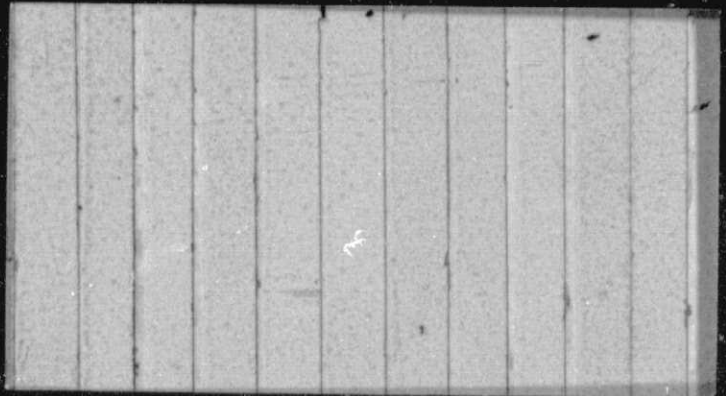


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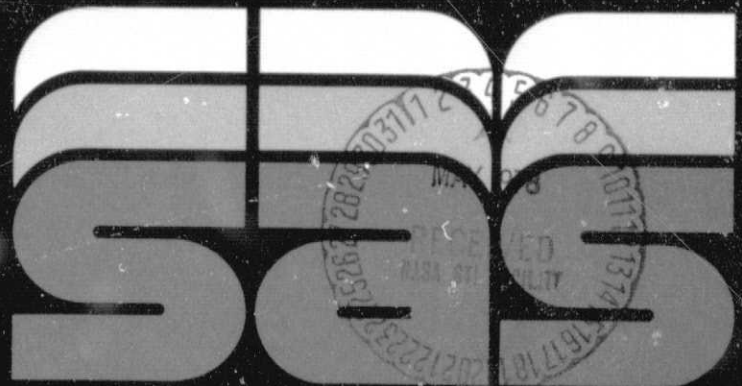
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SOFTWARE DEVELOPMENT

FOR

STRATOSPHERIC MODELING

(Final Report)

**Software Development
for
Stratospheric Modeling**

(Final Report)

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FOREWORD

This report describes work performed by Systems and Applied Sciences Corporation (SAS) under NASA Contract No. NAS5-24255. The work involves development of an improved two-dimensional model of chemical and physical processes in the stratosphere.

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SECTION 1 - INTRODUCTION

A more comprehensive model for stratospheric chemistry and transport theory is being developed for the purpose of aiding predictions of changes in the stratospheric ozone content as a consequence of natural and anthropogenic processes. This new and more advanced stratospheric model is time dependent and the dependent variables are zonal means of the relevant meteorological quantities which are functions of latitude and height. The model is constructed by the best mathematical approach on a large IBM S360 in American National Standard FORTRAN. It will be both a scientific tool and an assessment device used to evaluate other models. Program blocks are kept under a maximum of 100 statements per routine and each routine has but one function. The report sets out the detailed formulation of a numerical model both in physics and mathematics. The interactions of dynamics, photochemistry and radiation in the stratosphere can be governed by a set of fundamental dynamical equations which will be described in Section 2. Some physical ideal is obtained from an existing FORTRAN computer source deck of Crutzen's two-dimensional model of the stratosphere which is subsequently applied in building new and more comprehensive models. Section 3 describes the numerical method used in the integration. Some preliminary results and discussions are presented in Section 4.

SECTION 2 - BASIC EQUATIONS

The model is an integration of an extensive set of fundamental equations which can be used to predict the future state of the atmospheric circulation from knowledge of its present state. In an (x, y, ξ) coordinate system in which $x =$ distance eastwards, $y =$ distance northwards, and $\xi = \log (p_0/p)$; with $p_0 = 1000$ mb and $p =$ pressure, u , v , and w are the three corresponding velocity components respectively. In this log-pressure system the eastward component of the momentum equation is:

$$\frac{\partial}{\partial t} u + u \frac{\partial}{\partial x} u + v \frac{\partial}{\partial y} u + w \frac{\partial}{\partial \xi} u = \frac{uv}{a} \tan \varphi + 2 \Omega v \sin \varphi - \frac{\partial Z}{\partial x} \quad (1)$$

where $a =$ radius of the earth, $\Omega =$ rate of rotation of the earth, $\varphi =$ latitude, Z is geopotential. The thermodynamic equation is:

$$\frac{\partial}{\partial t} \theta + u \frac{\partial}{\partial x} \theta + v \frac{\partial}{\partial y} \theta + w \frac{\partial}{\partial \xi} \theta = q \quad (2)$$

where $\theta = T (p_0/p)^k$, $T =$ temperature, q is the rate of change of potential temperature, K is the ratio of gas constant for dry air R to specific heat of air at constant pressure C . The equation for conservation of matter is:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} - \frac{v}{a} \tan \varphi + \frac{\partial w}{\partial \xi} - w = 0 \quad (3)$$

Since our aim is to deal explicitly with zonal mean quantities only.

Accordingly let a over bar denote the zonal mean and a dash denote the departure therefrom, then equations (1) to (3) yield, after taking an average around a latitude circle:

$$\frac{\partial}{\partial t} (\bar{\tau} e^{-\xi} \cos \varphi) + \frac{\partial}{\partial y} (\bar{v} \bar{\tau}) + \frac{\partial}{\partial \xi} (\bar{w} \bar{\tau}) = - \frac{\partial}{\partial y} (\overline{v' \tau'}) - \frac{\partial}{\partial \xi} (\overline{w' \tau'}) \quad (4)$$

$$\frac{\partial}{\partial t} (\bar{\theta} e^{-\xi} \cos \varphi) + \frac{\partial}{\partial y} (\bar{v} \bar{\theta}) + \frac{\partial}{\partial \xi} (\bar{w} \bar{\theta}) = \bar{q} e^{-\xi} \cos \varphi - \frac{\partial}{\partial y} (\overline{v' \theta'}) - \frac{\partial}{\partial \xi} (\overline{w' \theta'}) \quad (5)$$

$$\frac{\partial}{\partial y} \bar{v} + \frac{\partial}{\partial \xi} \bar{w} = 0 \quad (6)$$

where $\tau = (\Omega a \cos \varphi + u) a \cos \varphi$

$$v = v e^{-\xi} \cos \varphi$$

$$w = w e^{-\xi} \cos \varphi$$

Note that the continuity equation (3) takes the simple form (6) which is the advantage of using the pressure coordinates.

Equations (4) to (6) may become a complete set by adding the y component momentum and hydrostatic equations. For our own purpose of not introducing the gravity waves we introduce an approximation to the y component

momentum equation that the zonal mean wind is in geostrophic equilibrium with the zonal mean geopotential field. Combining this with the hydrostatic equation leads to the thermal wind relationship:

$$\frac{\partial}{\partial \xi} \bar{v} = - \frac{R \exp(-k \xi)}{2 \Omega \tan \varphi} \frac{\partial \theta}{\partial y} \quad (7)$$

Equations (4) to (7) can be regarded as a closed set which completely determines the relationships among the dependent variables τ , θ , V , W . The other variables can be written in terms of the relevant quantities and are held as functions of time, latitude and altitude.

SECTION 3 - NUMERICAL METHOD

It is convenient to make the equations dimensionless. The scaling quantities is given a subscript s. Equations (4) to (7) become:

$$\frac{\partial}{\partial t} (\bar{\tau} e^{-k\xi_s\xi} \cos \varphi) + \frac{\partial}{\partial \varphi} (\bar{\tau} \bar{V}) + \frac{\partial}{\partial \xi} (\bar{\tau} \bar{W}) = H \quad (8)$$

$$\frac{\partial}{\partial t} (\bar{\theta} e^{-k\xi_s\xi} \cos \varphi) + \frac{\partial}{\partial \varphi} (\bar{\theta} \bar{V}) + \frac{\partial}{\partial \xi} (\bar{\theta} \bar{W}) = \bar{q} e^{-k\xi_s\xi} \cos \varphi + Q \quad (9)$$

$$\frac{\partial}{\partial \xi} \bar{\tau} = - \frac{e^{-k\xi_s\xi}}{\tan \varphi} \frac{\partial \bar{\theta}}{\partial \varphi} \quad (10)$$

$$\bar{V} = - \frac{\partial \Psi}{\partial \xi} \quad \bar{W} = \frac{\partial \Psi}{\partial \varphi} \quad (11)$$

where H and Q are the divergence of eddy momentum and eddy heat flux, respectively. Ψ is a stream function which is introduced to rewrite equation (6) in the form of equation (11). The method of solution is to eliminate the time derivatives from (8) and (9) using (10). Substituting for \bar{V} and \bar{W} from (11) gives an equation for Ψ .

$$\begin{aligned} & -\bar{\tau}_\varphi \psi_{\xi\xi} + 2 \bar{\tau}_\xi \psi_{\xi\varphi} + \frac{\bar{\theta}_\xi e^{-k\xi_s\xi}}{\tan \varphi} \psi_{\varphi\varphi} - \left[\xi_s \bar{\tau}_\varphi + \frac{\bar{\theta}_\varphi e^{-k\xi_s\xi} (1 + \sin^2 \varphi)}{\sin^2 \varphi} \right] \psi_\xi + \\ & \left[\xi_s \bar{\tau}_\xi + e^{-k\xi_s\xi} s \bar{\theta}_\xi + k \xi_s e^{-k\xi_s\xi} s \bar{\theta}_\varphi / \tan \varphi \right] \psi_\varphi = H_\xi + \xi_s H + \\ & e^{-k\xi_s\xi} \left[e^{-k\xi_s\xi} s \cos \varphi q_\varphi + Q_\varphi + Q \tan \varphi \right] / \tan \varphi \end{aligned} \quad (12)$$

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The ξ and ϕ used as subscripts denote differentiation with respect to that quantity. It may be solved with suitable boundary conditions for Ψ which may be used in (8) and (9) to get new values of τ, θ at the advanced time step. Equation (12) is then solved at the new time value and the process repeated.

A Crank-Nicholson implicit finite difference scheme is used in the numerical calculations. The Alternate Direction Implicit method is adopted so that the finite difference equation can be solved by simply inverting a tridiagonal matrix in each of the two dimensions sequentially. The nonlinear coefficients in the equations can be taken into account by using a predictor - corrector procedure. A more detailed description is followed.

Eq. (12) is an elliptic type, second order partial differential equation which can be solved by running a marching method for the time-dependent equation out to a sufficiently large time. Equations (8) and (9) are time-dependent first order partial differential equations. A general form for the set of equations can be written as:

$$S_t = A S_{\xi\xi} + B S_{\xi\phi} + C S_{\phi\phi} + D S_{\xi} + E S_{\phi} + F \quad (13)$$

The ADI scheme for equation (13) is the following:

$$S^{n+\frac{1}{2}} = S^n + \Delta t \left[A \delta_{\xi}^2 (S^{n+\frac{1}{2}}) + B S_{\xi\phi}^n + C \delta_{\phi}^2 (S^n) + D \delta_{\xi} (S^{n+\frac{1}{2}}) + E \delta_{\phi} (S^n) + F \right] \quad (14)$$

$$S^{n+1} = S^n + \Delta t \left[A \delta_\xi^2 (S^{n+\frac{1}{2}}) + B S_\xi^n \phi + C \delta_\phi^2 (S^{n+1}) + D \delta_\xi (S^{n+\frac{1}{2}}) + E \delta_\phi (S^{n+1}) + F \right] \quad (15)$$

where:

$$\delta_\xi^2 S_{jk} = (S_{j+1,k} - 2 S_{j,k} + S_{j-1,k}) / \Delta \xi^2$$

$$\delta_\phi^2 S_{jk} = (S_{j,k+1} - 2 S_{j,k} + S_{j,k-1}) / \Delta \phi^2$$

$$\delta_\xi S_{jk} = (S_{j+1,k} - S_{j-1,k}) / 2 \Delta \xi$$

$$\delta_\phi S_{jk} = (S_{j,k+1} - S_{j,k-1}) / 2 \Delta \phi$$

A simple tridiagonal matrix inversion will solve equations (14) and (15) to give the solution of equation (13).

SECTION 4 - PRELIMINARY RESULTS AND DISCUSSIONS

Equation (12) is an elliptic type, boundary value problem so that the crossing term $\psi_{\xi\varphi}$ is not a dominant term which can be approximated at the old time step as shown in equation (14) and (15). This enables us to use the Crank-Nicholson scheme and the ADI method to solve equation (12) without changing the coordinates for getting rid of the crossing term. Equation (12) has been solved without over 100 total time steps before it reached the steady state solution.

We have taken the average for each two consecutive values of ψ in the process of getting fast convergence. The values of ψ are then used to determine V and W which are substituted in equations (8) and (9) for solving r and θ at the advanced time step. This process has been repeated many times.

The terms in the right hand side of equation (12) are source functions which drive the rate of heating due to absorption of solar radiation and the rate of cooling by thermal radiation. Eddy fluxes of heat and momentum are treated by large-scale diffusion coefficients. For these fixed driving terms the solutions of the set of equations do not converge very well. It may be due primarily to the poor initial data available. Therefore, we have to find the steady state solution first before seeking any time-dependent solutions.