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MET.O.15 INTERNAL REPORT

55

ON THE CHOICE OF HIGH ORDER
SCHEME FOR A FLUX-CORRECTED
TRANSPORT ALGORITHM

BY

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1. INTRODUCTION

In many physical problems quantities exist that are advected by the motion of a fluid and must always remain positive. The modelling of clouds in the atmosphere is such a problem where it is important that the numerical treatment of advection ensures positivity of the cloud water densities. This positivity requirement is a special case of the more general requirement that monotonicity should be preserved and that small regions with large gradients should not be spuriously dissipated. A number of methods have been proposed to deal with the general problem (Sod (1978)), but currently only the approaches embodied in the hybrid scheme of Harten (1978) and the flux corrected transport (FCT) algorithm of Boris and Book (1973) are amenable to generalization to arbitrary orders of accuracy. As described below monotonicity is achieved using a combination of an accurate high order scheme and a low order scheme having the desired property.

In this note the influence of the choice of high order scheme (HOS) on the FCT algorithm (as modified by Zalesak (1979)) is examined. Particular attention is paid to the occurrence of clipping; that is the tendency for an initially smooth function to become a square wave in regions of rapid change (see e.g. Zalesak (1979)). In Section 3 two economical methods are proposed that maintain positivity, based on the hybrid and FCT approaches, and these are compared with earlier results.

The model problem is the linear advection equation in one dimension for some variable q

$$\frac{\partial q}{\partial t} = v \frac{\partial q}{\partial x} \quad (1)$$

Single time level schemes are considered, written in flux form

$$q_i^{n+1} = q_i^n - \frac{\Delta t}{\Delta x} [F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}] \quad (2)$$

i labels the spatial points, n the temporal. $F_{i+\frac{1}{2}}$ are the fluxes and will be a suitably weighted combination of fluxes calculated using a given HOS and by upstream differencing. The procedure, into which both the FCT and Hybrid algorithm can be cast, is (following Zalesak (1979)):

1. Compute the low order flux, $L_{i+\frac{1}{2}}$, by some low order scheme guaranteed to preserve monotonicity.
2. Compute the high order flux, $H_{i+\frac{1}{2}}$.
3. Define an antidiffusive flux,

$$A_{i+\frac{1}{2}} = H_{i+\frac{1}{2}} - L_{i+\frac{1}{2}}$$

4. Compute the updated low order solution,

$$q_i^L = q_i^n - \frac{\Delta t}{\Delta x} [L_{i+\frac{1}{2}} - L_{i-\frac{1}{2}}]$$

5. Choose scaling factors, $S_{i+\frac{1}{2}}$, that determine how much of the high order flux will be used at each point.

$$A_{i+\frac{1}{2}}^s = S_{i+\frac{1}{2}} A_{i+\frac{1}{2}} \quad 0 \leq S_{i+\frac{1}{2}} \leq 1$$

6. Apply this flux correction to the low order solution

$$q_i^{n+1} = q_i^L - \frac{\Delta t}{\Delta x} [A_{i+\frac{1}{2}}^s - A_{i-\frac{1}{2}}^s]$$

The specification of the $S_{i+\frac{1}{2}}$ is the most important step in the algorithm. The FCT method of Zalesak (1979) chooses the largest value for $S_{i+\frac{1}{2}}$ consistent with q_i^{n+1} remaining above one value q_i^{\min} , and below another, q_i^{\max} . There are a number of ways of choosing q_i^{\min} and q_i^{\max} . In this work they are chosen to ensure the preservation of monotonicity as

$$q_i^{\max} = \max(q_{i-1}^a, q_i^a, q_{i+1}^a)$$

$$q_i^a = \max(q_i^n, q_i^L)$$

$$q_i^{\min} = \min(q_{i-1}^b, q_i^b, q_{i+1}^b) \quad (3)$$

$$q_i^b = \min(q_i^n, q_i^L)$$

This choice ensures that the advected function values are bounded by the local values of the function at time (n) and also by the low order solution at time (n+1). This algorithm does result in clipping, though less than using the Boris and Book specification of $S_{i+\frac{1}{2}}$.

2. THE CHOICE OF HIGH ORDER SCHEME

The first choice considered for the high order fluxes is second order differences centred in space, as used by Nash and Thorpe (1984). Using a forward time-step this HOS is unstable, with amplification factor $1 + O(\nu \Delta t / \Delta x)^2$, but combination with the Zalesak limiter (equation (3)) ensures an overall stable scheme. The use of these fluxes should minimize the loss of amplitude suffered by advected profiles. Fig. 1 shows the result of advecting a peaked profile (resolved over 7 points, ^{FOR} 500 time steps with a Courant number, $\nu \Delta t / \Delta x$ of 0.5) by several schemes. This is a severe test but comparison with the analytical solution shows that the numerical result has very good phase and a peak value maintained at 45% of the original. It is evident however that the advected profile has flattened across its peak and the gradients have steepened on either side; this is the clipping phenomenon referred to in Section 1. With fixed Courant number the clipping becomes worse for a better resolved profile, over 11 points, as shown in Fig. 2. The peak amplitude is well described but the advected profile is almost a square wave. For smaller Courant numbers the clipping is much less severe as can be seen in Figs 3 and 4 which show the profile advected over the same number of time steps but with a Courant number of 0.1. The reduction in clipping is a result of the smaller amplification factor, since then the values at the points at the sides of the profiles do not increase at the expense of those points near the peak (the schemes are of course linearly conserving), and also of the smaller Courant number giving a much better resolution of the peak value(s) and thus these are not lost in the calculation of the bounds (equation (3)). The poorer phase speed for the smaller Courant number results from the phase lag of the space differencing scheme no longer being cancelled by the phase advance of the time differencing.

The second HOS was chosen to be Gadd's scheme (Gadd (1978)) which is stable and has second order phase properties. The tests described above were repeated and the results are also shown in Figs 1 to 4. Clearly the tendency to form square waves from peaked initial data is very much reduced but the peak amplitude is also less in all but the case of Fig 3, and the phase is slightly advanced.

Thus the clipping using centred space differencing can be attributed to the use of an unstable HOS. Nonetheless some clipping is also evident with the Gadd scheme and at the higher Courant number considerable asymmetries in profile slopes occur.

Carpenter (1982) and Collins (1983) have shown that the Gadd scheme can be modified in various ways to improve its accuracy and in particular its phase errors. Phase speed in the Carpenter scheme is third order and lagging (except for very short waves and large Courant numbers). For a Courant number of 0.1 Figs 3 and 4 show that using the Carpenter scheme gives the best approximation to the analytic solution, without the asymmetry given by the Gadd scheme. Clipping is minimal and the phase of the profile is good with little diffusion of wave amplitude to result in broadening. Figs 1 and 2 show the case of Courant number 0.5 when again the Carpenter scheme maintains the best shape though the amplitude loss is greater than when using the unstable HOS.

The asymmetric shape produced by the Gadd scheme and to a lesser extent by the other two HOS is due to the interaction of phase errors of the HOS with the FCT algorithm (more generally it is the difference in phase properties between the high and low order schemes, but for the Courant numbers considered here the LOS is accurate in phase). Consider the case of a HOS that produces a slower phase speed than the low order. On the downstream side of the profile the LOS will give values that are consistently higher than those of the (lagging) previous timestep value and so the upper bound (q_i^{\max} in equation (3)) will ensure that q_i^{n+1} is composed largely of the diffusive low order scheme. Conversely the upstream side of the profile will consist mostly of the HOS solution and be much sharper. The result of this interaction is an asymmetric shape with one side much more diffused than the other (eg the results for the second order HOS in figures 1 to 4). For an HOS that advances the phase the effect is reversed as can be seen from the upstream tails produced by the Gadd scheme.

Thus the choice of HOS is seen to have a strong influence on the accuracy of an FCT algorithm. Small errors in phase can lead to significant asymmetries in advected profiles. Using an unstable HOS can have some advantages by minimising damping but accentuates the formation of square waves. The FCT algorithm, while ensuring monotonicity, does not relax the need to find the best HOS possible.

3. MINIMAL FCT AND HYBRID ALGORITHMS

The switched hybrid algorithms (Harten (1978), Clark (1979)) define $S_{i+1/2}$ as an explicit function of the field values at time n , for example Clark's switch takes the form:

$$S_{i+1/2} = 1 - \frac{1}{2} \frac{|\delta x q^n|}{|q_n| x} \Delta x \quad (4)$$

The criterion of choice for the switches should be that the low order scheme is used strongly in regions where monotonicity is not likely to be preserved and minimally elsewhere. Nevertheless the form of $S_{i+1/2}$ in equation (4) means that it is inevitable that some extra damping is applied everywhere there is a non-zero gradient of q (however the results of section 2 show that this also happens in FCT algorithms). Also, as Clark pointed out, this function does not guarantee monotonicity though it does ensure positivity to a good approximation.

In this section Clark's switch will be used with Carpenter's scheme as the HOS and compared with two forms of FCT algorithm. The first is that defined in Section 2 while the second has a modified calculation of $S_{i+1/2}$ eliminating the constraint of the upper bound. This is done by choosing $q_i^{\max} = \infty$ and $q_i^{\min} = 0$. This minimal FCT is considerably more economical to calculate than the full FCT but imposes the constraint which is in practice most important.

Fig 5 shows the results of these three schemes together with the analytic solution after 500 steps on our first test problem (Courant number 0.1, 7 point profile). The relative behaviour of the schemes in this figure is typical of that found at other resolutions and Courant numbers. The full FCT has the most accurate phase despite the fact that the same HOS is used in each case. To some extent all the schemes are diffusive with the minimal FCT least so and the hybrid method of Clark most. Only the Clark scheme predicts negative values to the sides of the peak through these are small enough to ignore in practice. Both FCT algorithms give a small positive tail trailing from the rear of the hump and that from the minimal FCT is seen to slightly violate monotonicity. Fig 6 shows a similar profile resolved on 11 points, also with a Courant number of 0.1 and after 500 steps. The peak amplitude for the minimal FCT is .95, for the full FCT .82 and .80 for the hybrid scheme. The phase is good in each case but the hybrid results again broaden more than the rest.

The results of the full FCT scheme in this problem are thus comparable with the hybrid scheme but the hybrid scheme form of the scaling factor, $S_{ct}/2$, (the only point at which the two differ) requires only one third of the computational effort. The minimal FCT requires the same effort as the hybrid scheme but has significantly better accuracy. The Boris and Book (1973) specification for $S_{ct}/2$ is computationally more efficient than that used here but unlike the other methods is not amenable for extension to more than one dimension. If positivity alone is not adequate strict monotonicity preservation demands the use of the full FCT.

3. CONCLUSIONS

It has been shown that the accuracy of FCT algorithms for one dimensional constant advection depends sensitively on the choice of HOS. Thus the use of an FCT scheme does not remove the need to consider the choice of HOS carefully. Schemes do not exist that are sufficiently accurate to prevent substantial reduction in amplitude and large apparent diffusion for poorly resolved fields. The use of a weakly unstable HOS was shown to reduce amplitude damping but maintenance of shape was poor with the formation of steep gradients and flattened peaks. It was shown that, although a stable HOS avoids the formation of a square wave, significant spurious distortions may still be induced by poor phase properties.

Choosing a scheme to be stable and to have good phase properties greatly improves shape but there is still amplitude loss. It was demonstrated that the performance of the Harten and Clark switched schemes and the relatively expensive FCT method then becomes similar. For the case of advection when monotonicity is unnecessary but positivity is still important, a reduced FCT has been proposed which is competitive with hybrid schemes, and more generally applicable, but with minimal damping.

APPENDIX

The high order schemes used in this note are

- a. second order centred differencing
- b. Gadd's (1978) variation of the Lax-Wendroff scheme
- c. Carpenters' (1981) variation of Gadd's scheme

The fluxes calculated from second order centred differencing are

$$H_{i+\frac{1}{2}} = \frac{1}{2} v (q_i + q_{i+1})$$

assuming constant advection and unit Δx and Δt

The Gadd and Carpenter fluxes are calculated from the two step procedure

$$q_{i+\frac{1}{2}}^{n+\frac{1}{2}} = (\bar{q}^x)_{i+\frac{1}{2}}^n - \frac{1}{2} v (S_x q)_{i+\frac{1}{2}}^n$$

$$H_{i+\frac{1}{2}} = v \left\{ \left(1 + \frac{2}{3} a\right) q_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{a}{3} (q_{i+\frac{3}{2}}^{n+\frac{1}{2}} + q_{i-\frac{1}{2}}^{n+\frac{1}{2}}) \right\}$$

where, for the Gadd scheme, $a = \frac{3}{4} (1 - v^2)$

and for the Carpenter scheme, $a = \frac{1}{2} (1 - v^2)$

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FIGURE CAPTIONS

Figure 1: Comparison using different high order schemes in FCT algorithm. Courant number is 0.5, resolution 7 points, after 500 time steps. Tick marks on horizontal axis are every grid point. Solid line is analytic solution. High order schemes: O = Second order centred space; X = Gadd; Δ = Carpenter.

Figure 2: As for Fig 1. Resolution is 11 points.

Figure 3: As for Fig 1. Courant number is 0.1

Figure 4: As for Fig 1. Courant number is 0.1 and resolution is 11 points

Figure 5: Comparison of FCT and hybrid algorithms. Courant number is 0.1, resolution 7 points, after 500 time steps. Tick marks on horizontal axis are every gridpoint. Solid line is analytic solution. O = full FCT algorithm, X = Clark hybrid, Δ = minimal FCT. High order scheme is Carpenter.

Figure 6: As for Fig 5. Resolution is 11 points.

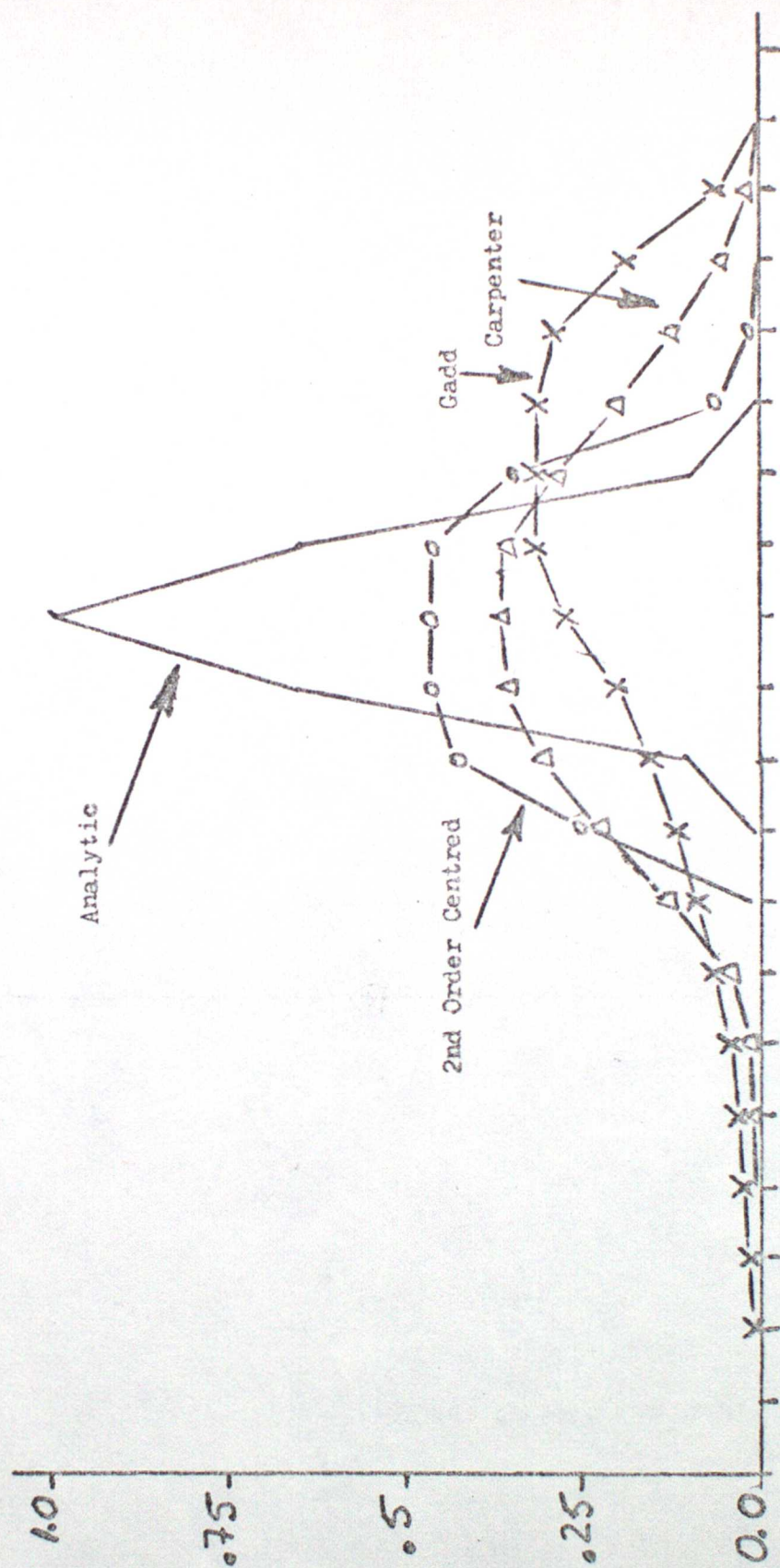


FIGURE 1

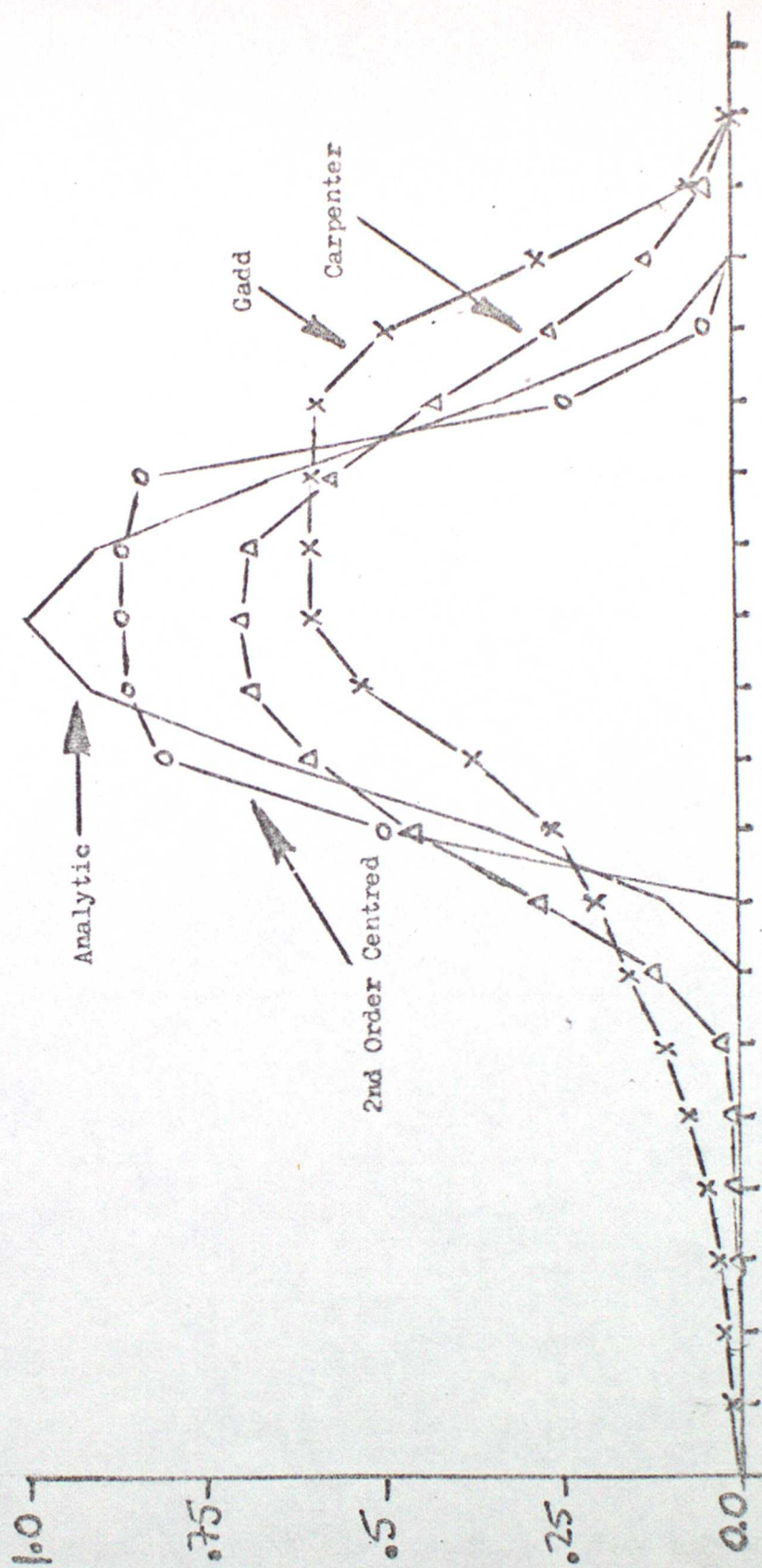


FIGURE 2

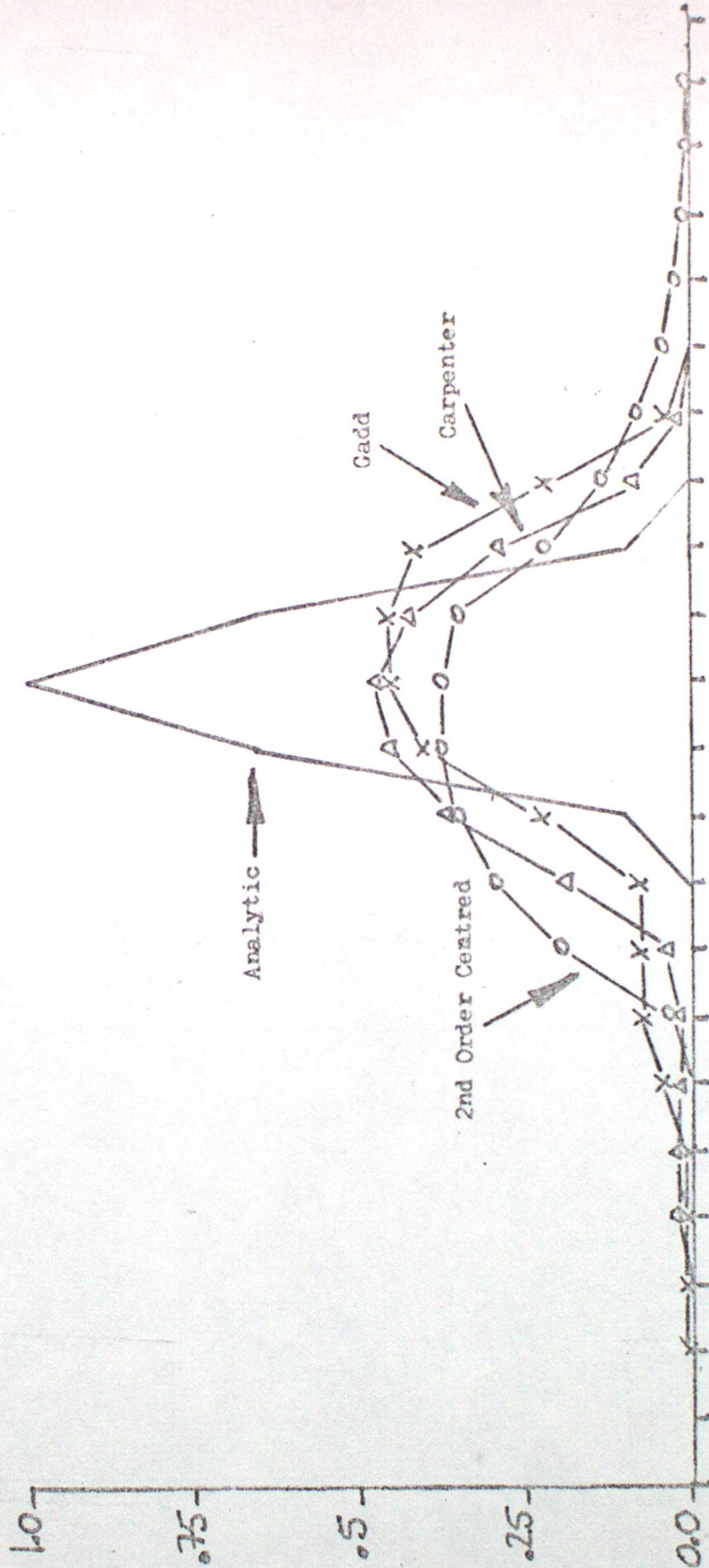


FIGURE 3

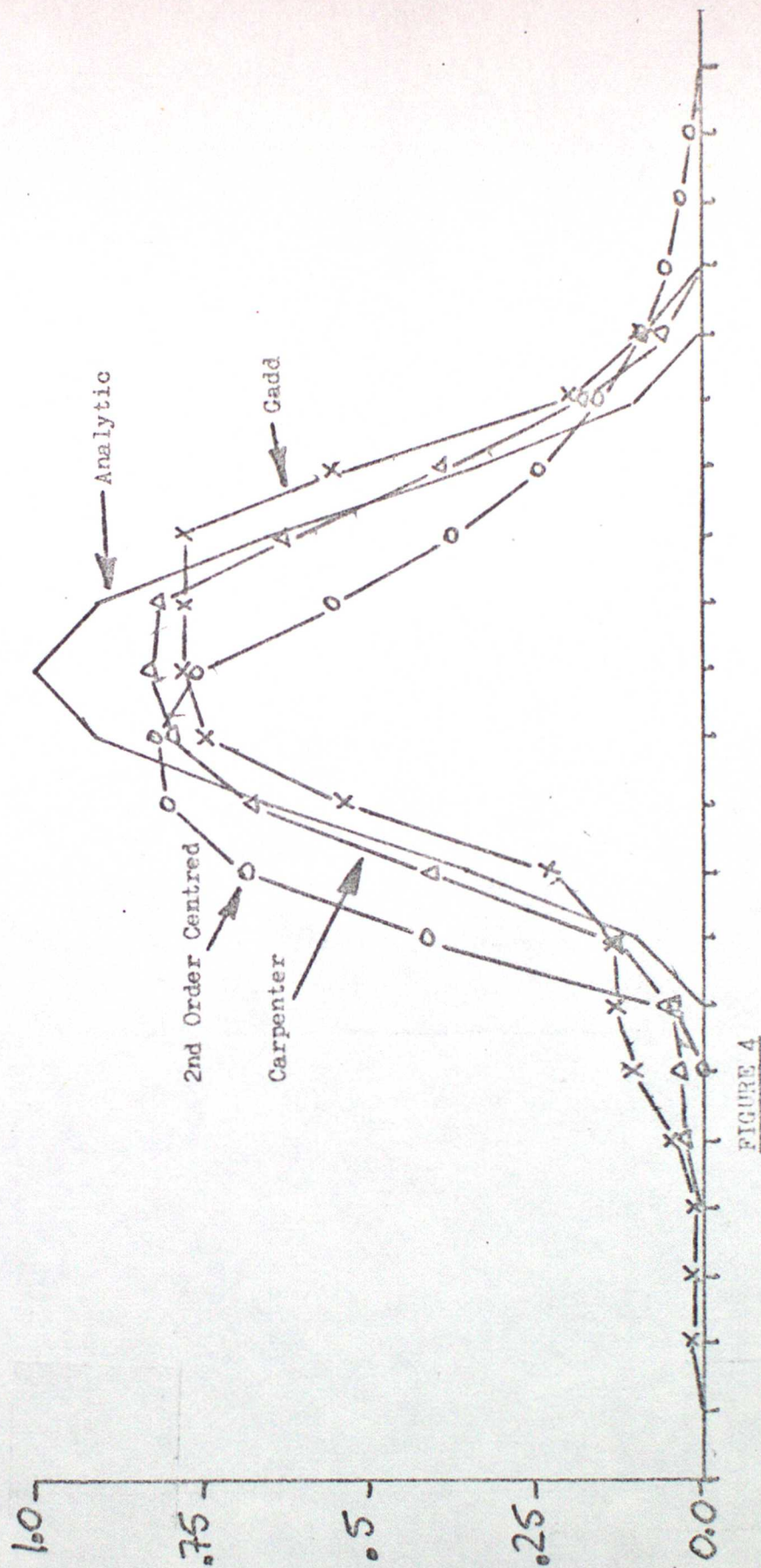


FIGURE 4

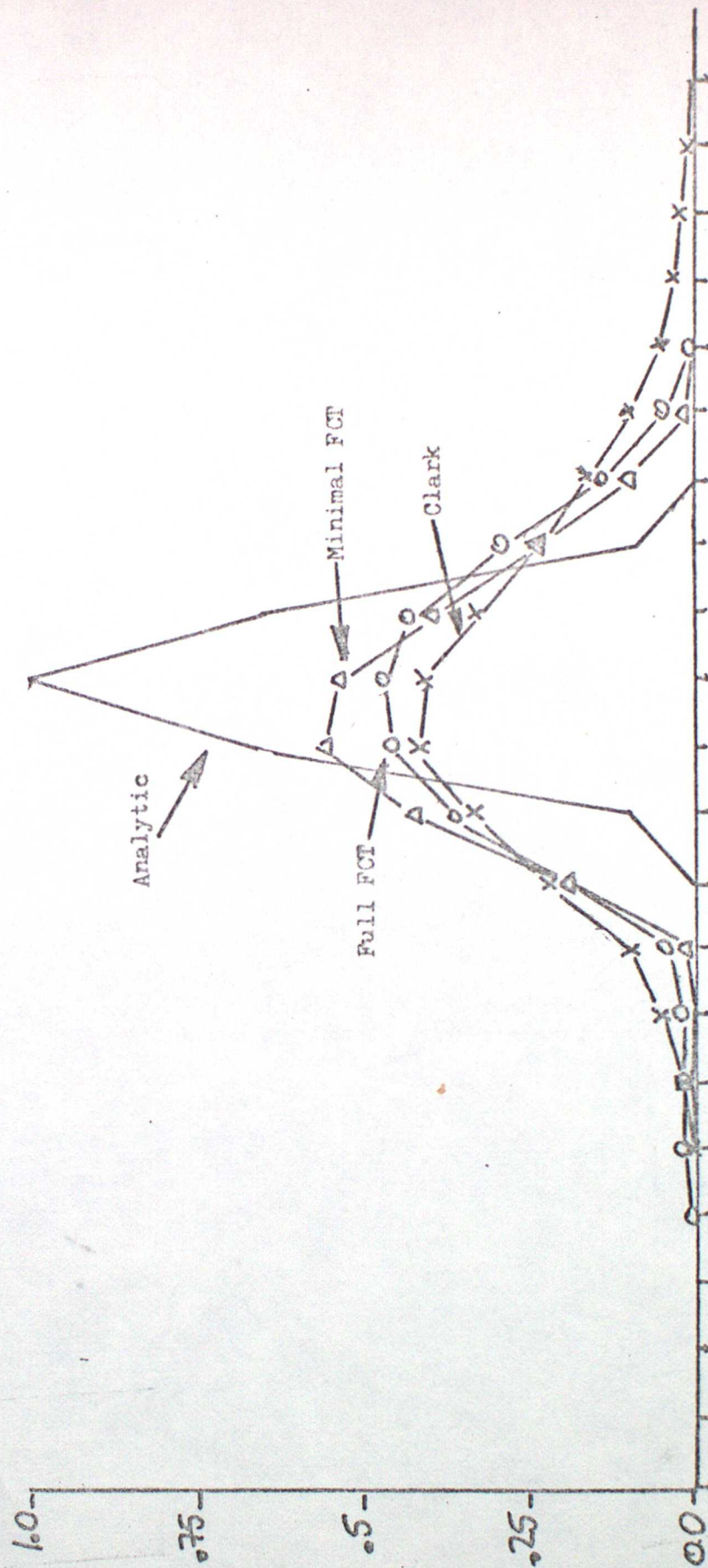


FIGURE 5

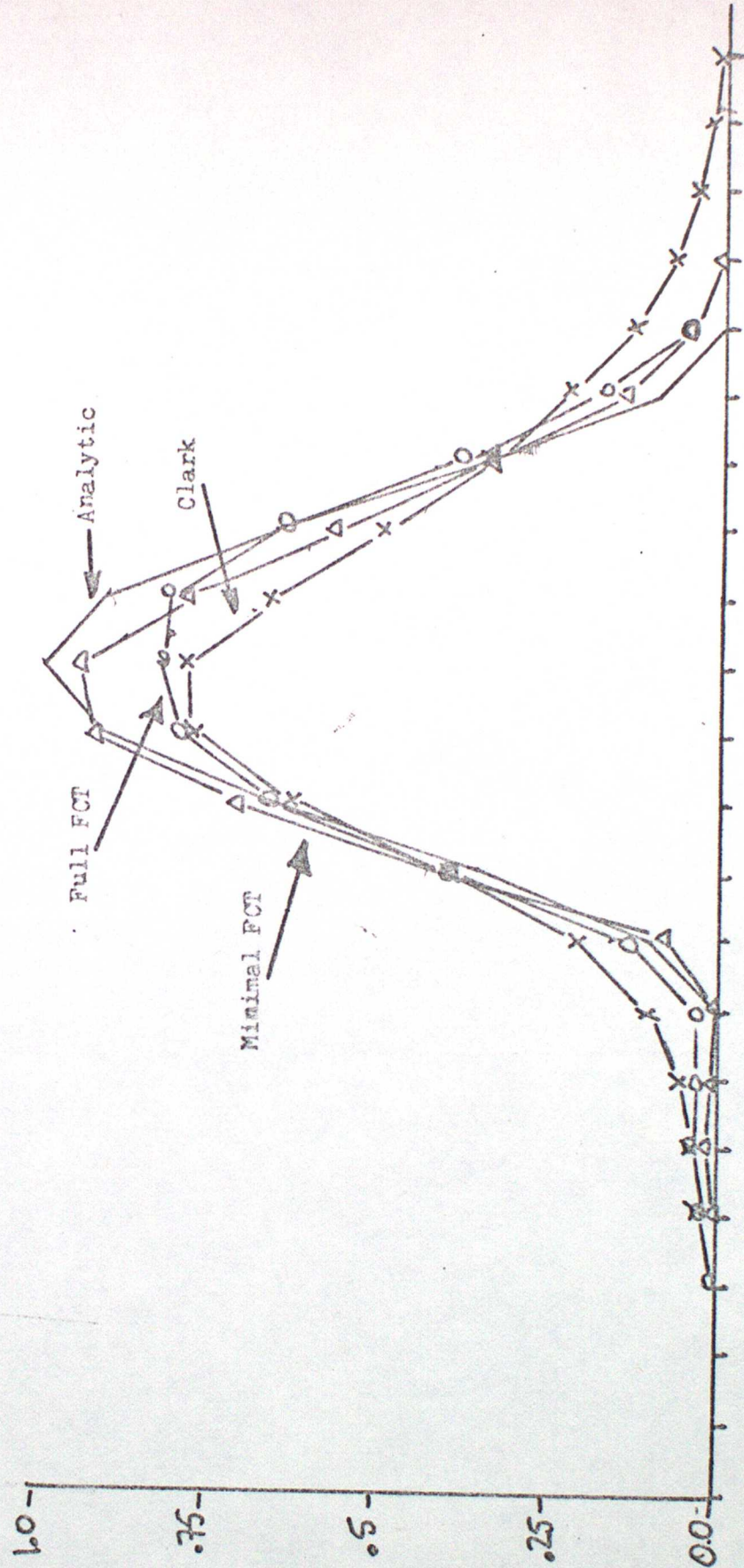


FIGURE 6