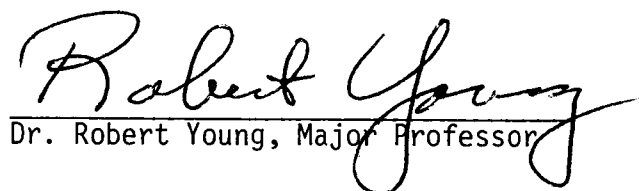
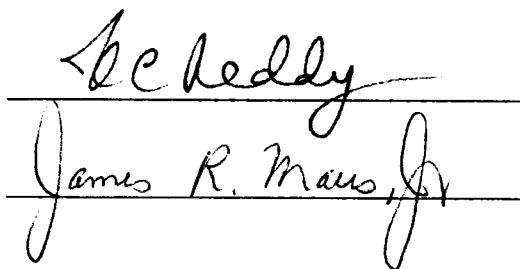


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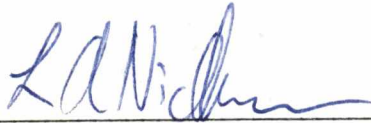

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PSEUDOSPECTRAL APPROXIMATION IN A PARABOLIZED
NAVIER-STOKES CODE

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

Lynn Alan Nicholson

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ABSTRACT

A pseudospectral method which is a combination of a spectral method and a collocation method offers an alternative to finite difference and finite element methods for problems with complex geometries. Spectral methods have the potential of yielding high accuracy for a given number of spatial nodes or collocation points. In this thesis, a parabolized Navier-Stokes code known as the Air Force Wright Aeronautical Laboratories Parabolized Navier-Stokes Code (AFWAL PNS Code) has been modified to make it pseudospectral in the circumferential direction. This modification uses a Fourier spectral method to obtain an accurate solution. Numerical solutions of the three-dimensional parabolized Navier-Stokes equations were obtained for a shuttle-like geometry at Mach 7.4 at an angle of attack of 20 degrees for comparison of finite difference and spectral approximations in the circumferential direction. These computations indicate that the spectral approximation required approximately 4% more computing time while achieving results essentially identical to a second-order finite difference scheme. The second-order accurate finite-difference terms on the left hand side of the solution algorithm in the AFWAL PNS Code are suspected of dominating the accuracy of the solution and causing the spectral approximation results to be less accurate than expected. The smoothing terms in the numerical algorithm also have an influence on the accuracy of a solution. Further study would be necessary to determine how to optimize the AFWAL PNS Code numerical algorithms to obtain the potential accuracy of the spectral technique.

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LIST OF SYMBOLS

a	Speed of sound
A_n	Spectral coefficient
$\tilde{A}_s, \tilde{B}, \tilde{C}, \tilde{S}$	Transformed flow-variable Jacobian Matrices
C_n	Spectral coefficient
C_v	Specific heat at constant volume
e	Total energy per unit volume
e_i	Internal energy
E, F, G	Cartesian flux vectors
$\tilde{E}, \tilde{F}, \tilde{G}$	Transformed flux vectors
$f(x)$	General function
J	Jacobian of transformation
M	Mach number
$\tilde{M}$	Transformed Jacobian matrices
N	Number of nodes
$\bar{N}_1, \bar{N}_2$	Block tridiagonal operators
P	Pressure
Pr	Prandtl number
q	Flow variable vector
$\hat{R}, \hat{S}, \hat{T}$	Transformed viscous flux vectors
Re	Reynolds number, per foot
T	Temperature
u, v, w	Cartesian velocity components
U, V, W	Contravariant velocities

x, y, z	Cartesian coordinates
α	Angle of attack; also used to determine the type of differencing in the marching direction
γ	Ratio of specific heats
δ	Central difference operator
Δ	Forward difference operator
Δq^*	Intermediate flow variables
ϵ_A	Ensures non-zero primary diagonal
ϵ_B	Alters smoothing with grid size
ϵ_I	Implicit damping parameter
ϵ_e	Explicit damping parameter
ξ, η, ζ	Transformed coordinates
ρ	Density
Φ_e	Explicit smoothing term
Φ_{IX}	Implicit smoothing term
∇	Backward difference operator

Subscripts

e	Denotes explicit quantity
I	Denotes implicit quantity
∞	Free-stream value
s	Sub-layer
w	Wall condition

I. INTRODUCTION

A pseudospectral method which is a combination of a spectral method and a collocation method offers an alternative to finite difference and finite element methods for problems with complex geometries. A finite difference method can be improved by reducing the nodal spacing or by using a higher-order approximation that uses information from more nodes plus additional boundary conditions. Either of these choices can be very expensive and the choice of boundary conditions for the higher order methods can be a source of errors. A spectral method does not require additional boundary conditions. For these reasons, spectral methods can be particularly attractive. With complex problems in several dimensions, spectral methods have the potential of yielding high accuracy for a given number of spatial nodes or collocation points. Gottlieb and Orszag (1)¹ have shown that spectral and pseudospectral methods are formally finite-order accurate. For problems with periodic boundary conditions, Fourier spectral methods can be efficiently implemented using Fast Fourier Transforms (FFT) to obtain highly accurate solutions. The pseudospectral modifications (2) in the circumferential direction of a time dependent, three-dimensional Navier-Stokes Code achieved the desired accuracy with 50% fewer nodes than what is required for a fourth-order finite difference scheme, resulting in a significant cost reduction. In this thesis, a parabolized Navier-Stokes code based on an implicit finite

¹Numbers in parentheses refer to similarly numbered references in the List of References.

difference scheme has been modified to make it pseudospectral in one of the spatial directions and is compared with the finite difference results.

For steady supersonic flow over a body it is possible to simplify the full Navier-Stokes equations to the parabolized Navier-Stokes equations for certain problems. The simplified steady-state equations can be solved by a space marching technique with accuracy comparable to the full Navier-Stokes equations, but with greatly reduced storage and time requirements. A non-iterative, implicit, space marching, finite difference algorithm for the steady thin-layered Navier-Stokes equations has been developed by Schiff and Steger (3). The original code of Schiff and Steger has been refined and improved by Chausse and others (4) over a period of time. The evolved code is known as the Air Force Wright Aeronautical Laboratories Parabolized Navier-Stokes Code (AFWAL PNS Code) and is applicable to steady supersonic viscous flow over bodies of arbitrary shape. The PNS code uses an initial data surface where the flow is supersonic as a starting solution. A blunt body with an embedded subsonic region over the nose requires a three-dimensional time-dependent Navier-Stokes code to calculate a solution. The blunt body nose solution and initial data for starting the PNS code was computed using the three-dimensional, time-dependent, thin-layer Navier-Stokes code (AIR3D) developed by Kutler, et al. (5).

In the PNS formulation, the ideal gas high Reynolds number Navier-Stokes equations written in conservation law form are transformed from the physical domain to a rectangular computational volume. The Cartesian x, y, z coordinates are transformed to body-conforming ξ, η, ζ

coordinates where ξ, η , and ζ are the streamwise, circumferential and radial coordinates, respectively. This transformation results in the body, shock and outflow boundaries coinciding with the computational volume surfaces which simplifies the application of boundary conditions. The transformation also facilitates the application of both the thin-layered approximation and the PNS approximation.

A thin-layered approximation is physically valid for high Reynolds number flows, where the streamwise gradients in the viscous terms are negligible in comparison to those in the normal direction. By similar reasoning, the viscous derivative in the circumferential direction can be neglected although this is not essential to the development of the PNS approximation. In general, the viscous derivatives in the streamwise and circumferential directions along the body are not resolved unless the grid spacing is sufficiently small. Thus to simplify the computations while achieving consistent accuracy, all viscous derivatives in the ξ and η direction are dropped.

The PNS approximation allows the computation of steady supersonic viscous external flow fields as an initial boundary value problem. This simplification results in an algorithm which can be marched in space in the streamwise direction. The PNS approximation is reasonable if the viscous terms in the marching direction are negligible and the convection term in the marching direction has positive time-like behavior. The first condition is met by the thin-layer approximation and is justified for high Reynolds number flow and body conforming coordinates. The second condition is needed in viscous flow for positive viscosity to cause damping in the marching direction. To meet

this condition a viscous sublayer approximation is used. In this approach, the marching direction pressure gradient from the adjacent viscous supersonic flow is held constant through the thin viscous subsonic sublayer. An ideal gas equation of state is employed to relate energy to pressure, density and the velocity components, completing the system of equations.

An approximate factorization scheme with appropriate boundary conditions is used to solve the PNS equations. The equations are factored (spatially split) which reduces the solution process of two one-dimensional problems at a given spatial step. Smoothing terms are included to stabilize the solution. The use of a central difference approximation for the circumferential derivatives together with the periodic condition, leads to a periodic block-tridiagonal system of equations. Similarly, the use of a central difference approximation in the radial direction also results in a block-tridiagonal system of equations. The flow variables in the marching direction are found using a matrix L-U decomposition at each spatial step. It is in the circumferential direction with its inherent periodic behavior that the pseudospectral approximations based on Fourier series are used to compute the appropriate derivatives, while the rest of the algorithm is left in the finite difference form.

Spectral methods have been applied to a variety of problems (1) during the last decade and have been shown to be highly efficient for certain types of problems. Generally, it is possible to achieve a desired level of accuracy with fewer points using spectral methods. An overview of a finite difference method versus a spectral method shows

that in a finite difference algorithm the derivative at a discrete node can be approximated by a linear combination of the function at that node and the adjacent nodes. This local approximation of the derivative can be obtained by using a Taylor series expansion of the function. For a pseudospectral algorithm which in this thesis will be a discrete Fourier series, the derivative at a node can be approximated by a linear combination of the function at all the nodes in the circumferential direction. A spectral algorithm results in a global approximation of the function.

The function is approximated at each step by a discrete truncated Fourier series. The Fourier coefficients are determined by equating the functional value and the Fourier approximations at the collocation points. A set of collocation points or nodes is chosen such that the spectral coefficients can be determined efficiently and accurately. With a Fourier expansion, equally spaced nodes are the most efficient. Calculation of the coefficients in computational space with its inherent equal spacing satisfies the requirement for optimum performance. Thus, the physical variables are projected into spectral space where the spectral coefficients are computed. Then the spatial derivatives of the function at each point are evaluated by summing the derivatives of the truncated Fourier series. The derivative operation is computed in spectral space and then the spectral coefficients of the derivative are projected back into the physical space. Now that the derivative approximation at the node has been calculated, integration to the next spatial step follows from the approximate factorization algorithm and solution procedure.

The calculation of the Fourier spectral derivatives can be combined into one matrix operation. The spectral approximation matrix needs to be computed only once for a given problem. Then the spectral approximations to the derivatives at all the nodes can be calculated from a matrix multiplied by a vector and is applicable for any number of nodes N . The spectral derivatives can also be calculated by Fast Fourier Transforms (FFT) if the number of nodes N is a power of 2. The matrix multiplication technique is equal to or better than FFT when the number of nodes is less than 64 and it has an advantage on vector processors.

In the AFWAL PNS Code, the approximations to the circumferential derivatives in the left hand side operators are left in the finite difference form to preserve the block tridiagonal structure of the equations to be solved in the factored scheme. This simplification is equivalent to approximating a spectral approximation matrix which is non-sparse by a block tridiagonal matrix. The result is a simplified space marching procedure. Orszag (6) has shown that this type of simplification does not degrade the convergence of the solution procedure if the solution is iterated at each marching step. The converged solution will still retain the accuracy of the spectral method in the circumferential direction.

The accuracy of the Fourier-spectral approximation depends on the smoothness of the function. Smoothness refers to the continuity of the function's derivatives. If the function is infinitely differentiable (i.e. smooth), then the difference between the function and the Fourier-spectral approximation to the function converges to zero

faster than any finite power of $1/N$ as N approaches infinity, where N is the number of collocation points. Tadmor (7) has shown that the error decays exponentially with N . Therefore, the approximation is called infinite order accurate.

If the function is discontinuous at a point then the convergence of the approximation is not uniform. Oscillations known as Gibbs phenomenon will occur around the point of discontinuity as N approaches infinity. These oscillations can be eliminated or reduced through proper filtering procedure. A low pass filter is used in the AFWAL PNS Code to stabilize the Fourier spectral method. This filter removes the high frequency components which contain most of the oscillations. For periodic boundary conditions, the Fourier-spectral method is stable (1) and will converge rapidly for smooth functions. However, for non-periodic boundary conditions, discontinuities at the end points may occur. These end point discontinuities can produce inconsistent results even though the Fourier-spectral method is stable.

For non-periodic boundary conditions, Chebyshev-spectral methods can be implemented effectively. As a consequence, these methods are used for Dirichlet or Neumann boundary conditions. A combination of Fourier and Chebyshev methods may be used for multi-dimensional problems depending on the boundary conditions. The convergence properties of Chebyshev approximations are similar to those of Fourier series. However, the Chebyshev approximation is inherently continuous at the end points and consequently will not exhibit Gibbs phenomenon there. But, if the function has a discontinuity in the interior, the Chebyshev approximation will exhibit Gibbs phenomenon there.

Numerical solutions of the three-dimensional parabolized Navier-Stokes equations were obtained for a shuttle-like geometry at Mach 7.4 at an angle of attack of 20 degrees for comparison of finite difference and spectral approximations in the circumferential (η) direction. The remaining free-stream conditions are: $T_\infty = 98^\circ\text{R}$, $T_w = 1500^\circ\text{R}$, and $\text{Re} = 3.0 \times 10^6$ per foot. Comparisons are made for pressure contours between the body and the shock, pressure distributions axially and circumferentially on the body, and total temperature distributions through the leeward boundary layer. The computations indicate that the spectral approximation gives results which are comparable to those obtained using a second-order finite difference scheme. These calculations have been performed on a Cray computer. The spectral version of the code required approximately 4% more computing time than the finite difference version while achieving essentially identical results.

II. METHOD

AFWAL PNS Code Governing Equations

In order to develop the PNS equations, the three-dimensional Navier-Stokes equations are first written in conservation law form for an ideal gas. If the density, energy, and Cartesian velocity components are retained as dependent variables, the steady three-dimensional Navier-Stokes equations can be transformed from Cartesian x,y,z coordinates to body-conforming ξ,η,ζ coordinates and written in non-dimensional form (8) as

$$\frac{\partial \hat{E}}{\partial \xi} + \frac{\partial \hat{F}}{\partial \eta} + \frac{\partial \hat{G}}{\partial \zeta} = \frac{1}{Re} \left(\frac{\partial \hat{R}}{\partial \xi} + \frac{\partial \hat{T}}{\partial \eta} + \frac{\partial \hat{S}}{\partial \zeta} \right) \quad (1)$$

where

$\xi = \xi(x,y,z)$ is the streamwise or marching direction,

$\eta = \eta(x,y,z)$ the circumferential direction, and

$\zeta = \zeta(x,y,z)$ the normal or radian direction.

This equation is written in terms of the transformed convective flux vectors $\hat{E}, \hat{F}, \hat{G}$ and viscous flux vectors $\hat{R}, \hat{S}, \hat{T}$. The transformation from the physical domain to a rectangular computational volume results in the body, shock, and outflow boundaries coinciding with computational volume surfaces which simplifies the application of boundary conditions. Thus $\zeta = 0$ plane corresponds to the body surface while the $\zeta = 1$ plane corresponds to the bow shock. This transformation also facilitates the application of both the thin-layered approximation and the parabolized Navier-Stokes approximation.

A thin-layered approximation has been incorporated into the AFWAL PNS Code. This approximation is physically valid for high Reynolds number flows, where the streamwise gradients of the viscous terms are negligible in comparison to those in the normal direction. By similar reasoning, the viscous derivatives in the circumferential direction can be neglected although this is not essential to the development of the PNS approximation. In general, the viscous derivatives in the streamwise and circumferential directions along the body are not resolved unless the grid spacing is sufficiently small. Thus to simplify the computations while achieving comparable results all viscous derivatives in the ξ and η direction are dropped. This reduces Equation (1) to

$$\frac{\partial \hat{E}}{\partial \xi} + \frac{\partial \hat{F}}{\partial \eta} + \frac{\partial \hat{G}}{\partial \zeta} = \frac{1}{\text{Re}} \left(\frac{\partial \hat{S}}{\partial \zeta} \right). \quad (2)$$

The PNS approximation allows the computation of steady supersonic viscous external flow fields as an initial boundary value problem. The PNS approximation is reasonable only if 1) the viscous terms in the marching direction ξ are negligible, and 2) the convection term in the marching direction $\partial \hat{E} / \partial \xi$ has positive time-like behavior. The first condition is met by the thin-layer approximation and is justified for high Reynolds number flow and body conforming coordinates. The second condition is the most difficult restriction to impose and is needed in viscous flow if positive viscosity is to cause damping in the marching direction. If the pressure term is properly split from the marching direction convection flux term, a stable subsonic marching process can be achieved whenever the pressure can be specified in subsonic regions.

The treatment of the marching direction pressure gradient controls the stability of the algorithm in subsonic regions and is the crucial condition to be met. The method used in the AFWAL PNS Code is called a viscous sublayer approximation. In this approach the marching direction pressure gradient from the adjacent viscous supersonic flow is impressed down through the thin viscous subsonic sublayer. Thus, the subsonic viscous sublayer pressure is not a function of the local flow field variables and an analysis of the eigenvalues of the appropriate Jacobian matrices (3) indicates that condition (2) will be satisfied. The sublayer approximation is introduced by substituting P_s for P in the marching direction flux vector $\hat{E}$ to obtain $\hat{E}_s$. P_s is the usual pressure P for supersonic flows and P_s is held constant normal to the body through the sublayer for subsonic flow. The constant is set to the value of the pressure at the edge of the subsonic sublayer.

In the space marching codes, it is convenient to choose

$$\xi = \xi(x)$$

$$\eta = \eta(x, y, z)$$

$$\zeta = \zeta(x, y, z)$$

Using this transformation, $\xi_y = \xi_z = 0$, the thin-layer approximation and the PNS approximation give

$$\frac{\partial \hat{E}_s}{\partial \xi} + \frac{\partial \hat{F}}{\partial \eta} + \frac{\partial \hat{G}}{\partial \zeta} = \frac{1}{Re} \left(\frac{\partial \hat{S}}{\partial \zeta} \right) \quad (3)$$

The transformed dependent variable vector is

$$\hat{q} = J^{-1} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \end{pmatrix} \quad (4)$$

$\hat{E}_s, \hat{F}, \hat{G}$ and $\hat{S}$ are the transformed flux vectors defined as

$$\hat{E}_s = J^{-1} \begin{pmatrix} \rho U \\ \rho u U + \xi_x P_s \\ \rho v U \\ \rho w U \\ (e + P_s) U \end{pmatrix} \quad (5)$$

$$\hat{F} = J^{-1} \begin{pmatrix} \rho V \\ \rho u V + \eta_x P \\ \rho v V + \eta_y P \\ \rho w V + \eta_z P \\ (e + P) V \end{pmatrix} \quad (6)$$

$$\hat{G} = J^{-1} \begin{pmatrix} \rho W \\ \rho u W + \zeta_x P \\ \rho v W + \zeta_y P \\ \rho w W + \zeta_z P \\ (e + P) W \end{pmatrix} \quad (7)$$

$$\hat{S} = J^{-1} \begin{pmatrix} 0 \\ m_1 u_\zeta + m_2 \zeta_x \\ m_1 v_\zeta + m_2 \zeta_y \\ m_1 w_\zeta + m_2 \zeta_z \\ m_3 \end{pmatrix} \quad (8)$$

U, V and W are the contravariant velocities given by

$$U = \xi_x u \quad (9)$$

$$V = \eta_x u + \eta_y v + \eta_z w \quad (10)$$

$$W = \zeta_x u + \zeta_y v + \zeta_z w \quad (11)$$

The parameters m_1 , m_2 and m_3 are related to the physical variables as

$$m_1 = \zeta_x^2 + \zeta_y^2 + \zeta_z^2 \quad (12)$$

$$m_2 = (\zeta_x u_\zeta + \zeta_y v_\zeta + \zeta_z w_\zeta)/3 \quad (13)$$

$$m_3 = \frac{km_1}{Pr(\gamma-1)} \frac{\partial a^2}{\partial \zeta} + \frac{1}{2} \frac{\partial}{\partial \zeta} [m_1(u^2 + v^2 + w^2)] \quad (14)$$

The Jacobian is given as

$$J^{-1} = x_\xi y_\eta z_\zeta + x_\zeta y_\xi z_\eta + x_\eta y_\zeta z_\xi - x_\xi y_\zeta z_\eta - x_\eta y_\xi z_\zeta - x_\zeta y_\eta z_\xi \quad (15)$$

An ideal gas equation of state is employed to relate energy to pressure, density and the velocity components, completing the system of equations. For a perfect gas, the total energy per unit volume e , is related to the other flow variables by the following equation

$$e = \text{total energy} = \text{internal energy} + \text{kinetic energy}$$

where

$$e = \rho e_i + \frac{\rho}{2} (u^2 + v^2 + w^2)$$

and

$$\rho e_i = \rho C_v T = \frac{P}{(\gamma-1)}$$

thus

$$e = \frac{P}{(\gamma-1)} + \frac{\rho}{2} (u^2 + v^2 + w^2). \quad (16)$$

Numerical Algorithm and Solution Procedure

Schiff and Steger (3) have developed an approximate factorization scheme to solve Equation (3) with the appropriate boundary conditions. The equations are factored (spatially split) which reduces the solution process to two one-dimensional problems at a given step. The algorithm produces block tridiagonal systems for each space coordinate and is written as follows

$$[\bar{N}_1 \bar{N}_2]^j \Delta q^j = f^j \quad (17)$$

where

$$\Delta q^j = q^{j+1} - q^j$$

and

$$\bar{N}_i^j = \left[\left(\frac{\chi_s^j + \epsilon_x^{j+1}}{j^{j+1}} \epsilon_A \right) - \Phi_{I\eta} + \frac{(1-\alpha)}{j^{j+1}} \Delta \xi \delta_\eta \tilde{B}^j \right] \quad (18)$$

$$\bar{N}_2^j = \left[\left(\frac{\tilde{A}_s^j + \xi_x^{j+1}}{J^{j+1}} \epsilon_A \right) - \phi_{I\zeta} + \frac{(1-\alpha)}{J^{j+1}} \Delta \xi \left(\delta_\zeta \tilde{C}^j - \frac{1}{Re} \delta_\zeta \tilde{M}^j \right) \right] \\ \left/ \left(\frac{\tilde{A}_s^j + \xi_x^{j+1}}{J^{j+1}} \epsilon_A \right) \right. \quad (19)$$

and

$$f^j = - \left(\frac{\tilde{A}_s^j - \tilde{A}_s^{j-1}}{J^{j+1}} \right) q^j + \alpha (\tilde{E}_s^j - \tilde{E}_s^{j-1}) + (1-\alpha) \Delta \xi \left(\frac{1}{Re} \delta_\zeta \tilde{S}^j \right) \\ - (1-\alpha) \Delta \xi \delta_\eta \left[\left(\frac{\eta_x}{J} \right)^{j+1} E^j + \left(\frac{\eta_y}{J} \right)^{j+1} F^j + \left(\frac{\eta_z}{J} \right)^{j+1} G^j \right] \\ - (1-\alpha) \Delta \xi \delta_\zeta \left[\left(\frac{\zeta_x}{J} \right)^{j+1} E^j + \left(\frac{\zeta_y}{J} \right)^{j+1} F^j + \left(\frac{\zeta_z}{J} \right)^{j+1} G^j \right] \\ + \left[\left(\frac{\xi_x}{J} \right)^{j+1} E_p^j - \left(\frac{\xi_x}{J} \right)^j E_p^{j-1} \right] + \phi_e . \quad (20)$$

The central, forward and backward difference operators are δ , Δ and ∇ , respectively. E, F and G are the Cartesian flux vectors. The $\tilde{A}_s, \tilde{B}, \tilde{C}, \tilde{S}$ and $\tilde{M}$ matrices are the Jacobian matrices which are the derivatives of the transformed flux vectors $\hat{E}_s, \hat{F}, \hat{G}$ and $\hat{S}$ with respect to the $\hat{q}$ variables. E_p is a vector which is zero in the supersonic region and non-zero in the subsonic region to account for the way the pressure is held fixed in the subsonic sublayer. In the marching direction $\alpha = 0$

for Euler implicit or $\alpha = 1/3$ for three-point backward differences in the ξ direction; this corresponds to first or second accuracy in the ξ direction, respectively. The radial (ζ) and circumferential (η) differential operators are second-order accurate. Factorization errors have been eliminated for the case of uniform flows by writing the equations in terms of the flow field variables Δq without normalization by the Jacobians.

The explicit smoothing term Φ_e is fourth order in both η and ζ directions and is given as

$$\Phi_e = \epsilon_e \left(\frac{\tilde{A}_s^j + \xi_x^{j+1}}{J^{j+1}} \epsilon_B \right) [(\nabla_\eta \Delta_\eta)^2 q^j + (\nabla_\zeta \Delta_\zeta)^2 q^j] \quad (21)$$

The implicit smoothing term Φ_{IX} has the form

$$\Phi_{IX} = \epsilon_I \left(\frac{\tilde{A}_s^j + \xi_x^{j+1}}{J^{j+1}} \epsilon_B \right) (\nabla \Delta) X \quad (22)$$

The explicit damping parameter ϵ_e sizes the explicit smoothing term Φ_e . ϵ_I is an implicit smoothing parameter required to damp high frequency oscillations. The ϵ_B parameter causes the smoothing terms Φ_e and Φ_{IX} to increase or decrease relative to grid changes, ϵ_A is included to ensure that the entire primary diagonal of the block tri-diagonal never goes to zero.

To advance the solution of Equation (17), first calculate Equation (20) which corresponds to the right hand side of Equation (17). Equation (20) requires data only from known j and $j-1$ levels. The use of a central difference approximation for the η derivatives in the $\bar{N}_1$

operator, together with the periodic condition, leads to a periodic block-tridiagonal system of equations. Thus, a circumferential implicit inversion can be performed for

$$\bar{N}_i^j \Delta q^* = f^j \quad (23)$$

The use of a central difference approximation for the ζ derivative in the $\bar{N}_2$ operator also results in a block-tridiagonal system of equations. Once the intermediate variables q^* are known, it is possible to proceed with an implicit ζ sweep by solving

$$\bar{N}_2^j \Delta q^j = \Delta q^* \quad (24)$$

The new flow variables at the interior points are found using

$$q^{j+1} = q^j + \Delta q^j. \quad (25)$$

Fourier-Spectral Method

In a finite difference algorithm, the derivative at a discrete node is approximated by a linear combination of the function at that node and the adjacent nodes. This local approximation of the derivative can be obtained by using a Taylor series expansion of the function. In this thesis, the pseudospectral algorithm is a discrete Fourier series. The spectral derivative at a node will be approximated by a linear combination of the function at all the nodes in the circumferential direction. This approach results in a global approximation of the function.

In Fourier analysis, a function $f(x)$ that is periodic can be represented by an infinite Fourier series. Consider a continuous function $f(x)$ on the interval $[0,1]$, for which the Fourier series converges pointwise. The complex form of the Fourier series can be written as

$$f(x) = \sum_{n=-\infty}^{\infty} C_n e^{\frac{i2\pi nx}{X}} \quad (26)$$

where

$$C_n = \frac{1}{X} \int_0^1 f(x) e^{-\frac{i2\pi nx}{X}} dx \quad (27)$$

and the period $X = 1$. The function $f(x)$ is composed of an infinite set of components where the coefficient C_n is the amplitude of the n^{th} component with a wavelength X/n . The same type of analysis can be applied to a discrete approximation of $f(x)$ where $f(x_j)$ for $j = 0, 1, 2, \dots, N - 1$. A discrete representation of the function will result in a Fourier interpolation of the function in terms of $f(x_j)$. Thus, $f(x_j)$ may be written as the sum of a finite set of N Fourier modes.

The complex form of the truncated discrete Fourier series may be written as

$$f(x_j) = \sum_{n=0}^{N-1} A_n e^{\frac{i2\pi jn}{N}} \quad (28)$$

where

$$A_n = \frac{1}{N} \sum_{j=0}^{N-1} f(x_j) e^{-\frac{i2\pi jn}{N}} \quad (29)$$

Note that in going from Equation (26) to Equation (28), X is replaced by $N \Delta x$ and x is replaced by $j\Delta x$. Since no wavelength

smaller than Δx can be calculated for the discrete approximation of $f(x)$, the infinite series becomes a finite series. Thus, the discrete Fourier series is made up of a finite set of Fourier components and no phenomena less than the wavelength Δx can be resolved.

In this application, derivative approximations are required for odd and even periodic functions. For problems with a plane of symmetry and no yaw angle, the velocity components u and w and the coordinates x and z are even functions in η and the velocity component v and the coordinate y are odd functions in η . Then, the third component of the flux vector $\hat{F}$ is an even function in η and the other components of $\hat{F}$ are odd functions in η . The Fourier-spectral approximation can be made using the appropriate sine or cosine expansion. The components of $\partial \hat{F} / \partial \eta$ are approximated spectrally by even or odd discrete Fourier transforms as follows.

The sine series approximation can be written as follows for real odd periodic functions. Let $f_j = f(\theta_j)$, where $\theta_j = \pi j / N$, $j = 0, 1, 2, \dots, N$. For an odd function, $f_j = -f_{2N-j}$ and periodicity implies $f_j = f_{2N+j}$ and it follows that $f_0 = f_N = 0$. So f_j can be expressed as

$$f_j = \sum_{n=1}^{N-1} A_n \sin \left(\frac{\pi j n}{N} \right), j = 1, 2, \dots, N-1 \quad (30)$$

where

$$A_n = \frac{2}{N} \sum_{j=1}^{N-1} f_j \sin \left(\frac{\pi j n}{N} \right), n = 1, 2, \dots, N-1 \quad (31)$$

The derivatives of the function f at the discrete nodes θ_j can be approximated by

$$\frac{df_j}{d\theta} \approx \sum_{n=1}^{N-1} nA_n \cos\left(\frac{\pi j n}{N}\right), j = 0, 1, 2, \dots, N \quad (32)$$

The cosine series approximation can be written as follows for real even periodic functions. Let $f_j = f(\theta_j)$, where $\theta_j = j/N$, $j = 0, 1, 2, \dots, N$. For an even function, $f_j = f_{2N-j}$ and periodicity implies $f_j = f_{2N+j}$. The function f_j can be expressed as

$$f_j = \frac{1}{2} A_0 + \sum_{n=1}^{N-1} A_n \cos\left(\frac{\pi j n}{N}\right) + \frac{1}{2} (-1)^n A_N, j = 0, 1, 2, \dots, N \quad (33)$$

where

$$A_n = \frac{2}{N} \left[\frac{1}{2} f_0 + \sum_{j=1}^{N-1} f_j \cos\left(\frac{\pi j n}{N}\right) + \frac{1}{2} (-1)^n f_N \right], \quad (34)$$

$$n = 0, 1, 2, \dots, N$$

The derivatives of the function f at the discrete nodes θ_j can be approximated by

$$\frac{df_j}{d\theta} \approx - \sum_{n=1}^{N-1} nA_n \sin\left(\frac{\pi j n}{N}\right), j = 0, 1, 2, \dots, N \quad (35)$$

Equations (31) and (34) represent the projection of the physical variables f_j to the spectral space for obtaining the spectral

coefficients A_n . The derivative operation is carried out in the spectral space and the spectral coefficients of the derivative nA_n are projected back to the physical space to obtain the derivative approximations at the nodes. Computing the derivatives of the function at the discrete nodes based on the spectral coefficients is termed pseudo-spectral approximation. The spectral approximation in the circumferential direction, replaces the central differencing terms $\delta_n^{\hat{f}j}$ in the right hand side of Equation (17). The approximations to the n derivatives on the left hand side of Equation (17) are kept in the central finite difference form to preserve the tridiagonal block structure of the equations to be solved in the factored scheme.

High-order accurate spectral methods tend to exhibit nonlinear instabilities in convection dominated flows and Gottlieb, Lustman and Orszag (9) have shown that they can be stabilized by damping high frequency waves. A low pass filter of the form

$$\text{filt}(n) = \begin{cases} 1 & , n < n_0; \\ e^{-\alpha(n-n_0)^4} & , n \geq n_0, n = 0, 1, \dots, N \end{cases} \quad (36)$$

has been applied to the spectral approximations by multiplying the spectral coefficients A_n of Equations (32) and (35) by $\text{filt}(n)$. n_0 is chosen to be approximately $2N/3$ so that the highest third of the modes are damped and α is chosen such that the damping factor ranges between 1 and 10^{-10} .

III. RESULTS

Numerical solutions of the three-dimensional parabolized Navier-Stokes equations were obtained for a shuttle-like geometry at Mach 7.4 at an angle of attack of 20 degrees for comparison of finite difference and spectral approximations in the circumferential (η) direction. Comparisons are made for pressure contours between the body and the shock, pressure distributions on the body, and total temperature distributions through the boundary layer. Figures 1 and 2 illustrate the geometry for which the computations are performed. Figures 3 and 4 represent grid distribution at $x = 71$ inches and $x = 545$ inches, respectively.

The major differences between the computational geometry and the actual orbiter geometry are as follows:

- 1) The wing sweep-back angle has been increased from 45 to 55 degrees in order to avoid the embedded subsonic region.
- 2) The trailing edge is squared off at the body flap hinge line.
- 3) The lee surface is elliptical causing the wing leading edge to be more blunt.
- 4) The rudder and OMS pods are not included in the model geometry.

The coordinate locations of grid points on the shuttle-like surface are obtained from the QUICK (10) geometry package. The PNS code requires a starting solution on an initial data surface where the flow is supersonic. The nose region with its embedded subsonic region

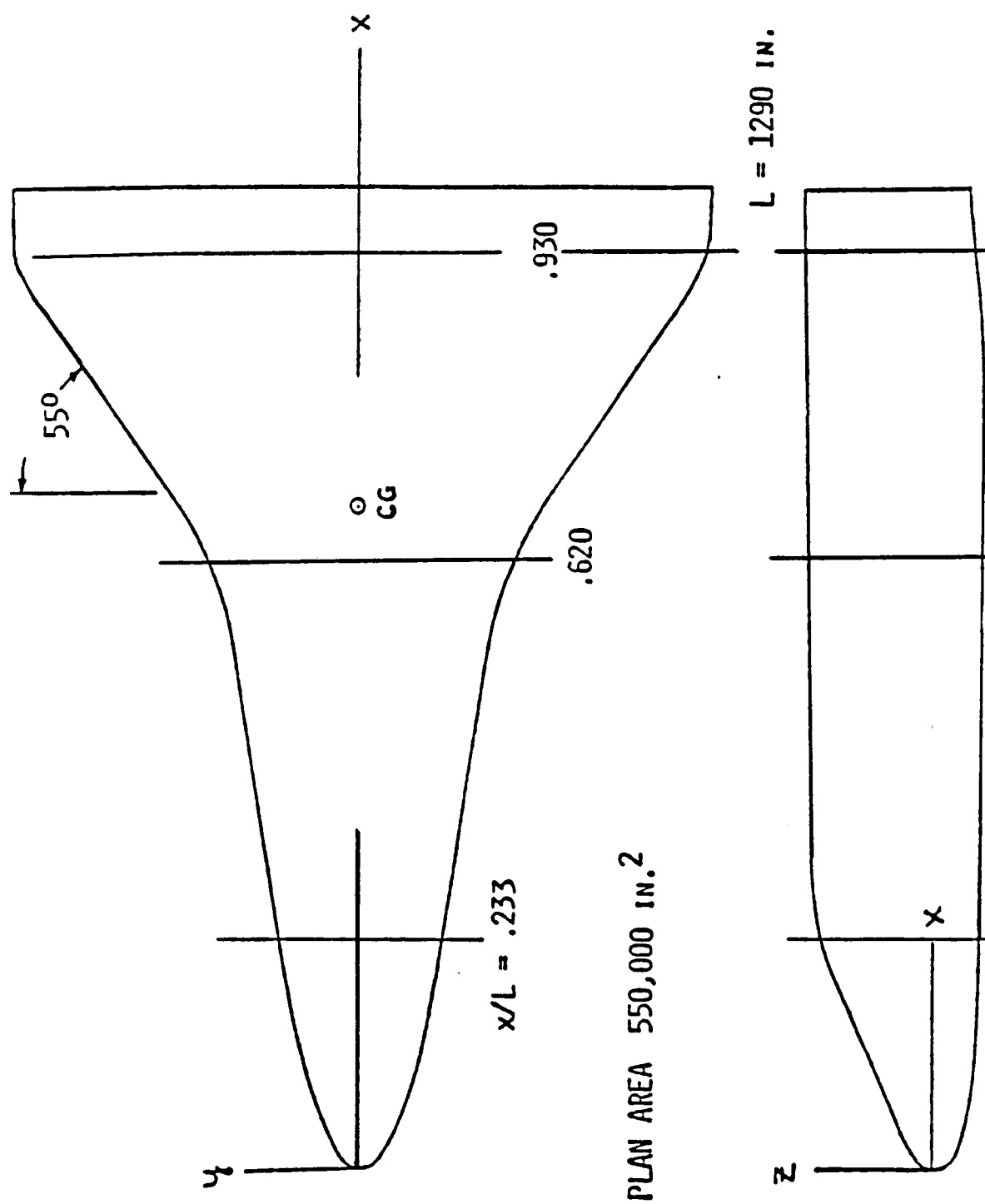


Figure 1. Computational Model Geometry

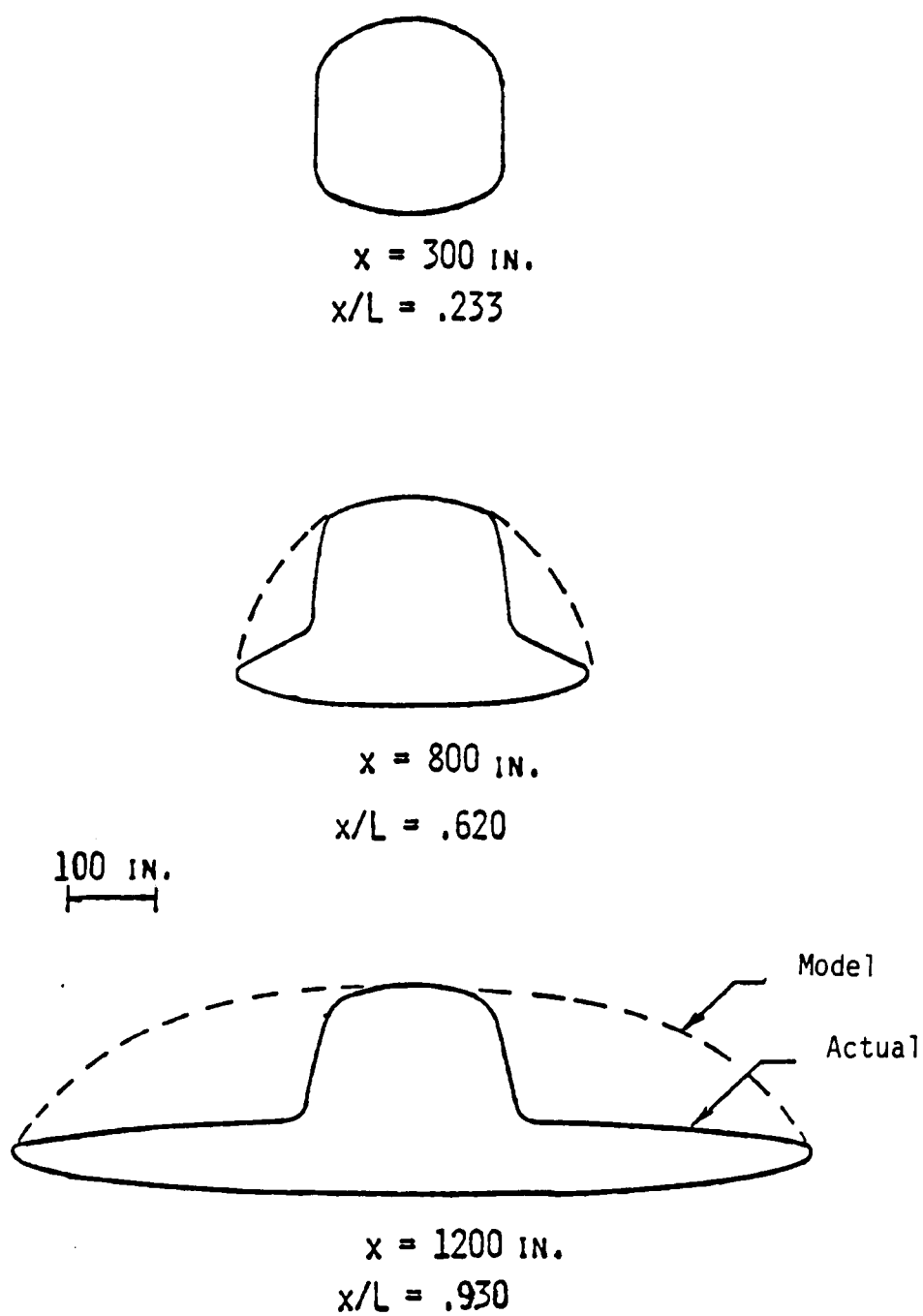


Figure 2. Computational Model Geometry Cross Sections

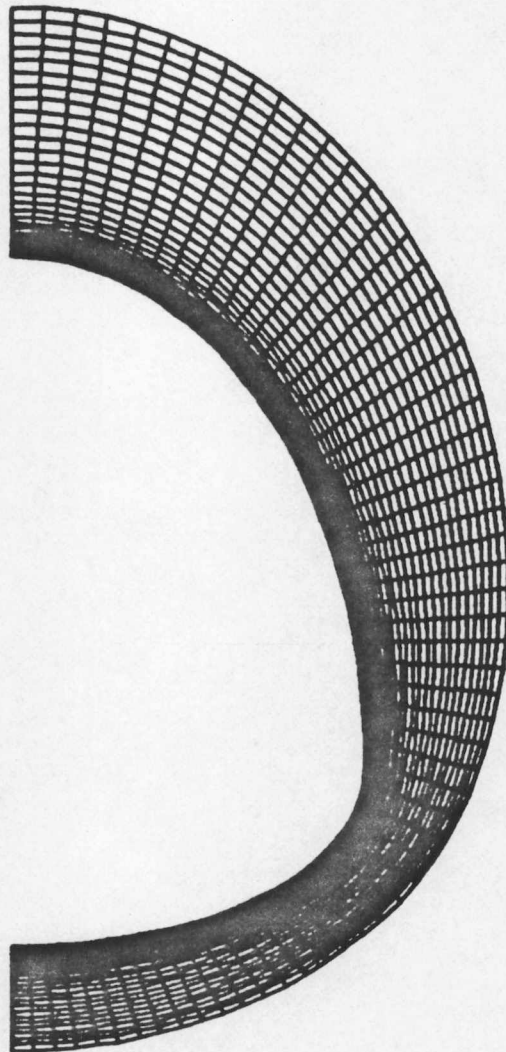


Figure 3. Grid (61x45) at $x = 71$ Inches

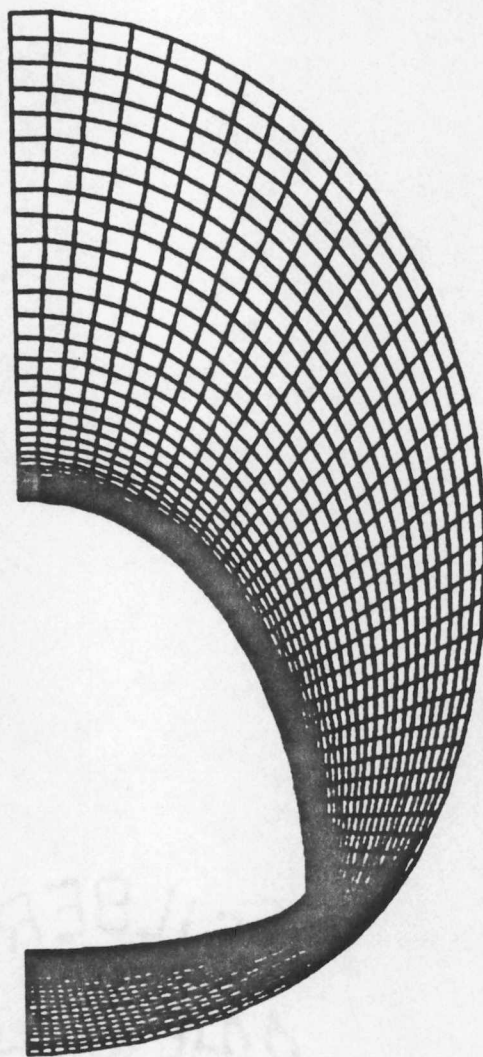


Figure 4. Grid (61x45) at $x = 545$ Inches

requires a three-dimensional time-dependent Navier-Stokes code to solve the blunt body nose flow. The three-dimensional time-dependent, thin-layer Navier-Stokes code (AIR3D) developed by Kutler, et al. (5) is used here to obtain the blunt nose solution and initial data plane for the PNS code. The free-stream conditions used throughout are: $M = 7.4$, $\alpha = 20$, $T_\infty = 98^\circ\text{R}$, $T_w = 1500^\circ\text{R}$, and $Re = 3.0 \times 10^6$ per foot. Due to significant crossflow separation a modified Baldwin-Lomax turbulence model has been used to obtain results closer to experimental values. The ratio of successive step sizes was increased by a ratio of 1.007 from 1.5 inches at the initial plane to 7.2 inches at $x = 850$ inches.

The nodes in the circumferential direction were varied to obtain three grids to compare the effect of grid spacing on the accuracy of spectral versus finite difference methods using the PNS code. The fine mesh (61x45) has 45 nodes in the normal direction ($L_{\max} = 45$) which are stretched out so that approximately 50% of the nodes are in the thin viscous layer, and 61 nodes in the circumferential direction ($K_{\max} = 61$ implies that half the circumference is divided into 60 intervals, or the circumferential nodes are 3 degrees apart from each other). Results were also obtained for meshes with 31 nodes (6 degrees apart) and 21 nodes (9 degrees apart) in the circumferential direction.

The computations indicate that the spectral approximation gives results which are comparable to those obtained using a second-order finite difference scheme. Due to the marching nature of the PNS code it is only necessary to compare results at an appropriate downstream location to determine the accuracy of the method. Figures 5 and 6

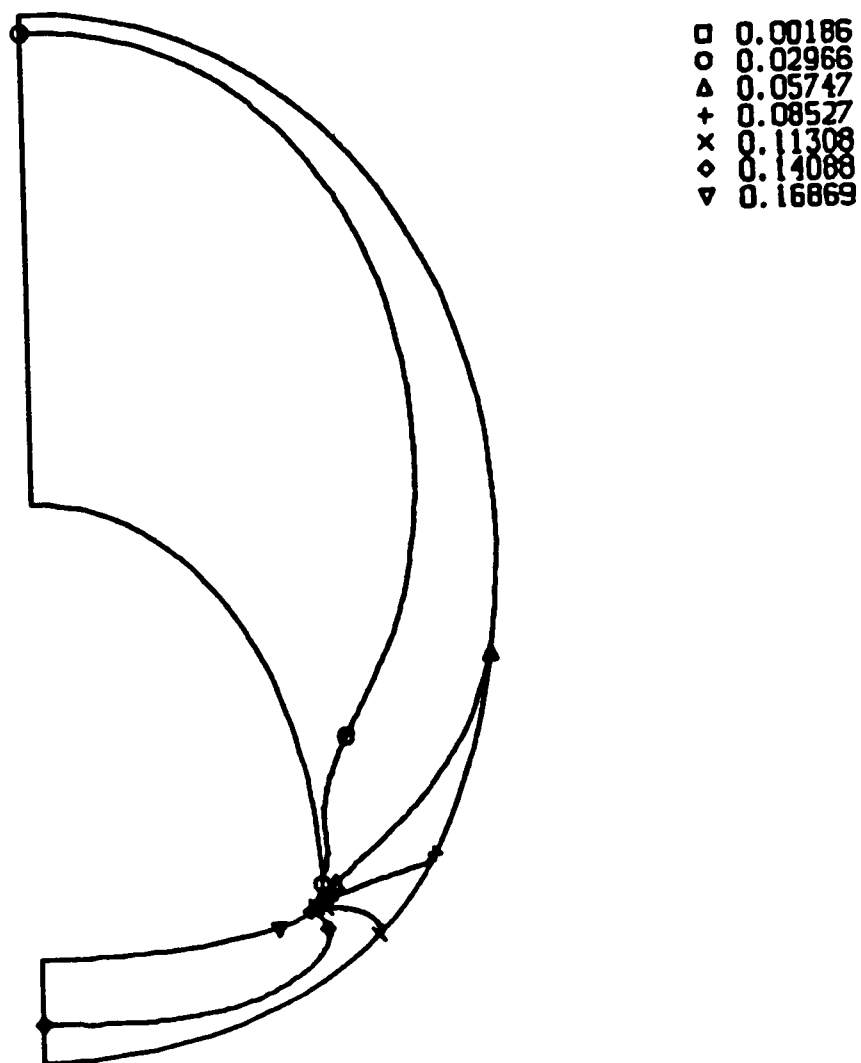


Figure 5. Finite Difference Pressure Contours (61x45)
at $x = 545$ Inches

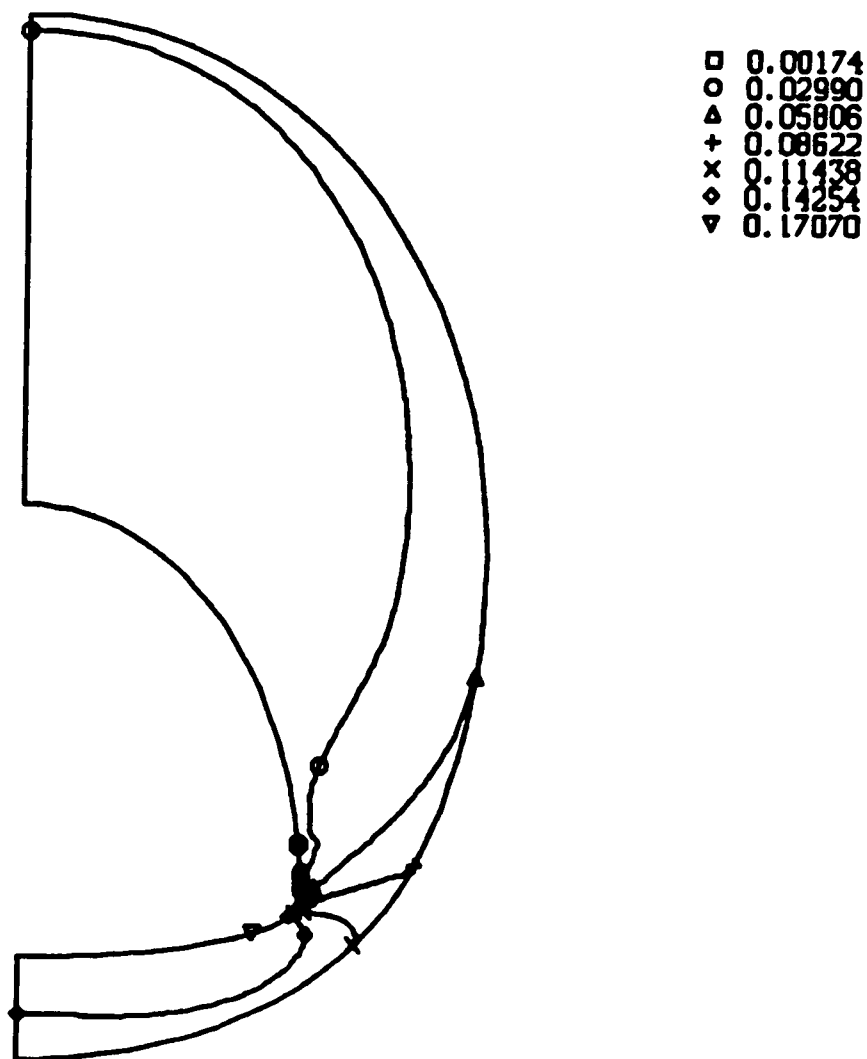


Figure 6. Spectral Pressure Contours (61x45)
at x = 545 Inches

show the pressure contours at $x = 545$ inches for the spectral and finite difference methods with a circumferential node distribution of 61 nodes. These contours are essentially identical. Figures 7 and 8 show the pressure distribution on the body in the circumferential direction for spectral and finite difference methods at $x = 545$ inches with a circumferential node distribution of 61 nodes. The spectral approximation shows a sharper transition on the leeward side but a smoother transition on the windward side. Figures 9, 10, and 11 show the pressure distribution along the body in the marching direction at the lee, middle and windward station for both spectral and finite difference methods. These plots are repeated for the cases of 61, 31 and 21 circumferential nodes. The curves overlap each other giving almost identical results. The total temperature distribution through the boundary layer on the leeward side shows the greatest variation due to the expanded viscous layer. There was no variation between finite difference and spectral methods for the total temperature through the boundary layer on the windward side. The total temperature distribution for the leeward side has been plotted for both finite difference and spectral methods at $x = 428$ inches. This plot is repeated for 61, 31 and 21 circumferential nodes and these curves also closely overlap as shown in Figures 12, 13, and 14.

The numerical algorithm used in the PNS code requires numerical viscosity terms to control numerical instabilities. The four smoothing terms in the AFWAL PNS Code have an influence on the accuracy of the solutions. The explicit damping parameter controls the amount of explicit smoothing. An implicit smoothing parameter is required to

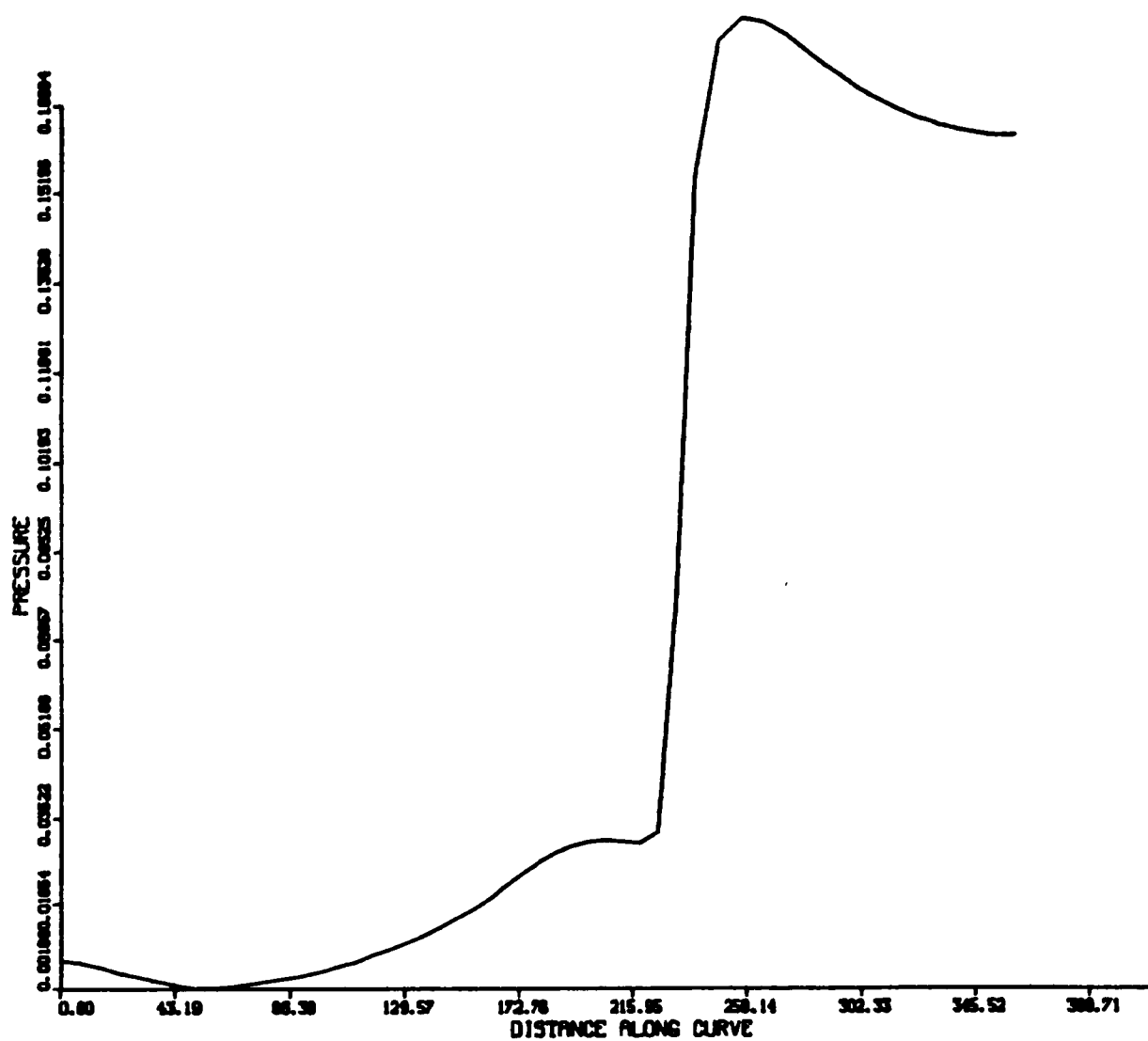


Figure 7. Finite Difference Circumferential Pressure Distribution (61x45) at $x = 545$ Inches

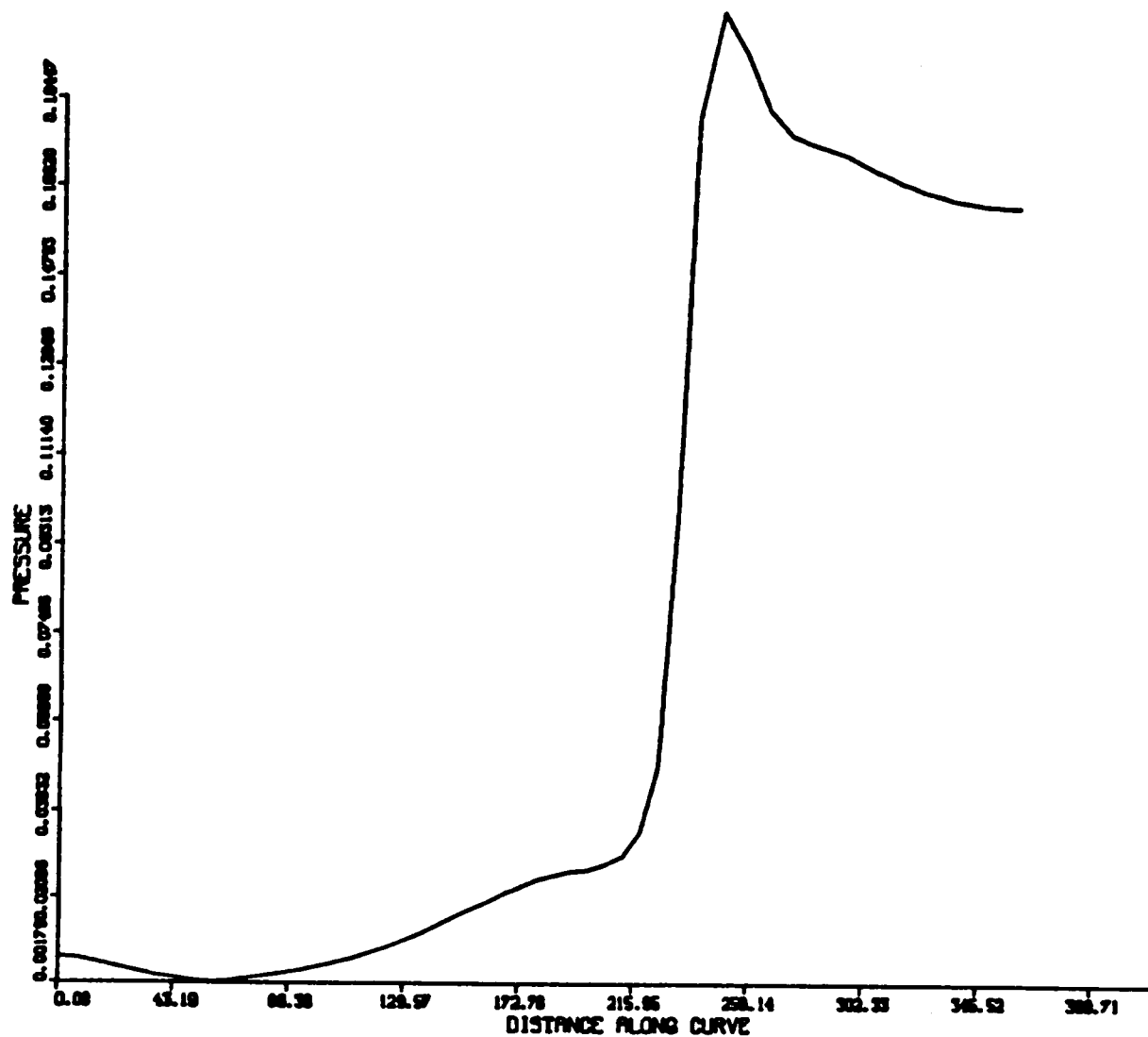


Figure 8. Spectral Circumferential Pressure Distribution (61x45) at x = 545 Inches

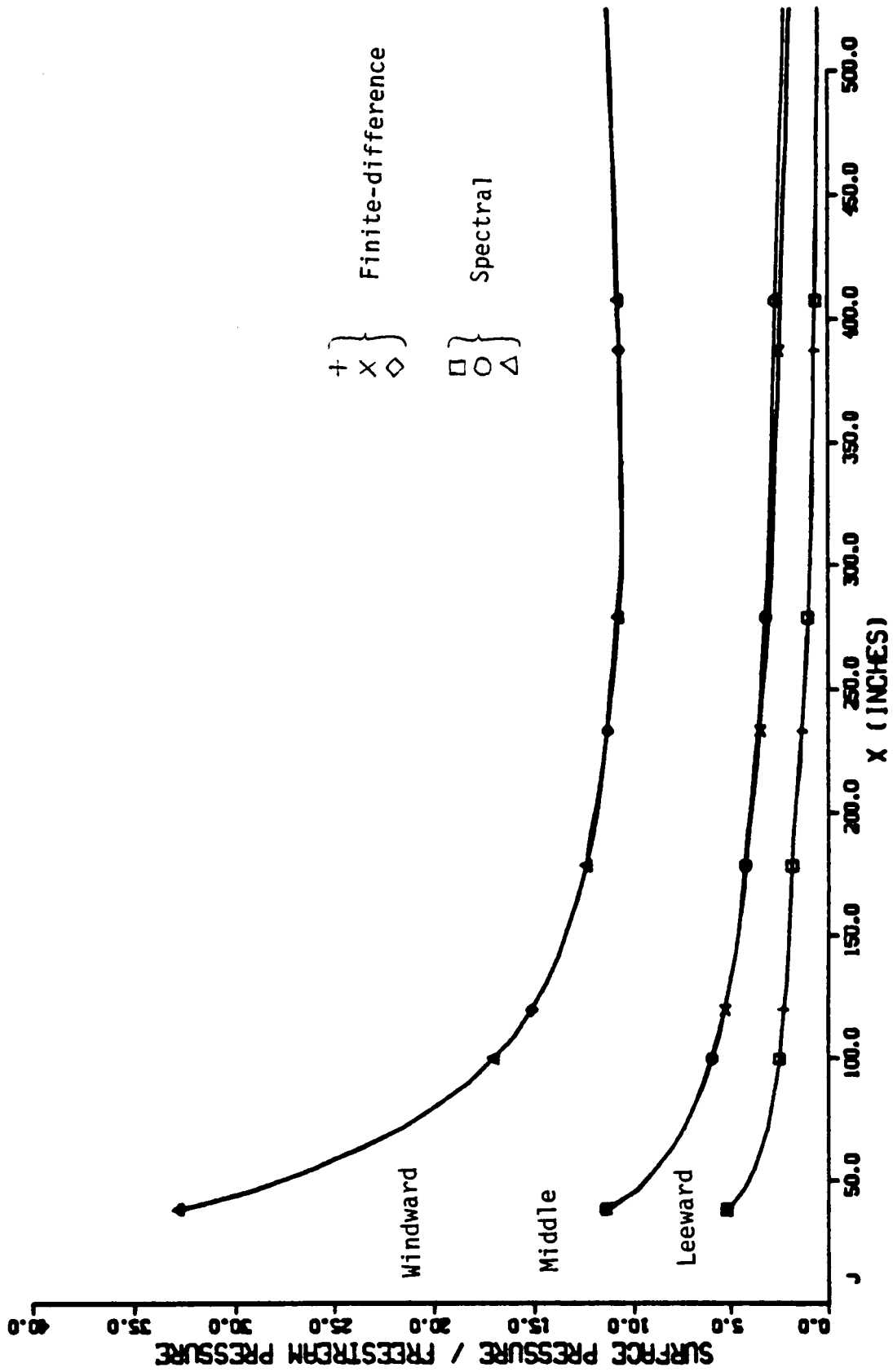


Figure 9. Finite Difference and Spectral Axial Pressure Distribution (61x45)

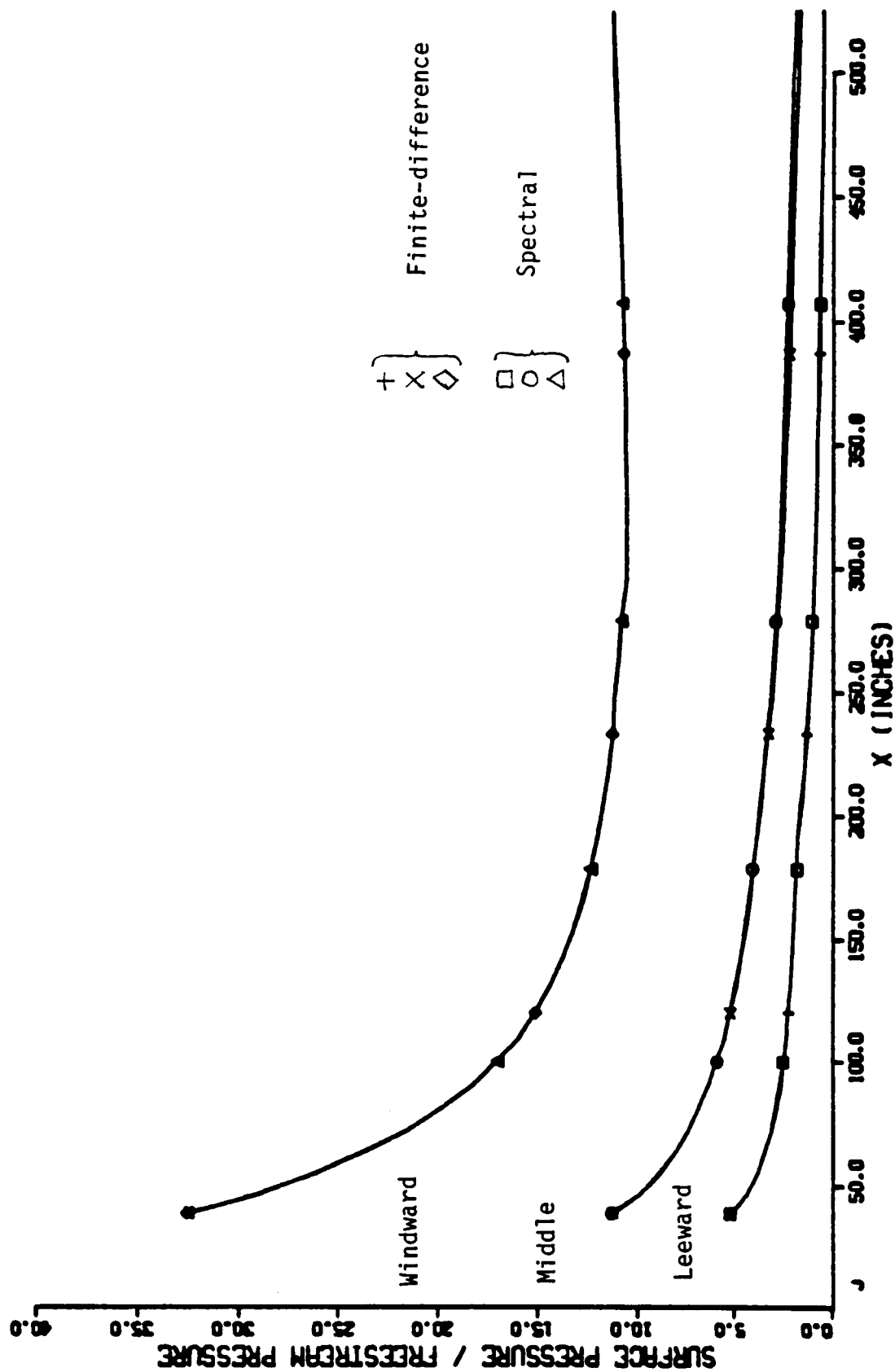


Figure 10. Finite Difference and Spectral Axial Pressure distribution (31x45)

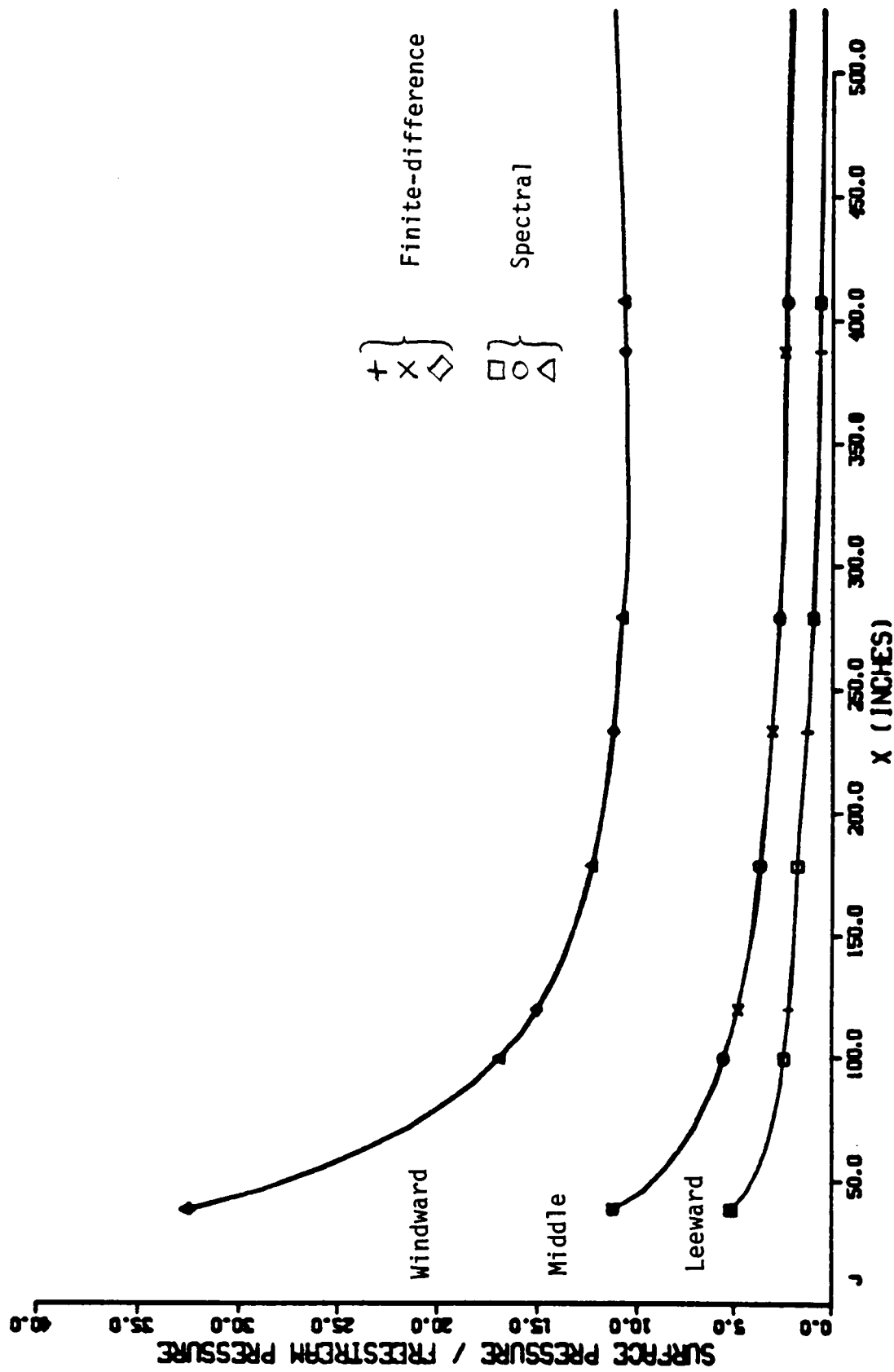


Figure 11. Finite Difference and Spectral Axial Pressure Distribution (21x45)

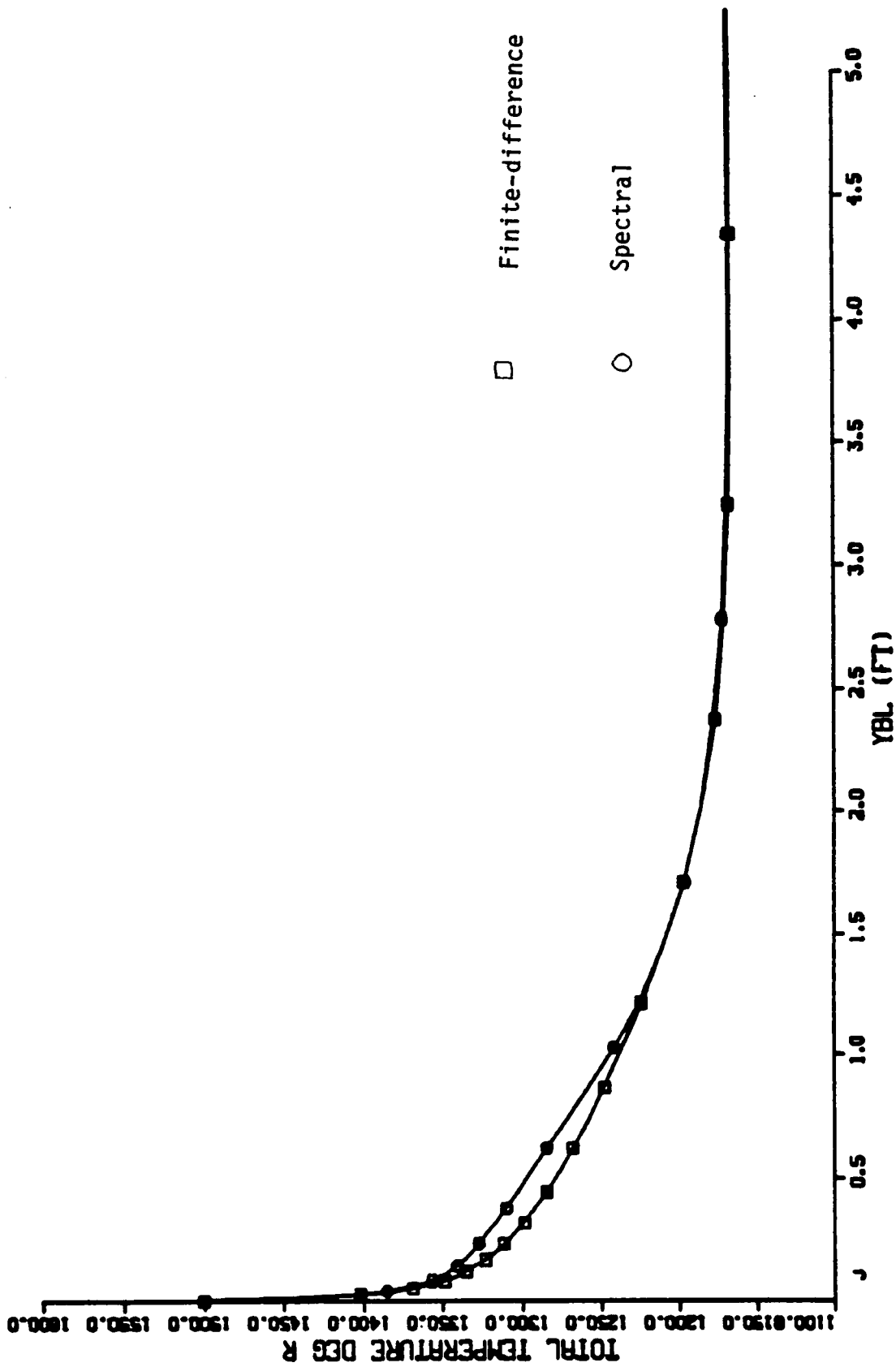


Figure 12. Leeward Finite Difference and Spectral Total Temperature Distribution (61x45) at x = 428 Inches

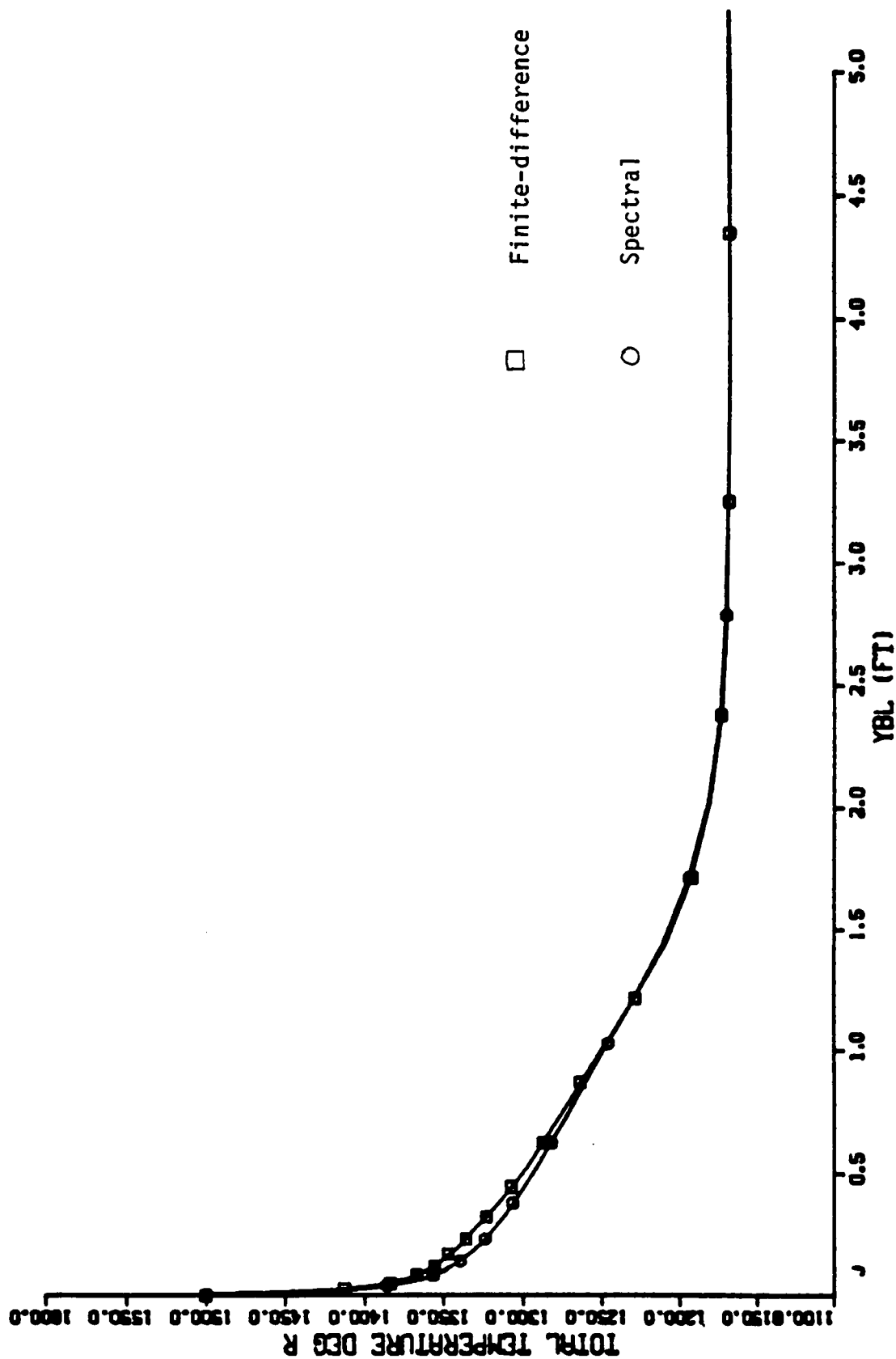


Figure 13. Leeward Finite Difference and Spectral Total Temperature Distribution (31x45) at $x = 428$ Inches

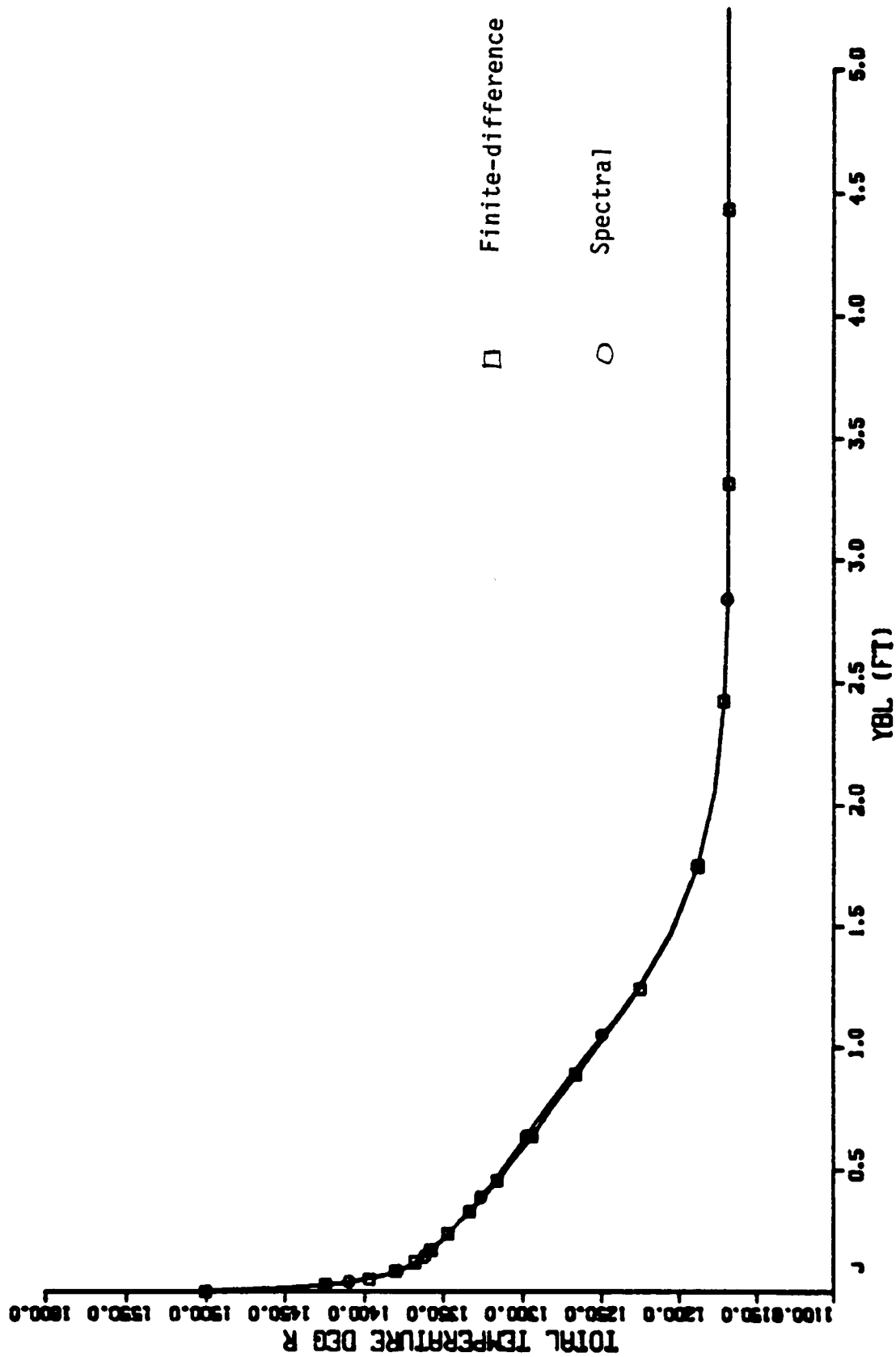


Figure 14. Leeward Finite Difference and Spectral Total Temperature Distribution (21x45) at $x = 428$ Inches

damp high frequency oscillations. There is another parameter to cause the smoothing terms to increase or decrease relative to grid changes. And, there is a smoothing parameter to ensure that the entire primary diagonal of the block tridiagonal never goes to zero.

These calculations have been performed on a Cray computer. The spectral version of the code required approximately 4% more computing time than the finite difference version while achieving essentially identical results.

IV. CONCLUSIONS

Numerical solutions of the three-dimensional parabolized Navier-Stokes equations using the AFWAL PNS Code were obtained for a shuttle-like geometry at Mach 7.4 at an angle of attack of 20 degrees for comparison of finite difference and spectral approximations in the circumferential direction. Comparisons were made for pressure contours between the body and the shock, pressure distributions on the body, and total temperature distributions through the boundary layer. Also, the nodes in the circumferential direction were varied to obtain three grids to compare the effect of grid spacing on the accuracy of spectral versus finite difference methods using the AFWAL PNS Code. Due to the marching nature of the code it was only necessary to compare the results at an appropriate downstream location. These computations indicated that the spectral approximation gives results which are essentially identical to those obtained using a second-order finite difference scheme. The spectral version of the code required approximately 4% more computing time than the finite difference version while achieving essentially identical results.

The smoothing terms in the AFWAL PNS Code which are necessary for numerical stability have a pronounced effect upon the solutions. These smoothing terms seem to have the effect of reducing the spectral accuracy to second-order accuracy. Also, another cause of the reduced spectral accuracy is the second-order accuracy of the left hand side of the solution algorithm. The approximations to the left hand operators were left in second-order accurate finite-difference form to

preserve the block tridiagonal structure of the equations to be solved in the factored scheme. This approximation simplifies the space marching procedure. But, the second-order accuracy of the left hand side of the solution algorithm also apparently dominates the accuracy of the entire solution. Hence, only second-order accuracy is obtained for both spectral and finite-difference methods. Further study would be necessary to determine how to optimize the AFWAL PNS Code numerical algorithms to obtain the potential accuracy of the spectral technique.

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VITA

Lynn Alan Nicholson was born in Grand Rapids, Michigan on December 20, 1950. His family moved from Ann Arbor, Michigan to Huntsville, Alabama in 1959. He attended Whitesburg Elementary and Huntsville High School. In 1970 he entered the University of Alabama in Huntsville. He transferred to Auburn University in 1974 and graduated in March 1979 with a Bachelor of Mechanical Engineering degree.

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