream pressure increases.

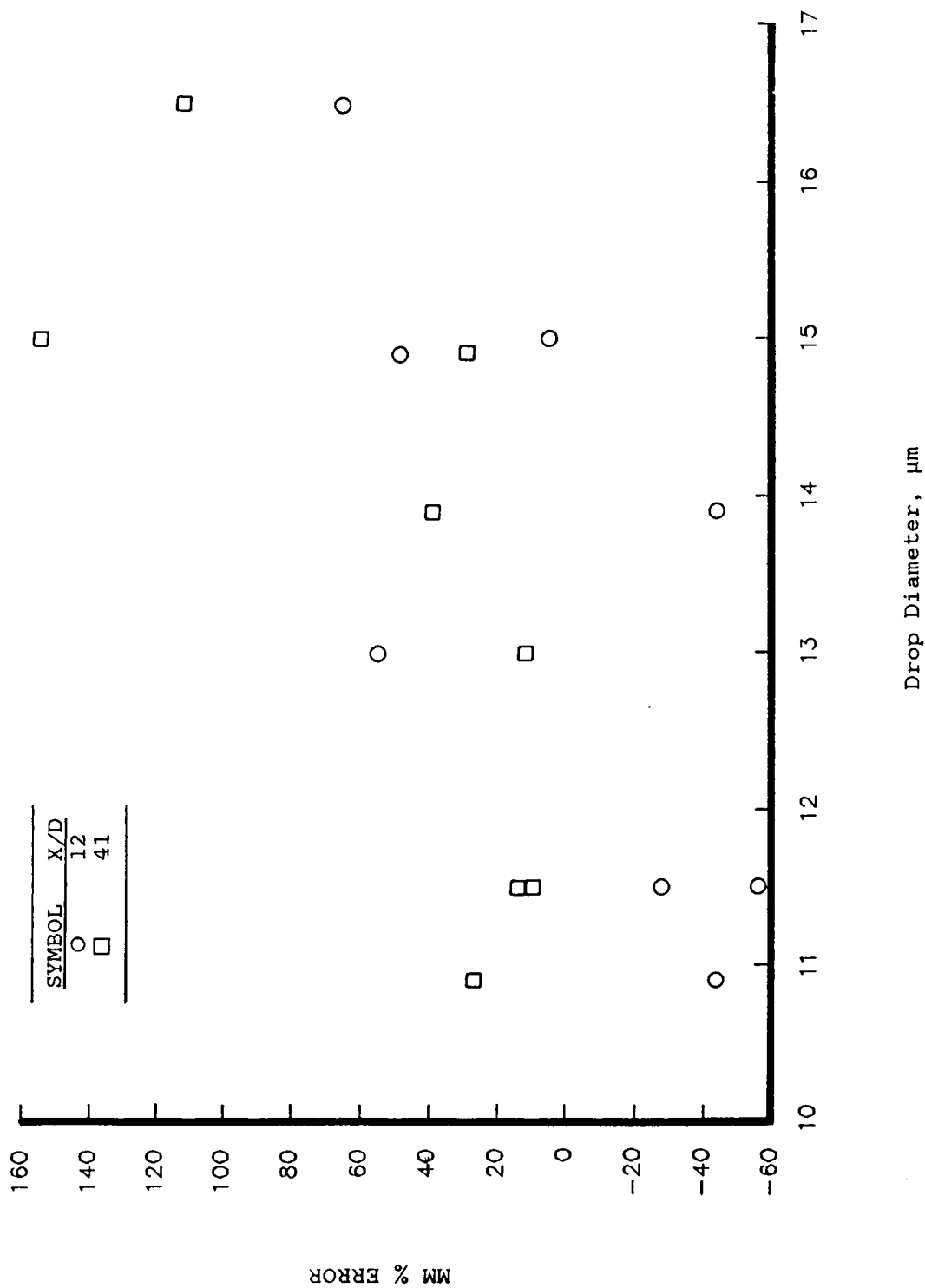


Figure 50. Correlation of Liquid Droplet Diameter Size with Model Accuracy of Predicted Mass Concentrations

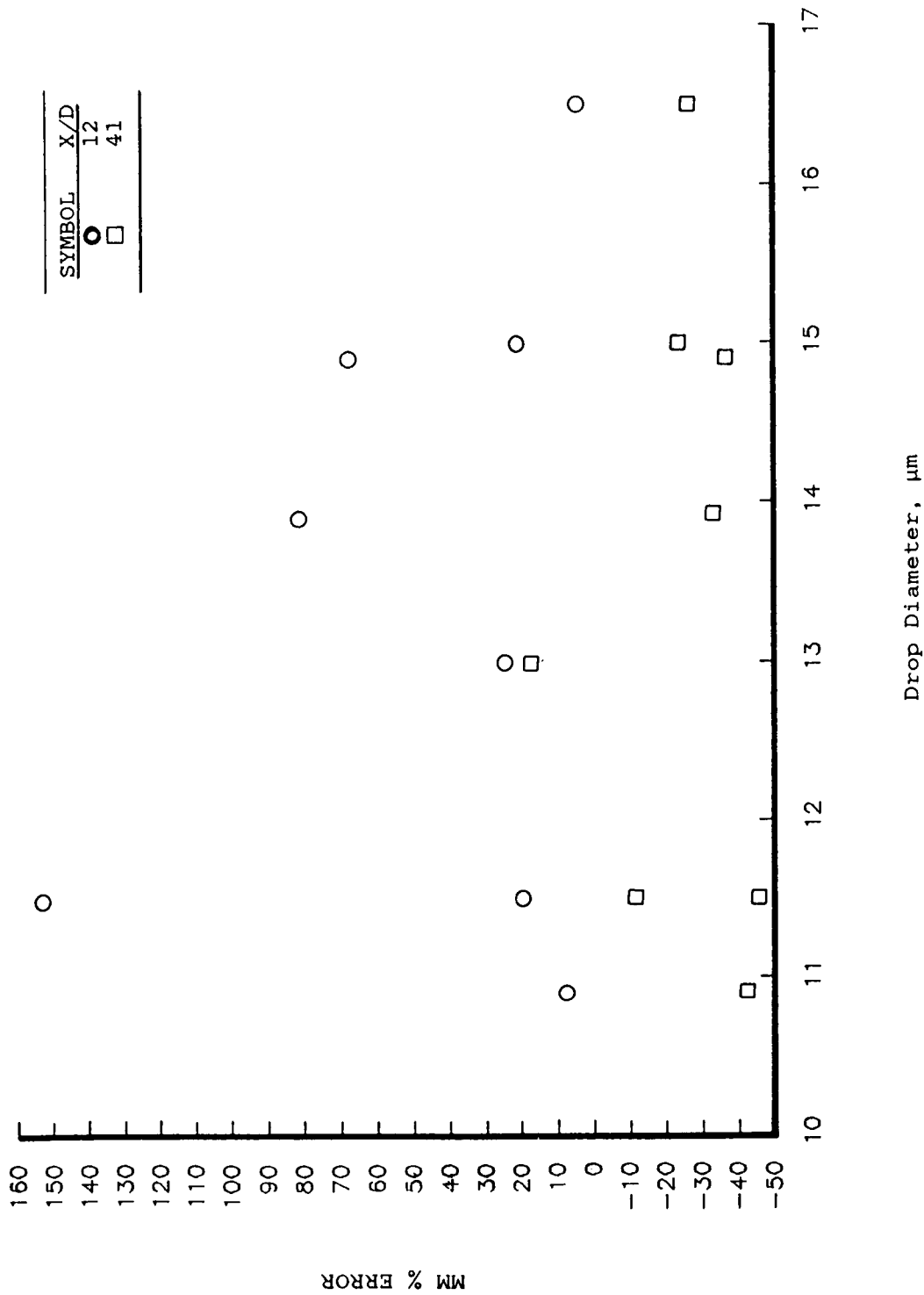


Figure 51. Correlation of Liquid Droplet Diameter Size with Model Accuracy of Predicted Spray Diameters

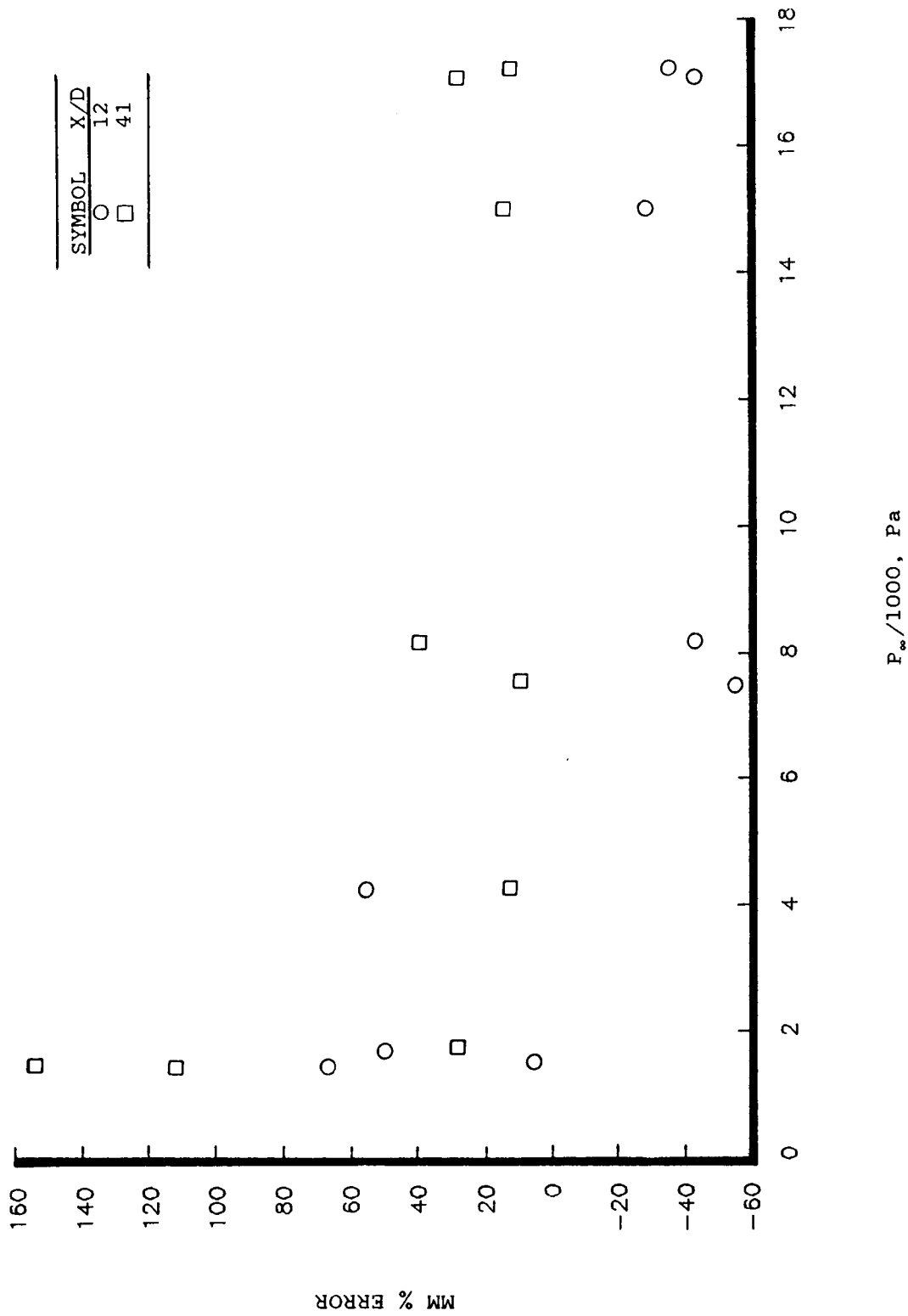


Figure 52. Correlation of Free-Stream Total Pressure with Model Accuracy of Predicted Mass Concentrations

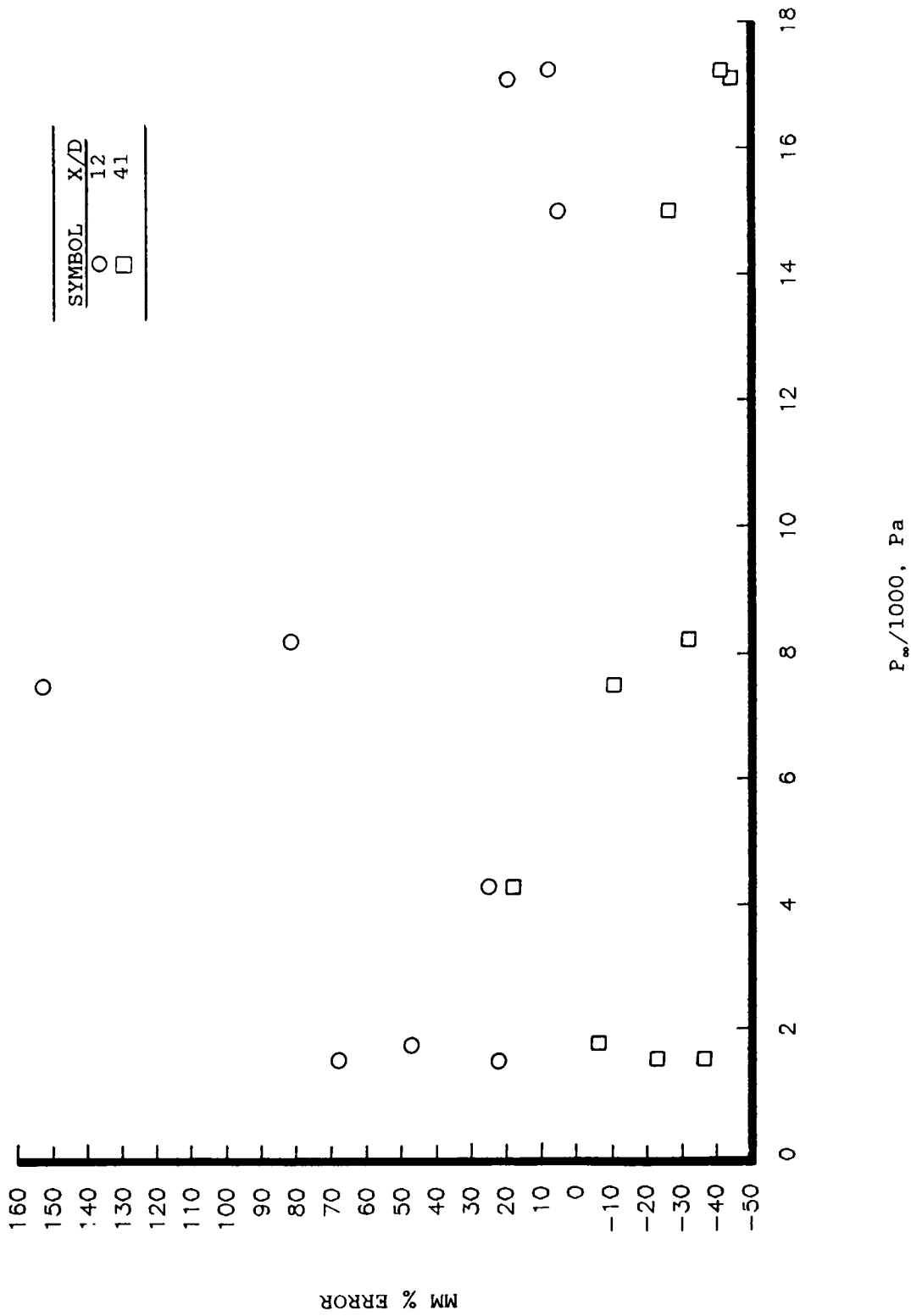


Figure 53. Correlation of Free-Stream Total Pressure with Model Accuracy of Predicted Spray Diameters

5.4 BASE PRESSURE

The base-pressure coefficients for the math model predictions and the experimental data for Cases 10 through 14 are presented in Table 2. The boundary layer velocity power law profile used in the mass concentration analysis was also used for the base pressure study to achieve a certain level of calibration of the model using these same profiles. The experimental data taken at the Ground Level Test Stand (GLTS) yielded base pressure coefficients between -0.060 and -0.085 [18]. This test data falls in the range of base pressure data from cylinders taken from several sources which measured base-pressure coefficients in the range of -0.05 to -0.17 for free-stream Mach numbers less than 0.4 [25,26]. The math model predicted a base-pressure coefficient for the data taken in GLTS of approximately -0.24 for all the tunnel air velocities tested for Cases 10 through 14. Since the model results are not within the experimental range, then these model predictions are not considered useful for any practical application. This disagreement could be the result of the initial velocity and turbulence kinetic energy profiles used in the model for these cases. A future study could investigate the effects of these profiles on the calculated base pressures in the hope of achieving predictions within the experimental range

and eventually within the measurement uncertainty of the experimental data.

5.5 DISCUSSION OF RESULTS

This LHF model invariably overestimated the spray diameters of the jet spray at 12 X/D downstream of the cylindrical body. However, the model predictions at 41 X/D downstream of the body almost invariably underestimated the jet spray diameters. The spray diameters were overestimated at 12 X/D by as much as 150%, and were underestimated at 41 X/D by as much as 45%. One possible explanation for the overestimated spray diameters at 12 X/D is the LHF theory approximation that the spray is assumed to be a perfect gas. This will cause the spray in the model to be much more susceptible to turbulent mixing than the actual spray which will cause higher mixing rates near the cylindrical body than existed in the actual experiment. Since the model results at 41 X/D were reversed from those at 12 X/D, i.e., the spray diameters were almost invariably underestimated at 41 X/D, it is possible that the mixing rate in the model was dramatically less than that in the actual experiment as the calculations progressed from 12 to 41 X/D downstream of the cylindrical body. The results at 41 X/D imply that the turbulent dissipation rate calculated in the model is too high. When the results at 12 X/D are considered in

conjunction with those at 41 X/D, it seems that model accuracy may be improved by decreasing the amount of turbulence in the recirculation zone while decreasing the rate of turbulent dissipation further downstream of the cylindrical body. This would decrease the spray diameters at 12 X/D and increase those at 41 X/D. The turbulence level in the recirculation zone may be decreased partly by simply decreasing the initial turbulence level set for the jet spray or the external flow field.

Previous evaluations of the LHF modeling technique presented by Faeth in Reference 1 showed that LHF models generally overestimated the rate of development of the spray. One of the experiments described by Faeth modeled a spray ejecting vertically downward into still air. The results of the present study showed that the model overestimated the rate of development of the spray at 12 X/D downstream of the cylindrical body, which agrees with the findings reported by Faeth, despite the difference in the test configurations.

The model predictions generally correlated best with the free-stream pressure of the external air flow. This is true for the spray diameters predicted at 12 and 41 X/D, as well as the mass concentrations predicted at the centerline when the overall results for both axial locations are considered. Since a good correlation of droplet diameters

versus model accuracy was not obtained, this suggests that the finite interphase transport rates which existed in the actual experiment but was not accounted for in the LHF approximations does not have a dominating influence on model accuracy for droplets having a mass mean diameter of $16.5\text{ }\mu\text{m}$ or less. No correlation in model performance was found versus altitude, and the model performance was generally better for the higher liquid ejection flow rates. Also, the difference in the liquid ejection velocity between experiment and model had no apparent influence on model accuracy.

The quantitative prediction by the model of the liquid mass concentrations at the centerline were anywhere from 5 to 155% in error. The best accuracy obtained when results at 12 and 41 X/D are considered were on the order of 30%. For those cases where the predictions were much better at one of the two axial locations, the results at the other location were much worse. Overall, the accuracy of the predictions for the liquid mass concentrations at the centerline for these test cases were roughly 70% at 12 X/D, and 150% at 41 X/D. This error can be partially attributed to the LHF approximations and the turbulent dissipation rate. The base pressure coefficients predicted by the model were constant for all tunnel air velocities tested, as they should be. However, the predictions were 200% high; no

explanation for an error of this magnitude is apparent. The base pressure coefficients may be sensitive to the initial body boundary layer velocity and turbulence kinetic energy profiles since these profiles effect the flow velocity and pressure in the body base region.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

A study of a modeling technique was conducted for a flow field downstream of a cylindrical body aligned with a low Mach number air stream with liquid mass ejecting from the base of the body. The STARPIC computer code which uses a Navier-Stokes solver developed for axisymmetric flow fields was modified to also predict the distribution of liquid mass ejection at the base of the body. The local homogeneous flow (LHF) modeling technique was applied to model the jet spray of the liquid mass ejection. This technique assumes that the interphase transport rates between the liquid and gaseous flows are infinitely fast. The comparisons made in this study between model predictions and experimental measurements indicates that this LHF model can predict the mass concentrations and spray diameters within 150% accuracy, and the base pressure coefficients without liquid mass ejection within 200%. Hence, it does not currently provide a reasonable qualitative or quantitative description of nonevaporating sprays in this type of flow field. However, this model has shown that it is capable of predicting the liquid mass concentrations and spray diameters with reasonable accuracy in some cases.

Therefore, it may have the potential to do so on a more consistent basis if further fine tuning of the code can be performed. The application of the LHF theory was simplistic in nature since no information concerning injector characteristics were required nor available. The predictions of the mass concentrations at 12 and 41 X/D were relatively insensitive to the initial jet spray velocity and body boundary layer velocity profiles. This indicates that the actual injector characteristics or body leading edge geometry, i.e., round-nosed or square-edged-nosed, did not significantly influence the model results, and therefore were not important for this study.

It is recommended that for flow fields of this type a separated phase model should be used to provide a better description of the flow field and should yield more accurate results. However, if the additional complications and computer time prohibit the use of a separated phase model, and a more detailed description of the flow field is not required, then this LHF model may yield more accurate results if further fine tuning of the model can be performed. This can be accomplished by studying the effect of the initial turbulence level and the turbulence dissipation rate in the k- ϵ model on the overall mixing pattern to achieve better quantitative and qualitative results at all axial locations. Finally, the initial

pressure of the liquid jet spray would be more realistic and may produce better model results if it is based on a predetermined base pressure coefficient rather than the free-stream pressure. However, the effects of the body boundary layer on the base pressure predicted by the model should be further investigated so that better agreement can be achieved between predicted and experiment base pressure coefficients.

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APPENDICES

APPENDIX A

A GRID REFINEMENT

It is obviously desirable in any computational computer code to have a solution which is not grid dependent. The following study was conducted to investigate the influence of grid geometry and numerical resolution on the model predictions of the flow properties. A typical test condition was modeled in the code and it was used for all of the cases run for the grid refinement investigation. A "standard" grid was defined that measured approximately four meters axially and one meter radially, with 62 axial grid lines and 38 radial grid lines; this grid was used as a baseline grid for the investigation. The axial length, radial width, axial grid density, and radial grid density were each varied systematically and evaluated independently while the other grid parameters were kept equal to that of the standard grid. To determine the minimum requirement for that grid geometry under investigation, the grid geometry was perturbed until the mass concentrations at 12 and 41 X/D did not change.

The axial grid density was evaluated by using 42, 62, and 82 grid lines. The results, presented in Figures 54 and 55, show that 42 axial grid lines did cause a grid dependent solution. However, since 62 and 82 axial grid lines

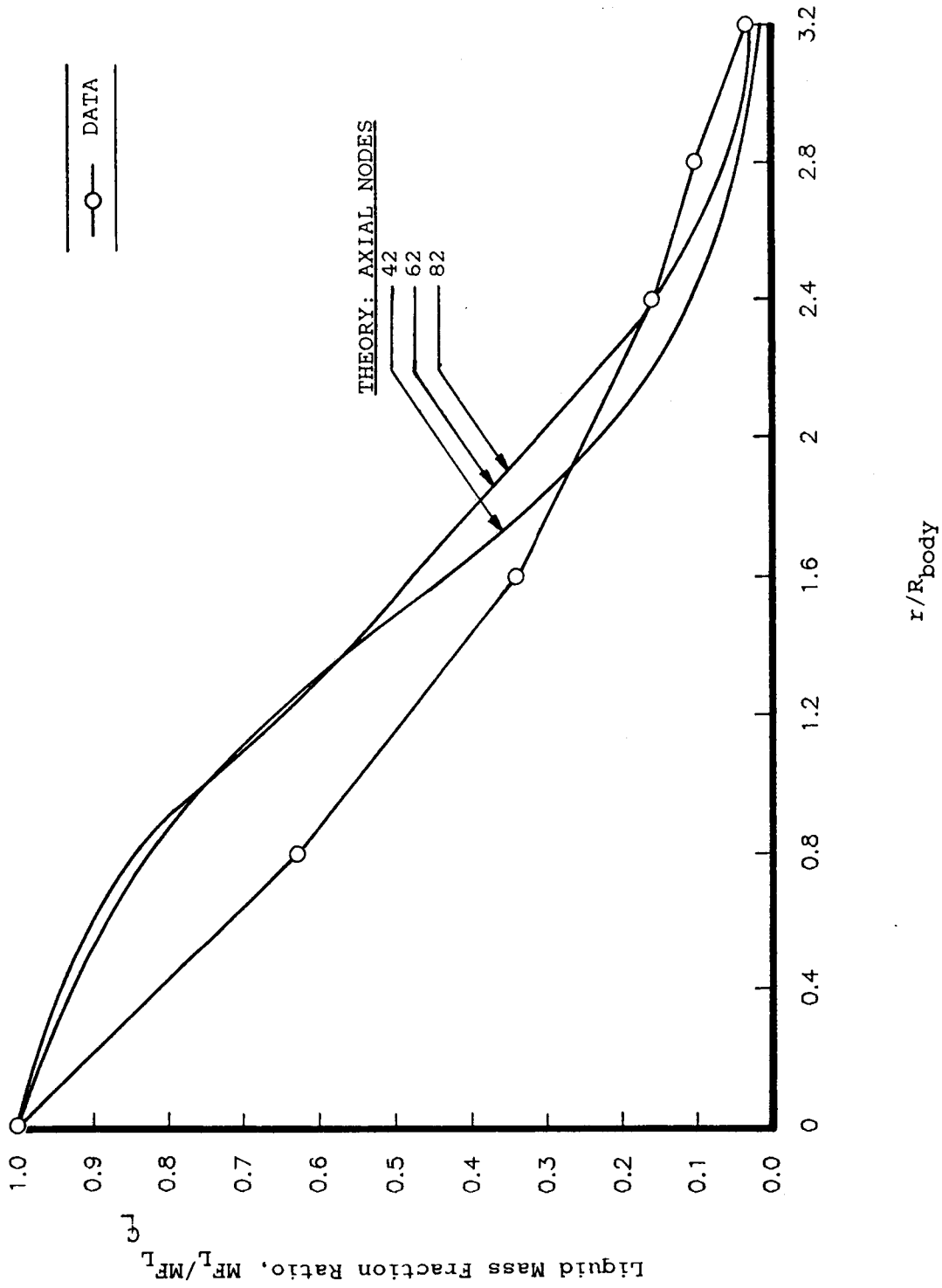


Figure 54. Grid Refinement of Axial Grid Density for Model Predictions at 12 X/D

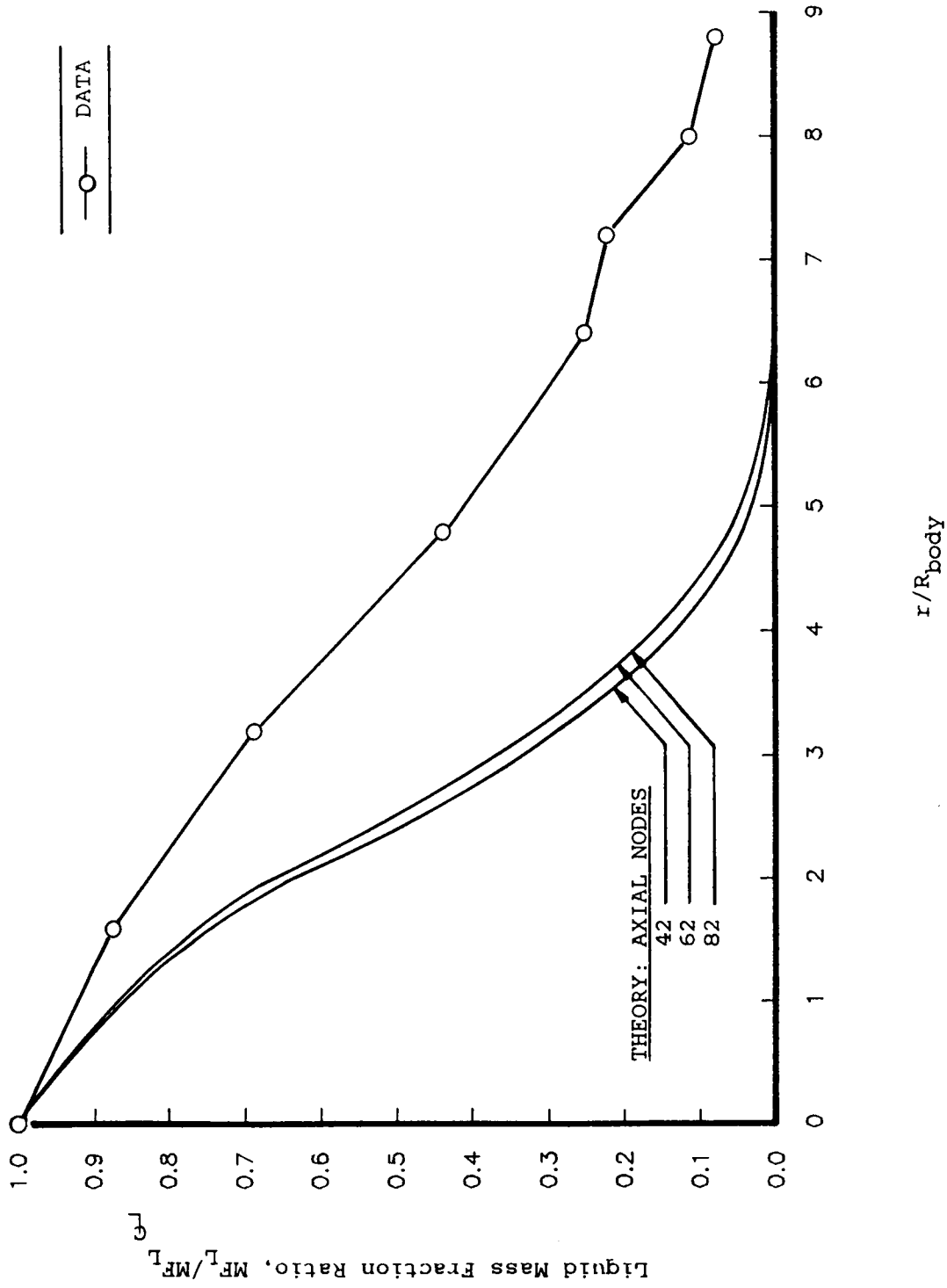


Figure 55. Grid Refinement of Axial Grid Density for Model Predictions at 41 X/D

resulted in identical solutions, it was concluded that 62 axial grid lines will provide a sufficient axial grid density for this application.

The radial grid density was evaluated by using 30, 38, and 46 radial grid lines. The results, presented in Figures 56 and 57, show that no variation in model outputs resulted. Hence, 30 radial grid lines provided a sufficient radial grid density for this application.

The axial grid length was evaluated by setting the grid length to 3, 4, and 5 meters. The results, plotted in Figures 58 and 59, show that a total grid length of three meters was sufficiently far enough downstream of the cylindrical body so that no influence of the exit boundary conditions were found in the model predictions.

The radial grid width was evaluated by setting the grid width to 0.5, 1, and 2 meters. The results, plotted in Figures 60 and 61, show that a grid width of 0.5 meters was a sufficient distance away from the cylindrical body so that the top boundary conditions did not influence the model predictions.

In concluding, the base grid, which utilized an axial grid length of four meters, a radial grid width of one meter, 62 axial grid lines and 38 radial grid lines, was found to have adequate grid definition so that the flow field calculated by the computational model was independent

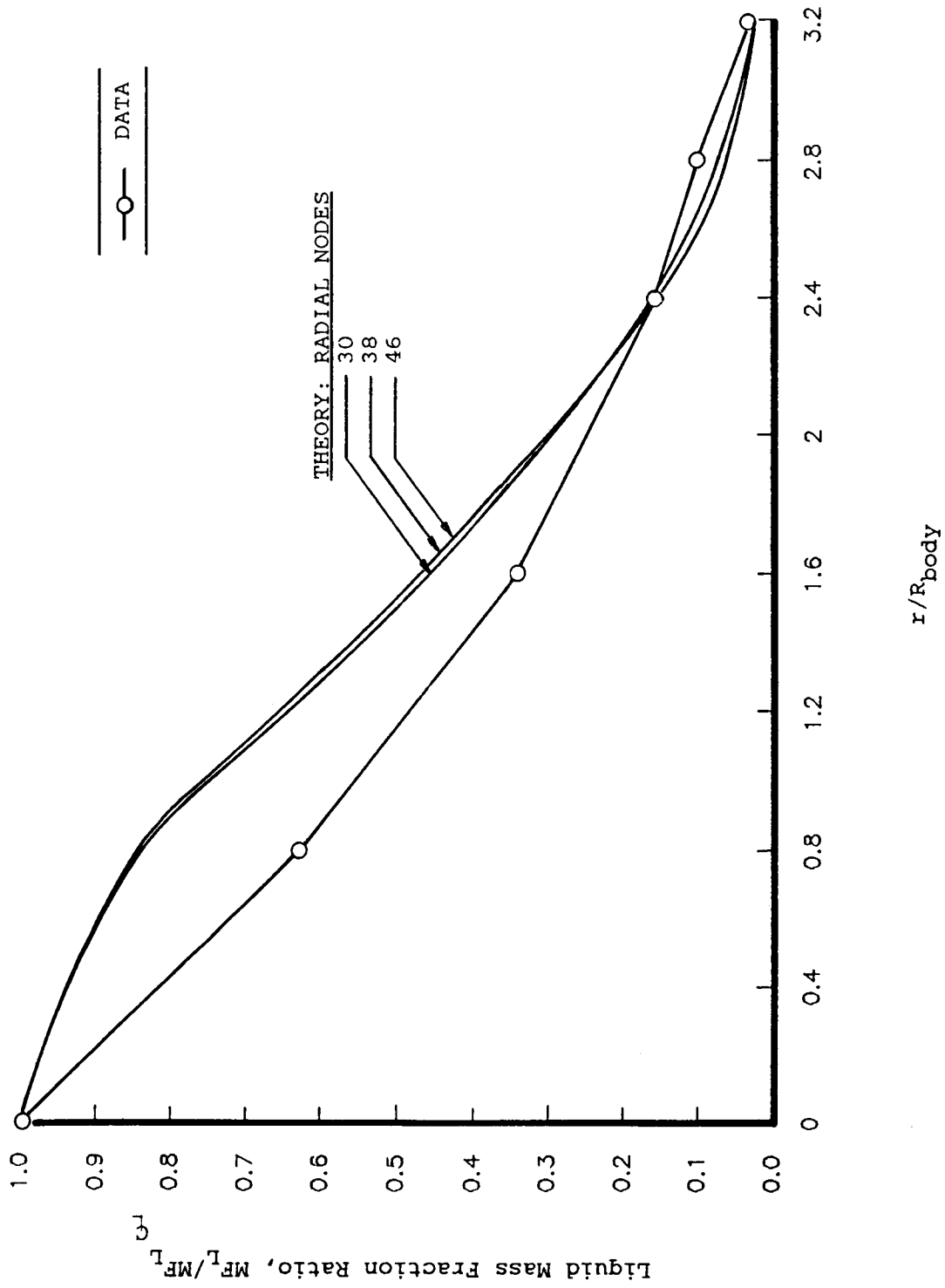


Figure 56. Grid Refinement of Radial Grid Density for Model Predictions at 12 X/D

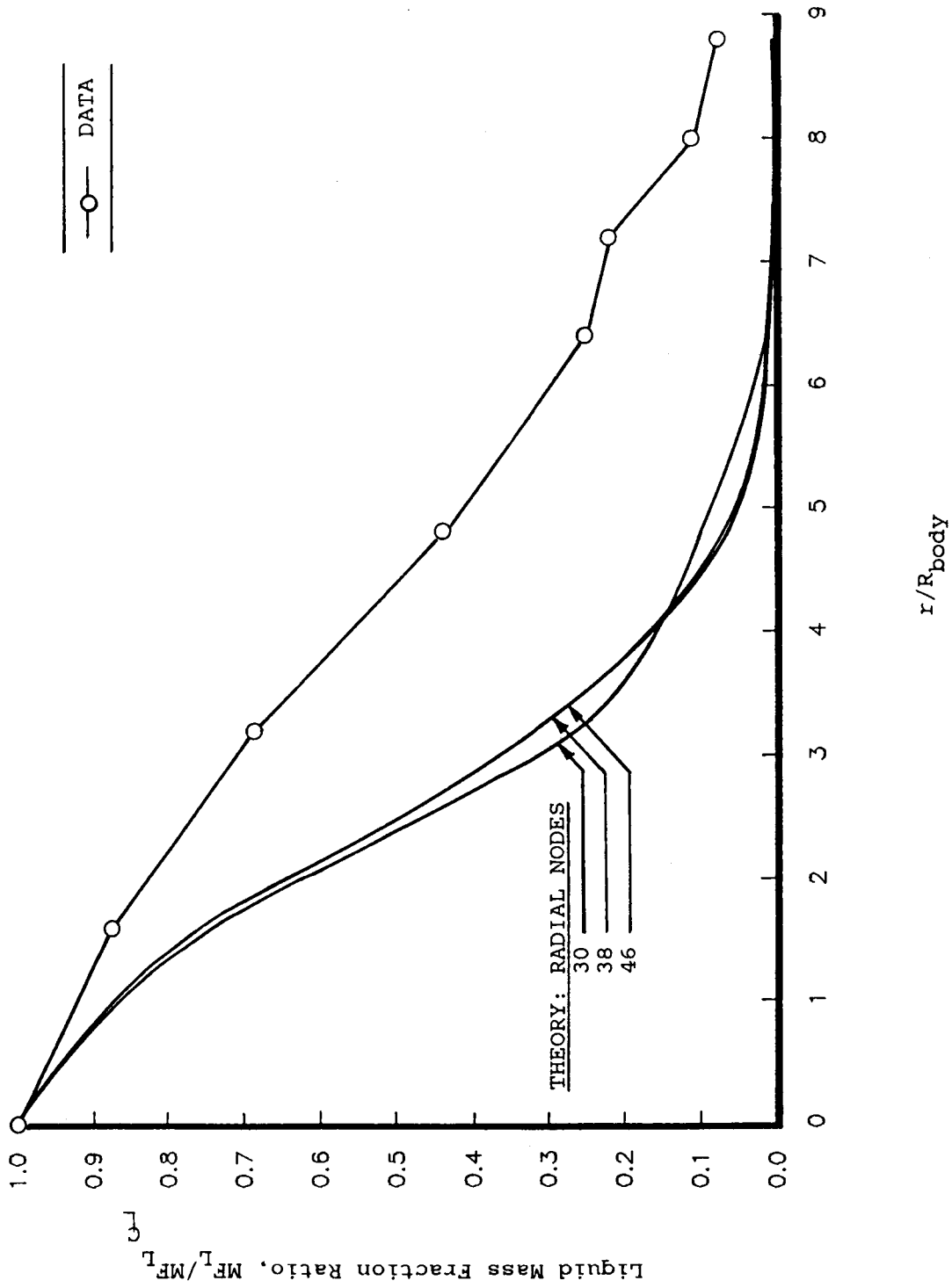


Figure 57. Grid Refinement of Radial Grid Density for Model Predictions at 41 X/D

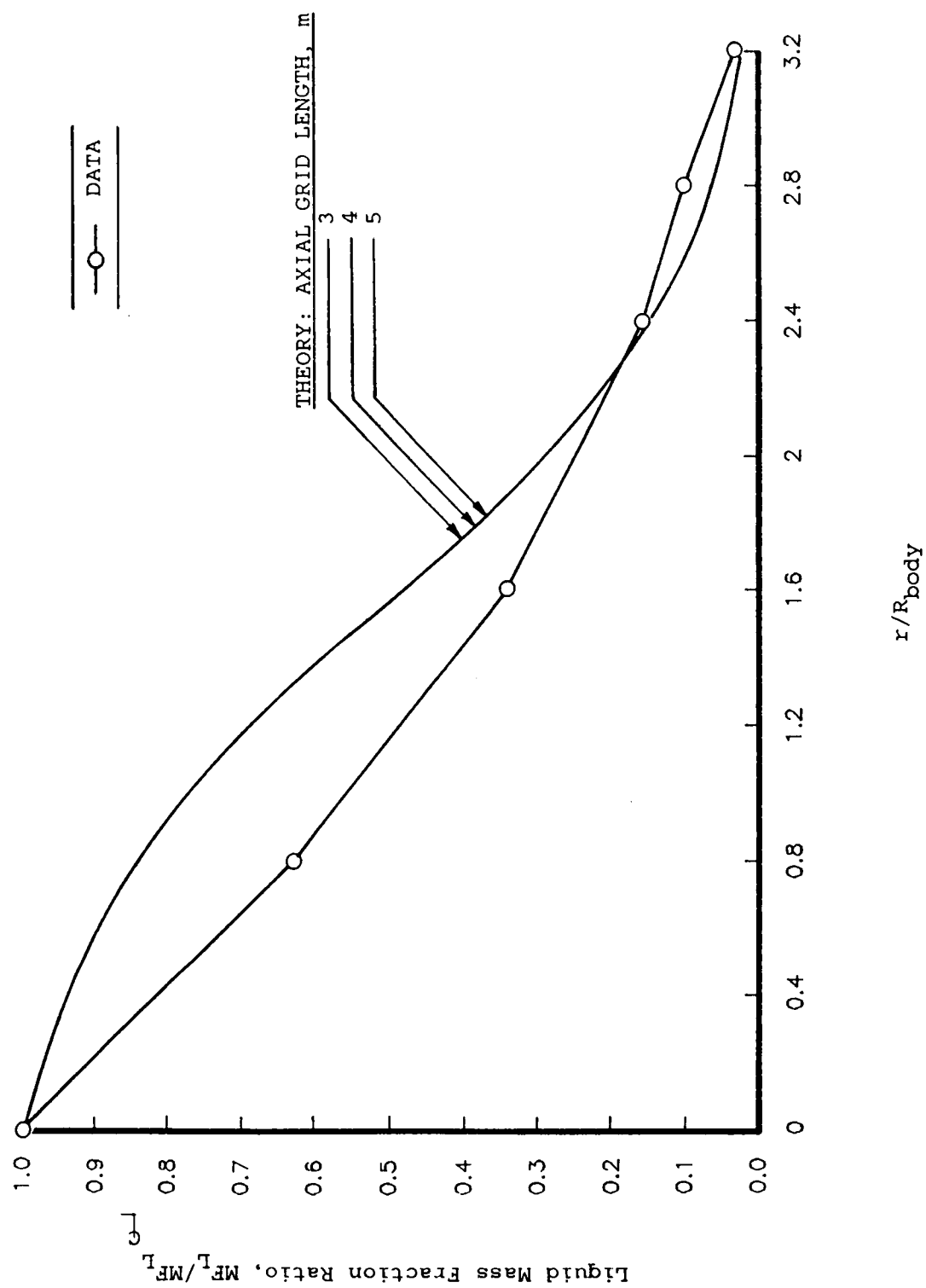


Figure 58. Grid Refinement of Axial Length of Grid for Model Predictions at 12 X/D

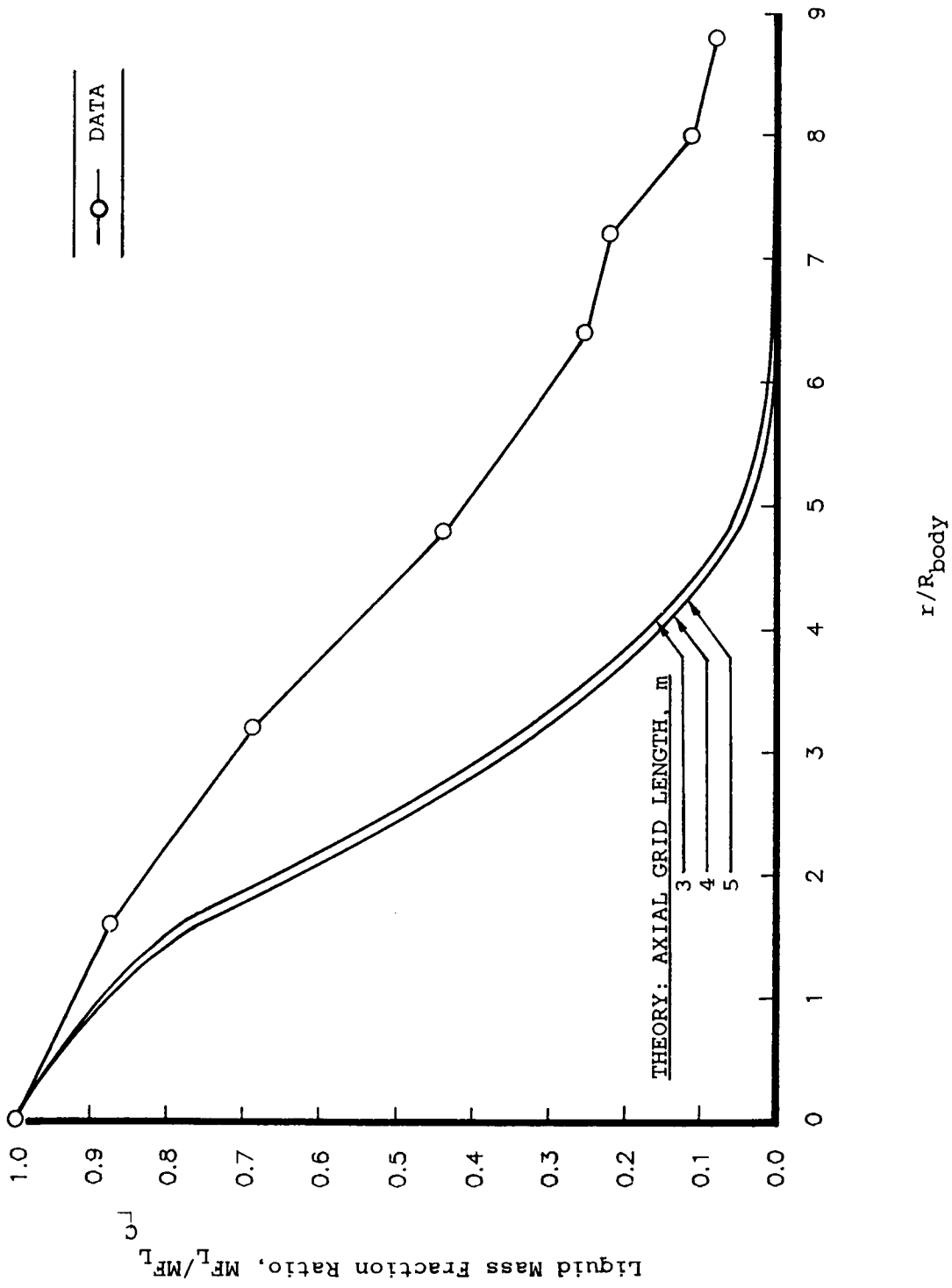


Figure 59. Grid Refinement of Axial Length of Grid for Model Predictions at 41 X/D

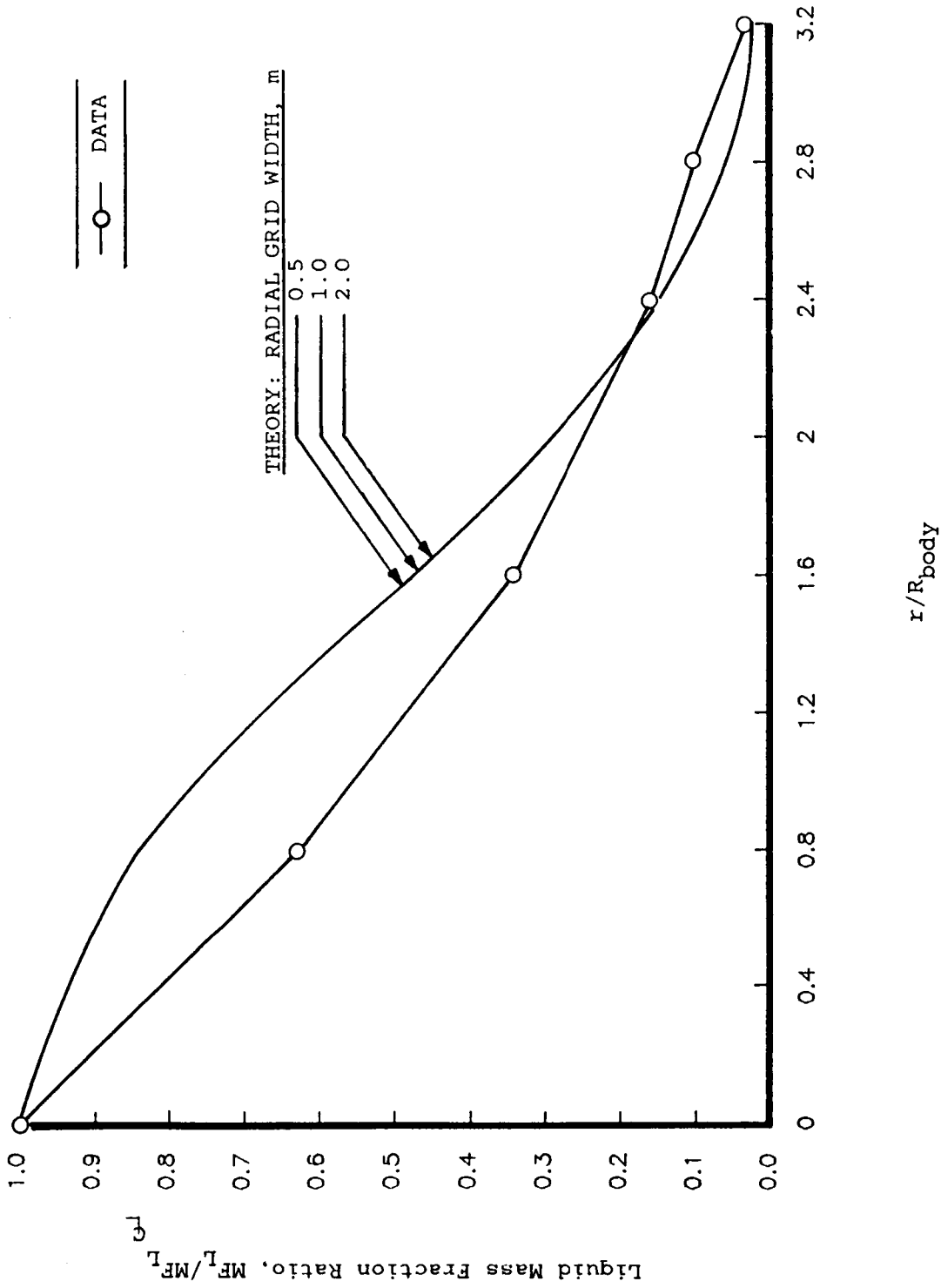


Figure 60. Grid Refinement of Radial Width of Grid for Model Predictions at 12 X/D

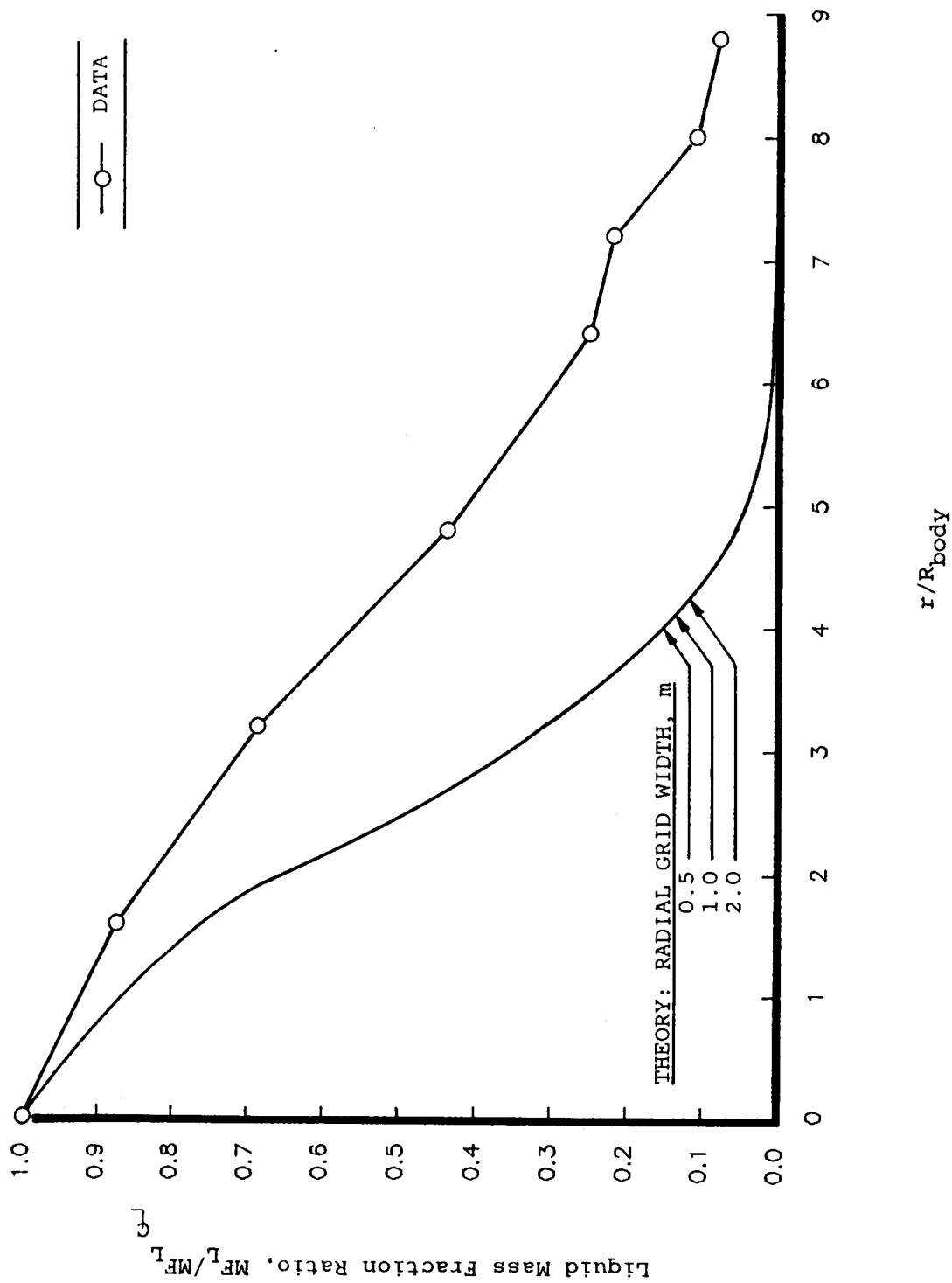


Figure 61. Grid Refinement of Radial Width of Grid for Model Predictions at $41 X/D$

of this grid geometry. It might be that further numerical experiment would yield a base grid containing fewer nodes that would be sufficient for adequate resolution. This would result in reduced computational times. However, the computer CPU time consumed for one test case was less than 900 seconds using the base grid. Also the memory allocation required for the 2356 nodes of the 62 X 38 base grid was less than 0.5 megabytes. Hence, without further experimentation the base grid was chosen as the standard grid which was used in all of the flow cases run for the model evaluation.

APPENDIX B

B ITERATION CONTROL AND CONVERGENCE OF SOLUTION

Investigation into the iteration control process was conducted to minimize the number of iterations necessary to achieve a converged solution. First, a study of the maximum residual source term necessary to achieve a converged solution for the mass concentrations was performed. Then the initial guesses of the solution and the under-relaxation factors which control subsequent model guesses were investigated.

B.1 Establishment of Solution Convergence

The maximum residual source term was optimized by forcing the model to run a high number of iterations (5000) and in the process, printing the mass concentrations every 500 iterations. The residual source term is essentially the change in the model solution of the variable ϕ from the previous iteration to the current iteration, i.e.,

$$\text{RESOR}_{\phi} = \frac{\phi_{\text{new}} - \phi_{\text{old}}}{\phi_{\text{old}}} \quad (44)$$

This residual source term is calculated at each node and then summed to yield the "sum of the residual source" (RESOR). The mass fractions at 12 X/D converged when the sum

of the residual source term for the mass fraction (RESORF) was 34 or less (Fig. 62). However, the mass fractions at 41 X/D did not converge until RESORF reached values of 0.0158 (Fig. 63). Therefore, to assure a converged solution, the maximum residual source was set equal to 0.005 for all of the model runs made for this thesis. From the residual source term investigation, it was apparent that all parameters were converging quickly except for the residuals of the mass concentration. Therefore, the remainder of the iteration control study focused on the variables concerning the mass concentration only.

B.2 Controlling the Iteration Process

The initial guesses of the mass concentrations for the internal flow field were investigated by setting two extreme guesses. The mass concentrations were set equal to zero everywhere for one model run, and set equal to one everywhere for another model run. No significant difference in the number of iterations required to reach a converged solution was found.

The under-relaxation factor for the mass fraction (URFF) was then investigated. The under-relaxation factor (URF) essentially controls the amount of change for the next guess of the solution from the previous guess, i.e.,

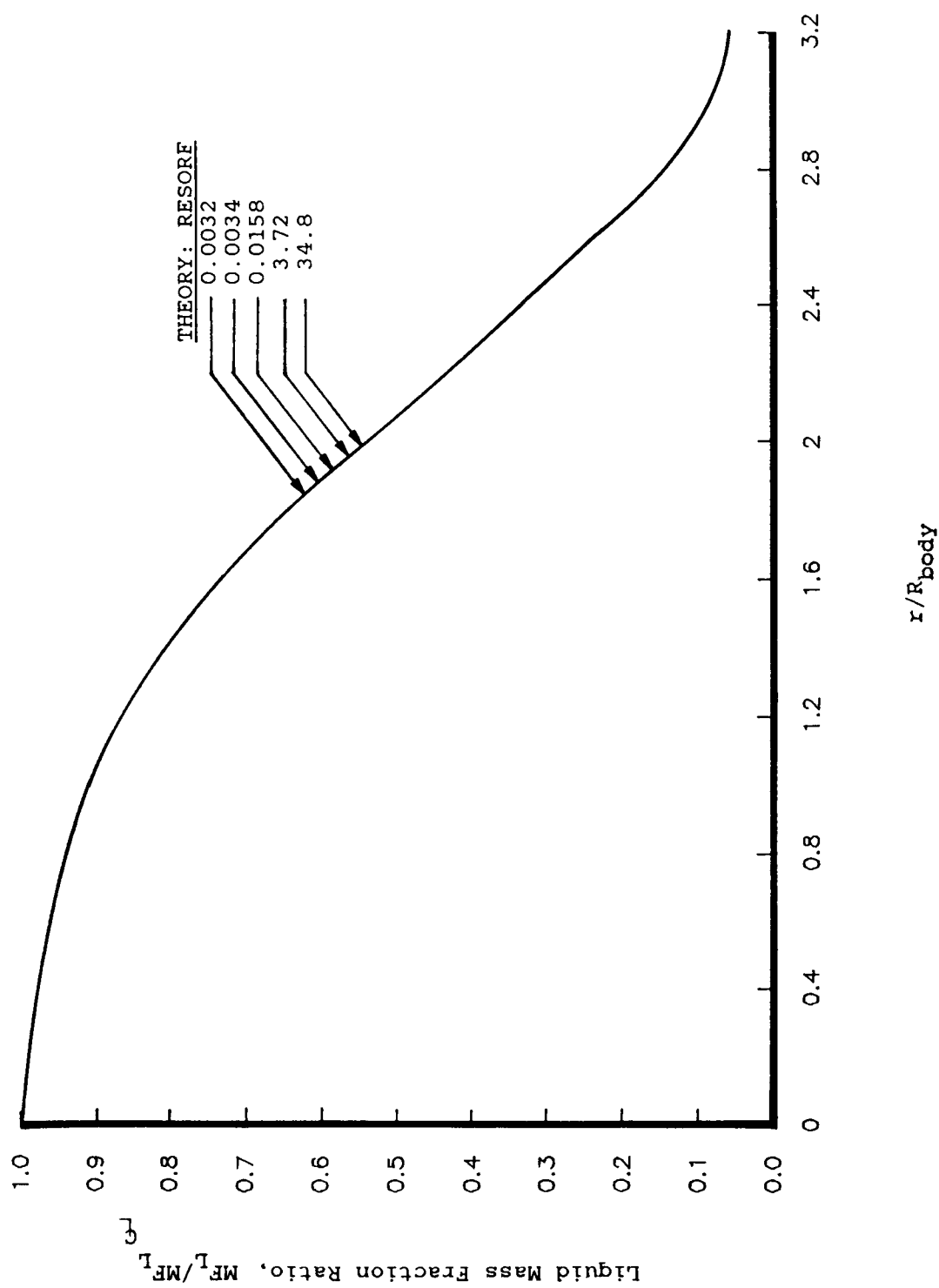


Figure 62. Residual Source Term for the Determination of Model Convergence at 12 X/D

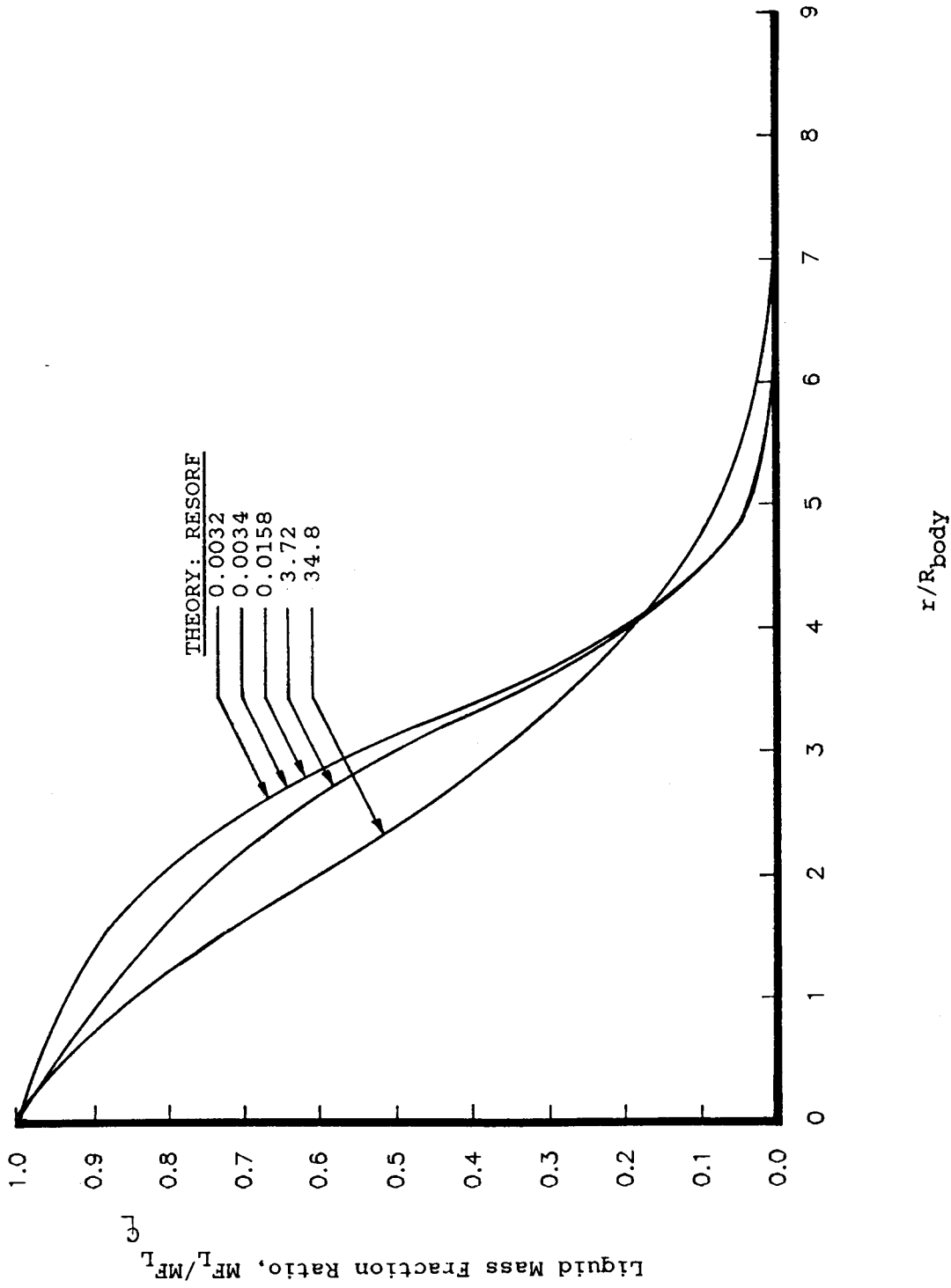


Figure 63. Residual Source Term for the Determination of Model Convergence at 41 X/D

$$\phi_{\text{next}} = \phi_{\text{next}} (\text{URF}_{\phi}) + \phi_{\text{prev}} (1 - \text{URF}_{\phi}) \quad (45)$$

Model runs were made where URFF was set equal to a range of values between 0.1 and 1.1. It was found that the model diverged when URFF was equal to 0.9 or greater. Also there was no significant improvement in the number of iterations necessary for a converged solution when URFF was less than 0.9. This was due to the fact that the RESORF term oscillates at all values of URFF. The lower the URFF term, the lesser the magnitude of the oscillations, but the total number of iterations for each oscillation did not change much. Hence, the total number of iterations did not vary significantly for a range of URFF's between 0.1 and 0.9. Finally, URFF was allowed to decrease as convergence neared. Once again, due to the same explanation given above, no significant difference in the total number of iterations occurred.

VITA

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