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REQUIEM FOR AN INTEGRATION PROCEDURE

by

J. P. Gerrity, Jr.
R. D. McPherson
and
P. D. Polger

Development Division
National Meteorological Center

OFFICE NOTE 53

1. Introduction

An effort to develop an implicit integration method suitable for application to a multi-level baroclinic model was initiated at NMC in the autumn of 1969. The initial stages followed the approach of Robert[1], who had been studying such methods for some time. The method he proposed treats implicitly, and therefore stably, *all* allowable gravitational oscillations, both external and internal. This treatment necessitates the solution at each time step of a boundary value problem consisting of one Helmholtz-type equation per layer in the model. Based on the results of experiments with a barotropic primitive equation model, he predicted a time advantage of 4:1 using this method, because of the longer time step permitted. This has subsequently been confirmed in preliminary experiments with a baroclinic model.[2]

After our own efforts to develop such techniques had been underway for some months, it occurred to us that further economies might be effected if one could somehow discriminate between the fastest modes and those with slower phase speeds in applying the implicit method. For example, in Office Note 47, it was shown that, in a four-layer model with an isothermal basic state, the two fastest modes have phase speeds in excess of 100 m sec^{-1}, while the two slower modes have phase speeds below 50 m sec^{-1}. It would not seem necessary to treat implicitly the latter two modes, for they are comparable to wind speeds found in the atmosphere which govern the linear stability criteria of the semi-implicit method. Further investigation revealed that, depending on whether one elected to use a Phillips- or Shuman-type 'sigma' vertical coordinate, the boundary-value problem to be solved at each time step reduced to one or two Helmholtz equations respectively, regardless of the number of layers in the model. It was a good idea.

But we write to bury Caesar, not to praise him, to adapt a phrase: the fact is, it didn't work. The reasons why the idea failed are sufficiently unusual to warrant an account of both the reason and the process of arriving at the fatal conclusion.

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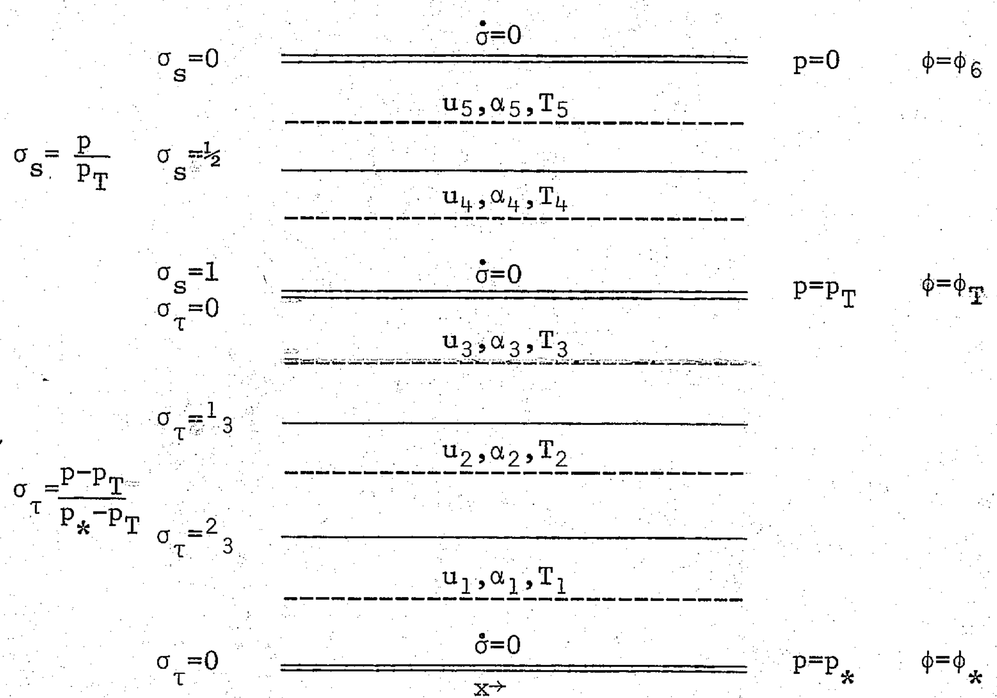
1 Unpublished manuscript.
2 Personal communication.

2. The 'Slab' Model

In our avarice to achieve further computational economies, we rather hastily programmed a model to test the idea. We elected to use the Shuman definition of the vertical coordinate, anticipating that we would be able to treat implicitly the fastest allowable mode, corresponding to the external gravity (Lamb) wave, and also the first internal mode corresponding to oscillations of the material surface separating the two σ-domains. The vertical structure is indicated schematically below:



The vertical plane is divided into two σ-domains. The lower one is composed of three layers and corresponds to the troposphere, while the upper has two layers and represents the stratosphere. Each domain is surrounded above and below by a material surface, on which $\dot{\sigma}$ $(=\frac{d\sigma}{dt})\equiv 0$. It was assumed that there was no variation in the y-direction; the integration was carried out only in the vertical plane. Hence, the model was colloquially dubbed the 'slab' model, and will be so referred to hereafter. In the development of the model, a flat, non-rotating earth was assumed.

It would go beyond the scope of this note to display the difference equations and to derive the Helmholtz equations resulting from the modified semi-implicit method. Suffice it to state that we obtained a system of two Helmholtz equations in p_* and p_T, which we were able to solve by relaxation. In retrospect, however, our original derivation was done in a rather awkward manner, which tended to obscure what was actually done to certain of the terms of the equations. This deficiency resulted in confusion in interpreting the results of subsequent attempts to analyze the model.

The slab model was eventually integrated to 100 hours using a one-hour time step and the customary Δx of 381 km. The initial data were uniform pressures and geopotentials, an isothermal stratification at T=250 K, and winds varying sinusoidally in the horizontal but without vertical shear. These integrations, for a range of horizontal wave numbers from unity to that corresponding to the wave of length $4\Delta x$, were successful in the sense that there was no evidence of exponential instability. We therefore concluded that the basic concept was a viable one.

There was, however, one problem: there was a tendency for the mean surface pressure to steadily decline throughout the calculation. The magnitude of this loss of mass seemed to be proportional to the horizontal wave number, as indicated in Figure 1. Because we had prescribed cyclic boundary conditions in the horizontal, and had $\dot{\sigma}=0$ at the upper and lower boundaries, it did not appear that a boundary flux of mass could be responsible. Instead, we attributed (incorrectly, it turns out) the difficulty to some unknown flaw in the relaxation procedure which we felt certain could be isolated and removed with a modest investment of time.

Efforts to locate the error in the relaxation procedure proved to be fruitless. Meanwhile, we had begun an effort to analyze the linearized system of equations in order to determine the allowable free modes in a model with a σ-vertical coordinate, and to examine the stability characteristics of implicit methods in such a model. These studies have previously been documented as Office Notes 45, 47, 49, and 52. The next section presents a brief summary of these studies.

3. Summary of Linear Stability Investigations

The analysis of the full five-layer slab model is not mathematically intractable in principle. Rather, it would be mainly a tedious exercise in algebra. At the outset, we therefore simplified the problem to a two-layer model using either Phillips' or Shuman's definition of the vertical coordinate. With the former, a two-layer model is very similar to the stratosphere of the slab model. It was therefore felt that the analysis of the simpler model would give some insight into the behavior of the slab model. The following summary of results is concerned exclusively with the Phillips σ-coordinate.

It should be noted, however, that parallel investigations with the Shuman definition have been conducted, with similar results.

Following the procedure outlined in Office Note 45, the equations governing the fluid are linearized about a barotropic state of no-motion. It is assumed that the underlying surface is flat and non-rotating, that the fluid is unbounded in the horizontal, and that slab-symmetry holds. We consider the isentropic flow of an ideal, inviscid gas. The perturbation equations are

$$u_t + \phi_x + \alpha\sigma(p_*)_x = 0 \tag{1}$$

$$(p_*)_t + \overline{p}_* u_x + \overline{p}_* \dot{\sigma}_\sigma = 0 \tag{2}$$

$$c_p T_t - \overline{\alpha}\sigma(p_*)_t + c_p\overline{\Gamma}\dot{\sigma} = 0 \tag{3}$$

$$\phi_\sigma + \overline{\alpha}\, p_* + \overline{p}_*\, \alpha = 0 \tag{4}$$

$$\overline{p}_*\alpha\sigma + \overline{\alpha}\sigma\, p_* = RT \tag{5}$$

where $\sigma = \frac{p}{p_*} = \frac{\overline{p}}{\overline{p}_*}$, with p_* the surface pressure. Also

$$\overline{\Gamma} = \frac{\partial\overline{T}}{\partial\sigma} - \frac{\overline{\alpha}\overline{p}_*}{c_p} \tag{6}$$

The overbar represents basic state variables; the unbarred quantities are perturbations. It will be noted that the system is not closed, because of the absence of an equation for the material derivative of the vertical coordinate, $\frac{d\sigma}{dt} \equiv \dot{\sigma}$. This can be remedied by differentiating (2) with respect to σ:

$$\dot{\sigma}_{\sigma\sigma} = - u_{x\sigma} \,, \tag{7}$$

since p_* is not a function of σ. For the same reason, and because $\dot{\sigma}$ vanishes at the upper ($\sigma = 0$) and lower ($\sigma = 1$) boundaries, eqn. (2) may be integrated vertically to obtain

$$(p_*)_t + \overline{p}_* \int_{\sigma=1}^{\sigma=0} u_x d\sigma = 0 \tag{8}$$

The temporal discretization appropriate to what was termed the semi-implicit and modified semi-implicit methods was then applied to eqns. (1-5). An ambiguity in nomenclature unfortunately exists: the semi-implicit method seeks to treat *all* the gravitational modes implicitly; the prefix 'semi' refers to the fact that in application to a non-linear model, the non-linear terms would be treated explicitly. The 'modified' method seeks to treat implicitly only the fastest gravitational modes. In a two-layer model, only two modes are permitted: one external, one internal. The 'modified' method attempts to treat implicitly only the external mode.

As presented in Office Note 45, the difference equations for the semi-implicit method are

$$\frac{u^{n+1}-u^{n-1}}{2\Delta t} + \tfrac{1}{2}(\phi^{n+1}+\phi^{n-1})_x + \tfrac{1}{2}\,\overline{\alpha}\sigma(p_*^{n+1}+p_*^{n-1})_x = 0 \qquad \text{S-1}$$

$$\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + \tfrac{1}{2}\,\overline{p}_*(u^{n+1}+u^{n-1})_x + \tfrac{1}{2}\,\overline{p}_*(\dot{\sigma}^{n+1}+\dot{\sigma}^{n-1})_\sigma = 0 \qquad \text{S-2}$$

$$c_p\,\frac{T^{n+1}-T^{n-1}}{2\Delta t} - \overline{\alpha}\sigma\,\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + \tfrac{1}{2}\,c_p\overline{\Gamma}(\dot{\sigma}^{n+1}+\dot{\sigma}^{n-1}) = 0 \qquad \text{S-3}$$

$$\phi_\sigma^n + \overline{\alpha}\,p_*^n + \overline{p}_*\,\alpha^n = 0 \qquad \text{S-4}$$

$$\overline{p}_*\alpha^n\sigma + \overline{\alpha}\,\sigma\,p_*^n = RT^n \qquad \text{S-5}$$

These equations may then be specialized for a two-layer model and solutions of the form

$$q^n = q\,\zeta^n\,e^{ikx} \qquad (9)$$

are assumed. Stability depends on the existence of non-trivial solutions for $|\zeta| \leq 1$. It should be noted at this point that the hydrostatic equation (S-4) and the ideal gas law (S-5) may be treated either completely explicitly, as is indicated in the above equations, or completely implicitly (i.e., perturbation quantities averaged over $(n+1)\Delta t$ and $(n-1)\Delta t$) without any impact on the stability characteristics. This is because all dependence on ζ vanishes following substitution of (9) into (S-4) and (S-5).

The substitution of (9) into (S-1)-(S-5) and subsequent manipulations demonstrated, as anticipated, unconditional stability. Then, a slight change was introduced to compute explicitly the terms in (S-2) and (S-3):

$$\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + \tfrac{1}{2}\,\overline{p}_*(u^{n+1}+u^{n-1})_x + \overline{p}_*\,\dot{\sigma}_\sigma^n = 0 \qquad \text{M-2}$$

$$c_p\,\frac{T_1^{n+1}-T_1^{n-1}}{2\Delta t} - \overline{\alpha}\sigma\,\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + c_p\,\overline{\Gamma}\,\dot{\sigma}^n = 0 \qquad \text{M-3}$$

the remaining equations being unchanged. This was called the 'modified' semi-implicit method, because it was reasoned that the $\dot{\sigma}$ terms were essentially associated with the internal mode. Since in the slab model we were attempting to effect such a treatment, it was thought that the modification embodied in (M-2) and (M-3) corresponded to the slab model method. It would therefore be reasonable to anticipate a conditional stability associated with this method; in fact, it too proved to be unconditionally stable.

Much later, it was realized that this behavior arose from the implied diagnostic equation in $\dot{\sigma}$ inherent in M-2. If that equation is differenced with respect to σ, one obtains a difference form of (7):

$$\dot{\sigma}^n_{\sigma\sigma} = -\tfrac{1}{2}(u^{n+1} + u^{n-1})_{x\sigma} \tag{10}$$

which, when substituted into (M-2) and (M-3), renders those equations completely implicit. It is not surprising that this system behaved stably; it was, in fact, not a 'modified' semi-implicit method at all.

At the time we obtained the results of the analysis, however, that fact was not understood. Rather, it was felt that the 'modified' method didn't really correspond to the slab model. For reasons which have become obscured by the passage of time, we became convinced that in the slab model the modified method consisted of, in addition to the explicit treatment of the stability term in (M-3), the following changes:

1. replacement of the pressure tendency term in the thermodynamic equation by an *explicit* approximation from the integrated continuity equation;

2. application of a mixed implicit-explicit approximation to the hydrostatic equation;

3. an *explicit* statement relating $\dot{\sigma}$ to the horizontal wind.

The difference equations become

$$\frac{p_*^{n+1}-p_*^{n-1}}{2\Delta t} + \tfrac{1}{2}\,\overline{p}_*\,\overline{(u^{n+1}+u^{n-1})_x}^{\sigma} = 0 \qquad \text{MI-2}$$

$$c_p\,\frac{T^{n+1}-T^{n-1}}{2\Delta t} + \overline{\alpha\sigma}\,\overline{p}_*\,[u^n_x + \dot{\sigma}^n_\sigma] + c_p\overline{\Gamma}\,\dot{\sigma}^n = 0 \qquad \text{MI-3}$$

$$\tfrac{1}{2}(\phi^{n+1}_\sigma+\phi^{n-1}_\sigma) + \tfrac{1}{2}\,\overline{\alpha}(p_*^{n+1}+p_*^{n-1}) + \overline{p}_*\alpha = 0 \qquad \text{MI-4}$$

$$\dot{\sigma}^n_{\sigma\sigma} = -\tfrac{1}{2}(u^n)_{x\sigma}, \qquad \text{MI-6}$$

where the "$-\sigma$" on the divergence term in MI-2 signifies the vertical average.

This version of the modified implicit method was analyzed in Office Note 52. The results were surprising at the time, and their interpretation far from clear. Briefly, the results were:

1. the method is conditionally stable, and the allowable time step is about 2.5 times that allowed by a completely explicit scheme;

2. the *external* mode became unstable first when the conditional criterion was violated, in direct contradiction to our expectations;

3. the instability occurred at a value of the numerical phase angle somewhat less than $\frac{\pi}{2}$, the value at which the instability occurs in a centered explicit scheme; this is manifested as a certain skewness when the loci of the roots of the frequency equation in ζ are viewed in the complex plane, as shown in Fig. 2.

These results were viewed with concern, for they indicated serious difficulties with the method. However, it seemed that especially (1) and (2) above were not compatible with our experimental integration of the slab model, suggesting that this second attempt still did not correspond to the method actually used in the model.

The change in the thermodynamic equation renders it completely explicit, which appeared to be in agreement with the slab model. We subsequently realized that it was not in agreement, and that making this approximation left an important term usually associated with the external mode treated explicitly. In retrospect, conclusion (2) is therefore not surprising.

If eqn. (9) is substituted into (MI-4) and (S-5), we obtain

$$(\zeta^2+1)\phi_\sigma + (\zeta^2+1)\overline{\alpha}\, p_* + 2\,\zeta\,\overline{p}_*\alpha = 0 \tag{11}$$

and

$$\overline{\alpha}\, p_*\sigma - RT + \sigma\,\overline{p}_*\alpha = 0 \tag{12}$$

It is evident that the mixed treatment of (11) results in an inconsistency in treating terms such as $\overline{p}_*\alpha$. This inconsistency was pointed out by Robert*, who suggested that it might be rectified by altering the form of the ideal gas law. Thus, Eqn. (S-5) was changed so that

$$\overline{p}_*\alpha^n\sigma + \tfrac{1}{2}\,\overline{\alpha}\sigma(p_*^{n+1} + p_*^{n-1}) = RT^n \tag{MII-5}$$

*Personal communication.

when Eqn. (9) is substituted into (MII-5), one obtains

$$\zeta\ \overline{p}_* \sigma\ \alpha + \tfrac{1}{2}(\zeta^2 + 1)\ \overline{\alpha}\ \sigma\ p_* = \zeta\ RT, \tag{13}$$

which is consistent with (11) in the $\overline{\alpha}\ p_*$ and $\overline{p}_*\alpha$ terms. The system comprised of (S-1), (MI-2), (MI-3), (MI-4), (MI-5), and (MI-6) was then reanalyzed. The results showed again that the system was conditionally stable, with the external mode becoming unstable first. But, the skewness referred to above was eliminated.

Our analyses to this point were still incompatible with our numerical integrations. We therefore returned to the original derivation of the slab model and retraced our steps carefully. The difference equations resulting from this exercise are presented in the next section.

4. The Final Solution to the Modified Implicit Problem

The slab model employed the equivalents of the following equations:

$$\frac{u^{n+1} - u^{n-1}}{2\Delta t} + \tfrac{1}{2}(\phi^{n+1} + \phi^{n-1})_x + \tfrac{1}{2}\ \overline{\alpha}\sigma(p_*^{n+1} + p_*^{n-1})_x = 0 \qquad \text{F-1}$$

$$\frac{p_*^{n+1} - p_*^{n-1}}{2\Delta t} + \tfrac{1}{2}\ \overline{\overline{p}_*(u^{n+1} + u^{n-1})_x}^{\,\sigma} = 0 \qquad \text{F-2}$$

$$c_p\frac{T^{n+1} - T^{n-1}}{2\Delta t} - \overline{\alpha}\sigma\ \frac{p_*^{n+1} - p^{n-1}}{2\Delta t} + c_p\ \overline{\Gamma}\ \dot{\sigma}^n = 0 \qquad \text{F-3}$$

$$(\phi_\sigma^{n+1} + \phi_\sigma^{n-1}) + \overline{\alpha}(p_*^{n+1} + p_*^{n-1}) + \overline{p}_*(\alpha^{n+1} + \alpha^{n-1}) = 0 \qquad \text{F-4}$$

$$\sigma\overline{p}_*(\alpha^{n+1} + \alpha^{n-1}) + \sigma\overline{\alpha}(p_*^{n+1} + p_*^{n-1}) - R(T^{n+1} + T^{n-1}) = 0 \qquad \text{F-5}$$

$$\dot{\sigma}_{\sigma\sigma}^n = \tfrac{1}{2}(u^n)_{x\sigma}\ . \qquad \text{F-6}$$

It will be noted that these equations are similar to those of the first 'modified' method: (S-1), (M-2), (M-3), (S-4), and (S-5), and an implied equation in $\dot{\sigma}$, (10). The exceptions are the fully implicit character of (F-4) and (F-5) which, as has been indicated previously, makes no difference in the stability analysis, and the *explicit* statement of the relationship between $\dot{\sigma}$ and the horizontal wind. It is the latter wherein the seeds of self-destruction for the modified method reside.

Note that this system of equations does not exhibit an explicit approximation of any term associated with the external mode; nor does it exhibit the inconsistencies Robert pointed out between the hydrostatic equation and the ideal gas law. It has only one such inconsistency, and that is the diagnostic equation in $\dot{\sigma}$ (F-6) which is not compatible with the equation for $\dot{\sigma}$ implied in the continuity equation. Eqn. (F-6) is *uncentered* in a sense, whereas all other terms are centered.

Because of the similarity of this set to the first 'modified' method, it was anticipated that the analysis would show the external mode unconditionally stable, but a conditional stability associated with the internal mode. However, it was expected that because of the one inconsistency, the skewness referred to earlier would be present but that this would not adversely affect the stability characteristics.

The analysis was carried out after substitution of eqn. (9) into (F-1)-(F-6), and resulted in the two equations

$$\left\{(\zeta^2-1)^2 + (k\Delta t)^2\left[\tfrac{1}{12}R\overline{\Gamma}\ \zeta(\zeta^2+1) + \tfrac{1}{8}\,\alpha_1(3+\kappa)\overline{p}_*(\zeta^2+1)^2\right]\right\}u_1$$

$$- \left\{(k\Delta t)^2\left[\tfrac{1}{12}R\overline{\Gamma}\ \zeta(\zeta^2+1) - \tfrac{1}{8}\,\overline{\alpha}_1(3+\kappa)\overline{p}_*(\zeta^2+1)^2\right]\right\}u_2 = 0 \qquad (14)$$

and

$$\left\{(k\Delta t)^2\left[\tfrac{5}{12}R\overline{\Gamma}\ \zeta(\zeta^2+1) + \tfrac{1}{8}[2\kappa\overline{\alpha}_1 + \overline{\alpha}_2(\kappa+1)]\overline{p}_*(\zeta^2+1)^2\right]\right\}u_1$$

$$+ \left\{(\zeta^2-1)^2 - (k\Delta t)^2\left[\tfrac{5}{12}R\overline{\Gamma}\ \zeta(\zeta^2+1) - \tfrac{1}{8}[2\kappa\overline{\alpha}_1 + \overline{\alpha}_2(\kappa+1)]\overline{p}_*(\zeta^2+1)^2\right]\right\}$$

$$= 0 \qquad (15)$$

Here, the subscripts 1 and 2 refer to the lower and upper layers of the model, respectively, and $\kappa = R/c_p$. The determinant of this pair of equations must vanish if non-trivial solutions exist, a condition which leads to the frequency equation, an eighth-order polynomial in ζ.

The roots of this polynomial have been determined for an isothermal atmosphere at 250 k. The procedure followed is that discussed in Office Note 52. We define

$$\varepsilon_m = mk\Delta t = \frac{2\pi m}{3.81} \cdot 10^{-5}(\mathrm{cm}^{-1}\mathrm{sec}) \qquad (16)$$

and then evaluated the determinant of eqns. (14) and (15) over the complex ζ-plane for m = 1,2,4,6,8,10.

For each value of m, we determined the loci of the zeros of the determinant, corresponding to the roots of the polynomial. It was anticipated that each root would lie on the unit circle until ε_m became large enough that the conditional stability criteria associated with the internal mode would be violated. The results of the evaluation are shown in Figure 3.

The roots in the right quadrant all lie sensibly close to the unit circle, indicating that the external and internal (physical) modes are stable to quite large values of Δt. The skewness is evident, but to a lesser degree than in Figure 2. Also, the root corresponding to the external computational mode lies on the unit circle.

But: the root corresponding to the internal computational mode is not on the unit circle, but on the negative real axis, and quickly takes on magnitude greater than unity. It is not clear why this occurs, but its impact on the results of the numerical integration of the slab model is quite evident. The fact that this root remains on the real axis means that its imaginary part is zero. This can only happen if the numerical phase angle is zero or π. Effectively, *this means that the aberrant behavior of the internal computational mode will be manifested in the mean.* Moreover, it can be shown that the rate of growth of instability is proportional to the horizontal wave number. These two facts appear to explain the loss of mass discussed in the second section.

It seems evident that, barring some unforeseen technique for counteracting the instability of the internal computational mode, the modified semi-implicit method is dead and not resurrectable. We hereby officially inter it; R.I.P.

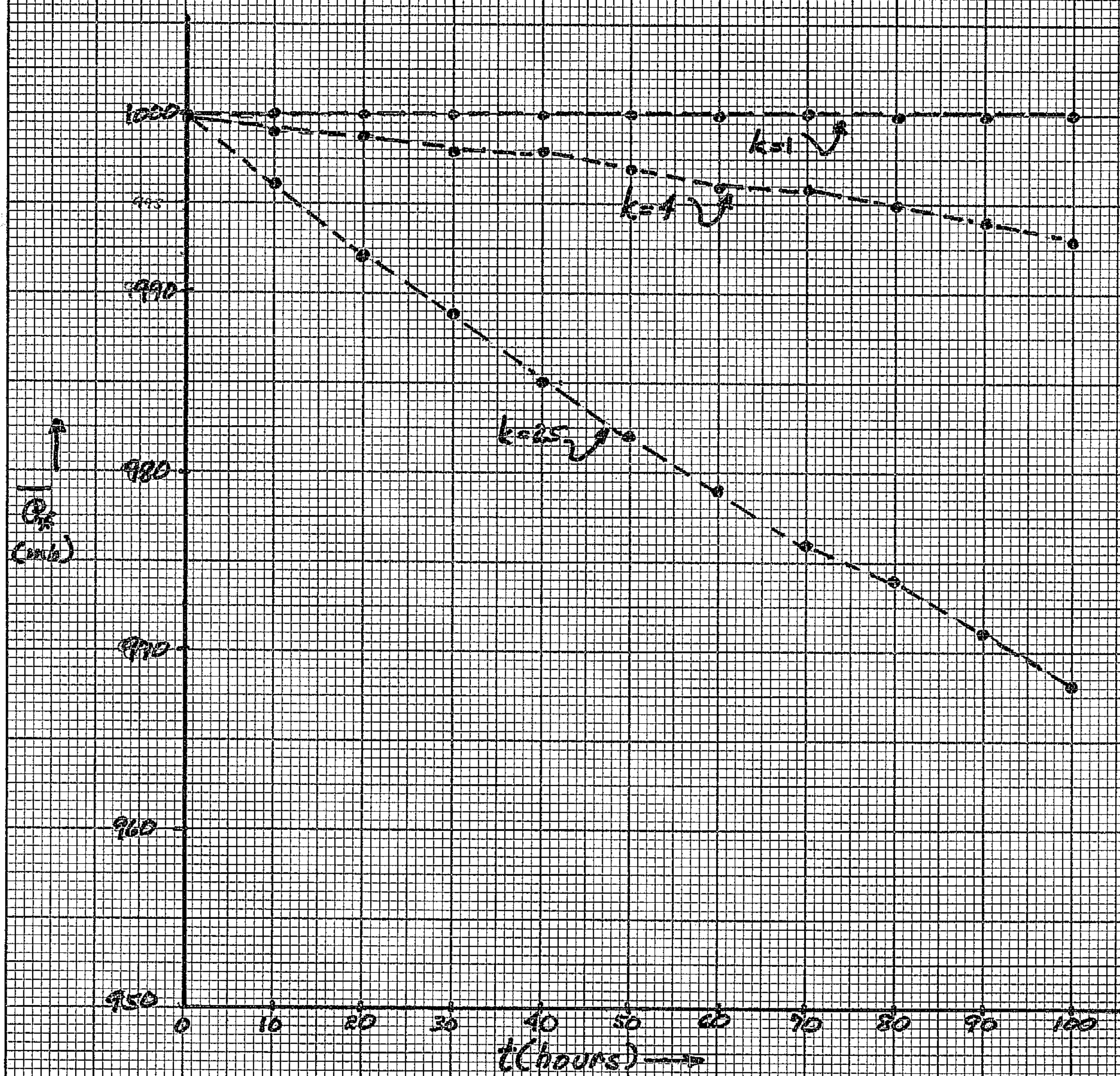


FIGURE 1. MEAN SURFACE PRESSURE $\overline{P_s}$ IN THE 'SLAB' MODEL AS A FUNCTION OF TIME AND HORIZONTAL WAVE NUMBER k.

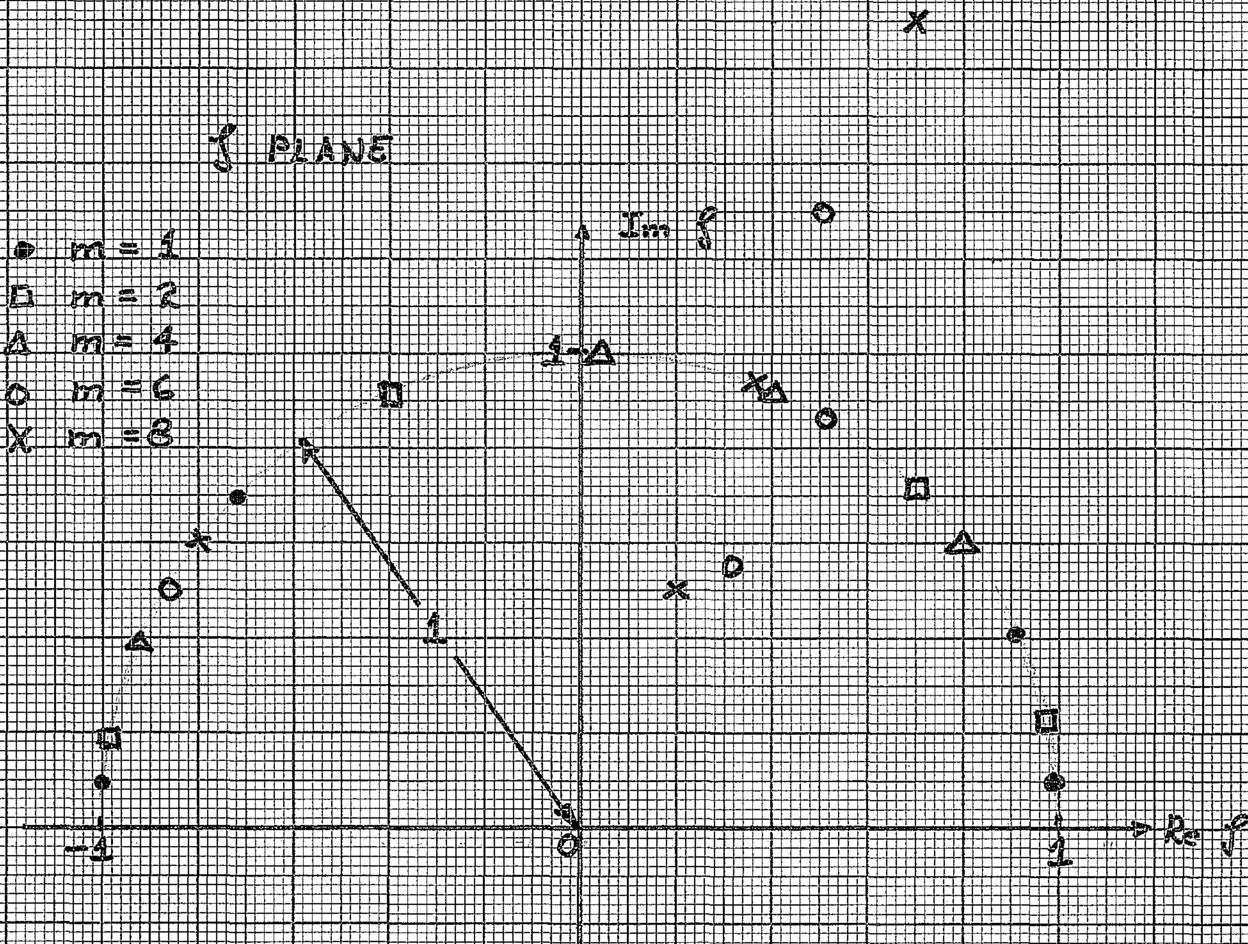


FIGURE 2. LOCI OF THE ZEROES OF THE POLYNOMIAL IN ζ FOR AN ISOTHERMAL ATMOSPHERE, $\bar{T} = 250K$, $\bar{P}_* = 1000mb$, AS A FUNCTION OF $\epsilon = k\Delta t$; $\epsilon_m \equiv 2\pi m / 3.81 \times 10^5$ (cm^{-1} sec). THIS SYSTEM IS CHARACTERIZED BY THE EXPLICIT REPLACEMENT OF THE PRESSURE TENDENCY IN THE THERMODYNAMIC EQUATION.

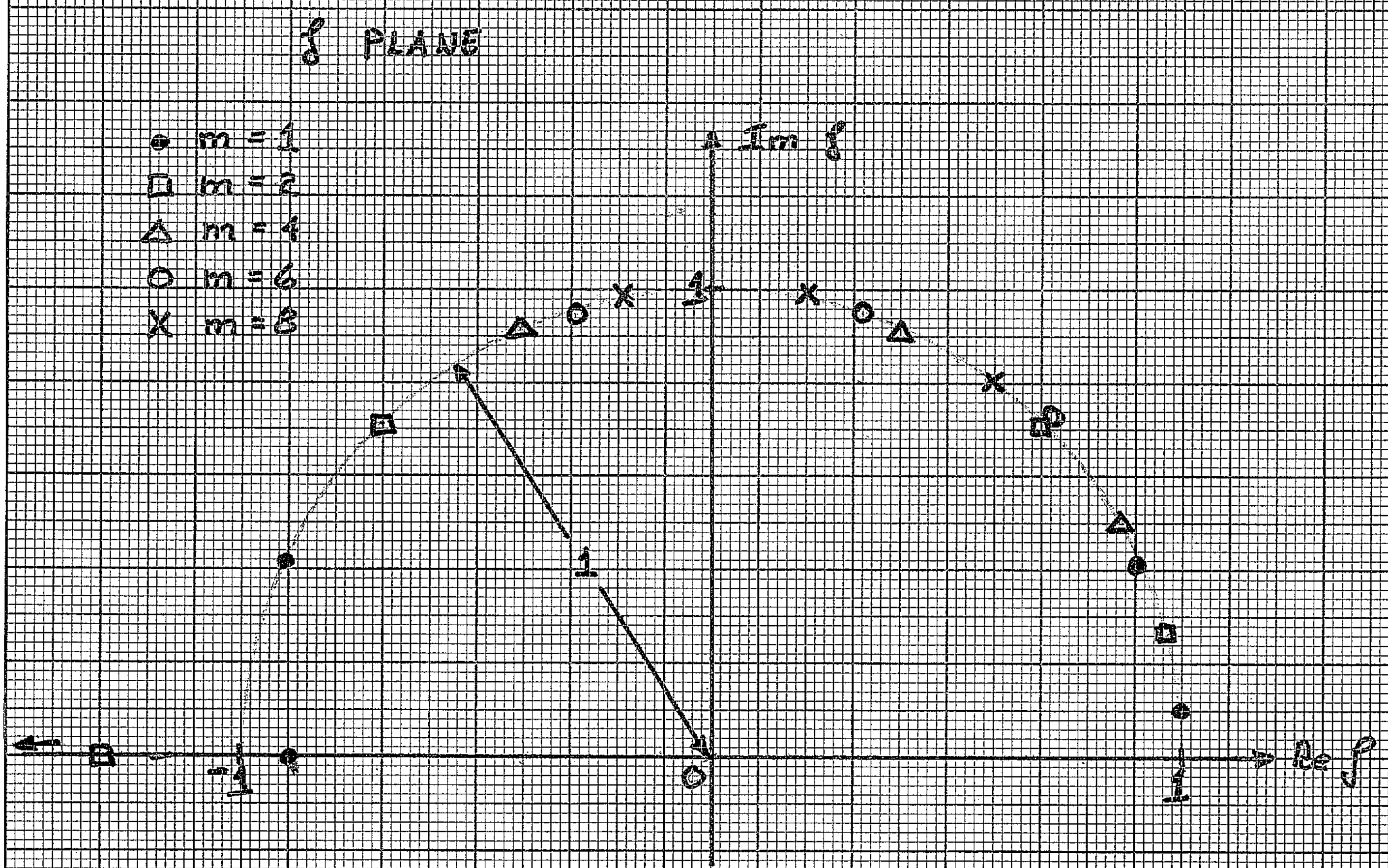


FIGURE 3. LOCI OF THE ZEROES OF THE POLYNOMIAL IN ζ FOR AN ISOTHERMAL ATMOSPHERE, $\bar{T}=250K$, $\bar{p}_* = 1000mb$, AS A FUNCTION OF $\epsilon \equiv k\Delta t$; $\epsilon_m = 2\pi m / 3.81 \times 10^5$ $(cm^{-1}\,sec)$. THIS IS FOR THE SYSTEM USED IN THE 'SLAB' MODEL.