

A TRANSFORMATION TO ASSIST NUMERICAL SOLUTION  
OF DIFFUSION EQUATIONS

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NUMERICAL ANALYSIS REPORT 5/86

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Abstract

A transformation of the dependent variable of the non-linear diffusion equation

$$C_t = \nabla \cdot (D(C) \nabla C)$$

for a concentration  $C$ , is presented which allows straightforward numerical calculations in cases where  $D(C)$  has pathological behaviour such as discontinuities or changes by orders of magnitude.

The transformation consists of introducing a velocity potential,  $\varphi$ , related to the diffusing substance via

$$\varphi = - \int D(C)/C \, dC$$

yielding the transformed equation

$$\varphi_t = D(C) \nabla^2 \varphi - \nabla \varphi \cdot \nabla \varphi$$

The use of this transformed equation, with its hyperbolic behaviour for small  $D(C)$  explicitly represented, avoids the numerical problems associated with a rapidly varying diffusion coefficient.

Numerical examples are given as well as methods of avoiding explicitly inverting  $\varphi(C)$  when  $D(C)$  is non-trivial.

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## 1 Introduction

The non-linear diffusion equation

$$C_t = \nabla \cdot (D(C) \nabla C) \quad (1.1)$$

or more generally

$$\frac{\partial C}{\partial t} = \nabla \cdot (D(C,x,t) \nabla C) \quad (1.2)$$

arises in many physically interesting problems. These typically come from situations where the flux of a substance with concentration  $C$  is  $-D(C) \nabla C$  and where  $C$  is a conserved quantity.

Examples are treacle spreading on a flat surface, for which  $D(C) = C^3$ , shallow flows in porous media, for which  $D(C) = C$ , and the diffusion of arsenic in silicon, for which

$$D(C) = \left[ \frac{1 + \beta(C + \sqrt{C^2 + 4})}{1 + \beta} \right] \quad (1.3)$$

Equations (1.2) is of parabolic type if  $D(C,x,t) > 0$  for all  $C,x,t$  and is of degenerate parabolic type if  $D(C,x,t) = 0$  for some values of its arguments. In all cases, including those where  $D$  is discontinuous, a solution is sought where both  $C$  and the flux  $-D(C,x,t) \nabla C$  are continuous functions. Much analysis exists for such problems and some can be found in [1],[4],[6].

The numerical solution of the degenerate problem has been examined in detail by Tomoeda [9] for the one-dimensional case with  $D(C)=C^m$  when an additional source term is present. The solution requires highly accurate tracking of the point where degeneracy first occurs. For the more general parabolic problem a number of methods, such as that of Meek & Norbury [8], are available if  $D(C,x,t)$  is sufficiently well behaved. In this paper we propose a method to accommodate less well behaved functions  $D$ .

The paper starts by introducing some of the properties of such equations and methods used in their solution. A section describing the proposed transformation and the reasons for its use then follows. Numerical examples are then given to show how the transformation can be implemented. In particular we give an approximate technique for cases where the functional form of  $D(C)$  makes inverting the transformation computationally time consuming.

## 2 Equation Properties and Existing Solution Techniques

An elegant method of solving a non-linear diffusion equation with  $D=D(C)$  is the use of the Kirchhoff transformation [5],

$$w = \int^C D(y) dy \quad (2.1)$$

which implies

$$\frac{\partial C}{\partial t} = \nabla^2 w \quad (2.2a)$$

or

$$\frac{\partial w}{\partial t} = D(C) \nabla^2 w \quad (2.2b)$$

The transformation ensures that if both  $w$  and  $\nabla w$  are continuous then  $C$  has the required continuity. The problem is typically solved numerically using the partial differential equation (2.2a) to step  $C$  in time and then the integral definition (2.1) to evaluate  $w$ . The method works well for moderate changes in  $D(C)$  including discontinuous changes. See for example Crank [4] or Buonomo & Di Bello [3].

The major benefit of this transformation is that if the problem tends towards a steady state then  $\nabla^2 w \rightarrow 0$  and hence the solution is well represented by low order polynomials and numerical methods based on such representations will work well. However, when considering highly transient problems, for example if  $D(C)$  gets very small for some value of  $C$ , then  $\nabla^2 w$  can become large. For instance consider the one-dimensional similarity solution for  $D(C)=C$ , (see Barenblatt & Zeldovich [2])

$$C = \begin{cases} t^2(A^2 - (x/t)^2) & |x| < At \\ 0 & |x| > At \end{cases} \quad (2.3)$$

so that

$$\frac{\partial^2 w}{\partial x^2} = \begin{cases} \frac{-A^2}{t(A^2 - (x/t)^2)^{3/2}} & |x| < At \\ 0 & |x| > At \end{cases} \quad (2.4)$$

The righthand side of (2.4) becomes unbounded as  $|x| \uparrow At$  and good representation of such behaviour is impossible using low order polynomials.

From the work of Tomoeda and others it is known that as  $D(C)$  tends to zero the equations behave in a hyperbolic fashion and at points where  $D(C)=0$  the equation is in fact hyperbolic. To examine this behaviour consider finding steep travelling wave solutions to the one-dimensional parabolic equation with very high speeds of propagation so that the hyperbolic nature is emphasized. Transforming from variables  $x, t$  to  $\eta, t$  where

$$\eta = x/\sqrt{\epsilon} - t/\epsilon, \quad (2.5)$$

with  $0 < \epsilon \leq 1$  to provide a high wave velocity, gives

$$\epsilon \frac{\partial C}{\partial t} + \frac{\partial C}{\partial \eta} = \frac{\partial}{\partial \eta} \left[ D(C) \frac{\partial C}{\partial \eta} \right] \quad (2.6)$$

Taking the limit  $\epsilon \rightarrow 0$  the solution to this equation can be written as

$$\eta = \int_b^C D(y)/(y+a) dy + O(\epsilon) \quad (2.7)$$

where  $a$  is the concentration in front of the wave and  $b$  is determined by the forces acting to propagate the wave. We now note that if the dependent variable being sought in a numerical solution was the integral on the right hand side of (2.7) then the solution would be very close to a straight line travelling at speed  $1/\epsilon$ .

### 3 Proposed Transformation

Following on from the comments of the last section it is proposed that a new dependant variable should be introduced to favour numerical representation of transient behaviour. We consider the case where  $D(C)$  is small for small  $C$  so that the concentration  $a$  in (2.7) can be chosen as zero. The new dependent variable,  $\varphi$ , is taken as:

$$\varphi = - \int_b^C D(y)/y dy \quad (3.1)$$

for some constant  $b$ . Putting this into the equation gives

$$\frac{\partial \varphi}{\partial t} = D(C) \nabla^2 \varphi - \nabla \varphi \cdot \nabla \varphi \quad (3.2)$$

As with the Kirchhoff transformation, the continuity of  $\varphi$  and  $\nabla \varphi$  ensures that  $C$  has the necessary continuity. It can now be seen that as  $D(C) \rightarrow 0$ ,  $D(C) \nabla^2 \varphi \rightarrow 0$  and a non-linear hyperbolic equation occurs for  $\varphi$ . Any other transformation of the form:

$$v = \int_b^C D(y) y^\alpha dy \quad \alpha \neq -1 \quad (3.3)$$

results in an equation where as  $D(C) \rightarrow 0$  either the coefficients of the equation become infinite and  $\nabla v$  and  $\nabla^2 v$  go to zero or vice versa, as was seen with the Kirchhoff transformation  $\alpha = 0$ .

This change of dependent variable is not unknown; e.g. Tomoeda [9] uses

$$v = C^n = n \int_0^C (y^n)/y dy \quad (3.4)$$

in his papers. It does not however seem to have been recognized as a general tool for treating more complex problems where  $D(C)$  may vary considerably but remain bounded away from zero.



A physical explanation for  $\phi$ , which may assist understanding, can be given for situations where the flux is given by

$$\text{FLUX} = - D(C) \nabla C \quad (3.5)$$

It is noted that locally the flux of material is its local concentration,  $C$ , times its average velocity,  $u$ , i.e.

$$\text{FLUX} = Cu. \quad (3.6)$$

Hence the velocity is a scalar times a divergence and can therefore be represented by a velocity potential,  $\phi$ , where

$$u = \nabla \phi \quad (3.7)$$

Using the definitions (3.5), (3.6) and (3.7) it follows that

$$\phi = - \int_b^C D(y)/y \, dy \quad (3.8)$$

where  $b$  is some arbitrary constant to precisely define the potential.

One final point concerning the variable  $\phi$  is worth noting. For the degenerate parabolic equation when  $D(C)=0$  the equation becomes

$$\frac{\partial \phi}{\partial t} = - \nabla \phi \cdot \nabla \phi$$

and this can be interpreted as stating that the front where  $D(C) = 0$  travels at the average velocity of the diffusing material at the front.

#### 4 Solution Technique

To solve this problem numerically the coupled system

$$\varphi = - \int_b^C D(y)/y dy \tag{4.1}$$

$$\frac{\partial \varphi}{\partial t} = D(C) \nabla^2 \varphi - \nabla \varphi \cdot \nabla \varphi$$

must be integrated in time. Appropriate methods to deal with the separate diffusive and hyperbolic terms of the equation can be employed. For the examples given here the method of moving finite elements has been adopted (see for example Miller & Miller [7] or Wathen and Baines [10]). The system (4.1) is far more complicated than (2.1) and (2.2a) associated with the Kirchhoff transformation since at each time step the concentration  $C$  must be computed from  $\varphi$  and this may not be easy for any reasonably complex  $D(C)$ . A method for avoiding this problem is to transform the original  $C$  equation using a variable  $\psi$  which closely approximates  $\varphi$  but is easily inverted. Such a function might be smooth but defined in a piecewise manner or be some algebraic expression which can be quickly inverted. Using this approximate transformation the equation (1.1) becomes

$$\frac{\partial \psi}{\partial t} = D(C) \nabla^2 \psi + \left[ \frac{d\psi}{dC} \right]^{-1} \frac{d}{dC} \left[ \frac{D(C) d\psi}{dC} \right] |\nabla \psi|^2 \tag{4.2}$$

The price of avoiding the inversion of the more complex integral definition (3.7) is the calculation of the coefficient of  $|\nabla \psi|^2$  which, because  $\psi$  is close to  $\varphi$ , will be a very slowly varying function of  $\psi$ . At any points where  $D(C)$  has infinite gradient or is discontinuous both  $d\psi/dC$  and  $d^2\psi/dC^2$  must be exactly equal to the corresponding terms in  $\varphi$ . This ensures that the problem solved with  $\psi$  and  $\nabla \psi$

continuous will give the correct continuity for  $C$ .

To extend this transformation to  $D(C,t)$  is straightforward just by introducing  $\varphi(C,t)$ , as can be done with the Kirtchoff transformation, assuming that  $D_t(C,t)$  is bounded. This introduces the necessity of calculating a source term

$$\int D_t(C,t)/C \, dC \quad (4.3)$$

which may easily be done. Extensions to allow for a general  $D(C,t,x)$  can be performed analytically: however this requires  $D$  to be at least twice differentiable in  $x$  and results in an awkward set of integrals to evaluate. It remains to be seen whether the additional computational effort required in both these cases is justified and in any event these should not be employed if  $D$  is only a slowly varying function of its arguments.

## 5 Numerical Examples

As an example of how the transformation assists the numerical solution of a diffusion problem we consider arsenic diffusion in silicon, which is governed by a diffusion coefficient of the form (1.3) with  $\beta = 100$ , solved using the Moving Finite Element method. The problem is solved on the interval  $x \in [0,1]$  with Neumann boundary conditions at both ends. As the initial distribution we take a Gaussian profile centred at  $x = 0.25$  and with a standard deviation of 0.05. The height of the Gaussian is approximately  $10^{21}$ , although the problem is solved in non-

dimensional form (giving an effective diffusion coefficient which varies over two orders of magnitude).

The solution to this problem consists of steep moving fronts which propagate outwards from the centre of the Gaussian, whilst the magnitude of the profile is attenuated. The left-moving front hits the  $x = 0$  boundary and the concentration on this boundary rises, while the right-moving front propagates unhindered.

If we proceed to solve the problem in the original (but normalised) variables Figure 1 illustrates what happens at large times ( $t = 4000, 8000, 12000, 16000$  and  $20000$ ). Although the top of the profile is well represented by the piecewise linear solution obtained from MFE, the tail is very badly modelled indeed. (Note that all plots shown have a logarithmic vertical axes and hence the piecewise linear representation appears as a curve.) All results shown use 21 moving nodes but an increase in this number reaps no significant benefit.

Figure 2 shows the results using an approximate transformation as described in Section 4. The diffusion coefficient for the problem behaves like  $(1 + c)$  over much of the region, where the normalised concentration  $c \sim C/(5 \times 10^{18})$ . An approximation to the true velocity potential (3.8) is therefore

$$\psi = \int (1+c)/c \, dc = c + \ln(c).$$

As can be seen, using this transformation, a very good representation of the entire solution is obtained. The solution in the transformed variable is shown in Figure 3.

Other possible transformations of dependent variable are  $\ln(c)$  and the Kirchhoff transformation (2.1) (but based on  $1+c$ ). Unfortunately the MFE method breaks down when using these transformations when the left-moving front hits the  $x = 0$  boundary. This appears to be due to the close proximity of neighbouring nodes resulting in either impractically small timesteps or nodal collisions. However we do present results using these transformations prior to these problems.

Figures 4 to 7 illustrate output at  $t = 500$  and  $1000$ , using the velocity potential ( $c + \ln(c)$ ), the primitive variable ( $c$ ), the variable  $\ln(c)$ , and the Kirchhoff transformation ( $c + c^2/2$ ) respectively. As can clearly be seen, the results obtained by solving for the transformed variable of Section 4 are far superior to those using the other transformations.

## 6 Observation

The authors are indebted to Stan Osher for pointing out the following observation. Consider the 1-D case with  $D(C) \equiv \epsilon$ ,

$$C_t = (\epsilon C_x)_x = \epsilon C_{xx}$$

and apply the transformation. We have

$$\varphi = -\int \epsilon/C dC = -\epsilon \ln C$$

and the equation becomes

$$\varphi_t = \epsilon \varphi_{xx} - \varphi_x^2$$

If we now differentiate and make a further change of variables to  $u = 2\varphi_x$  we obtain

$$u_t + (u^2/2)_x = \epsilon u_{xx}$$

i.e. the viscous Burgers' equation. This combination of transformations is equivalent to

$$u = (-2\epsilon \ln(C))_x = -2\epsilon C_x/C$$

which is precisely the Cole-Hopf transformation [11] used to allow analytic investigation of the viscous Burgers' equation by transforming it to a linear parabolic equation. We note therefore, that for this special  $D(C)$ , the advocated transform is a partial inverse of the classical Cole-Hopf transformation.

## 7 Conclusions

A transformation has been proposed for the diffusion equation (1.1) which allows good numerical representation of the solution when it possesses a highly transient nature. The transformation consists of using the velocity potential of the diffusing material. Numerical examples have been shown to demonstrate how the transformation improves the solutions obtained when solving a practical problem.

## 8 Acknowledgements

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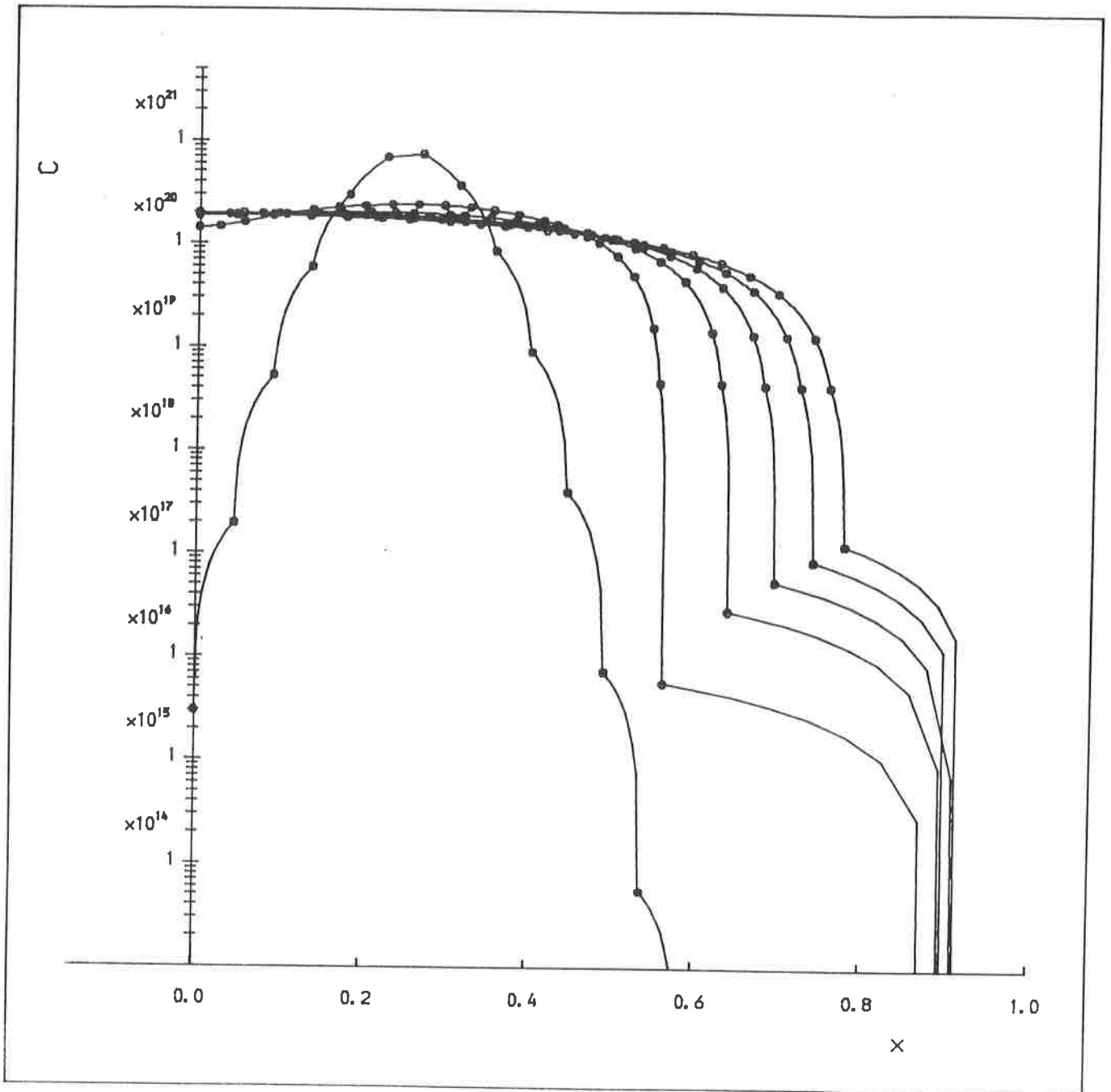


Figure 1: Calculations using the primitive variable.

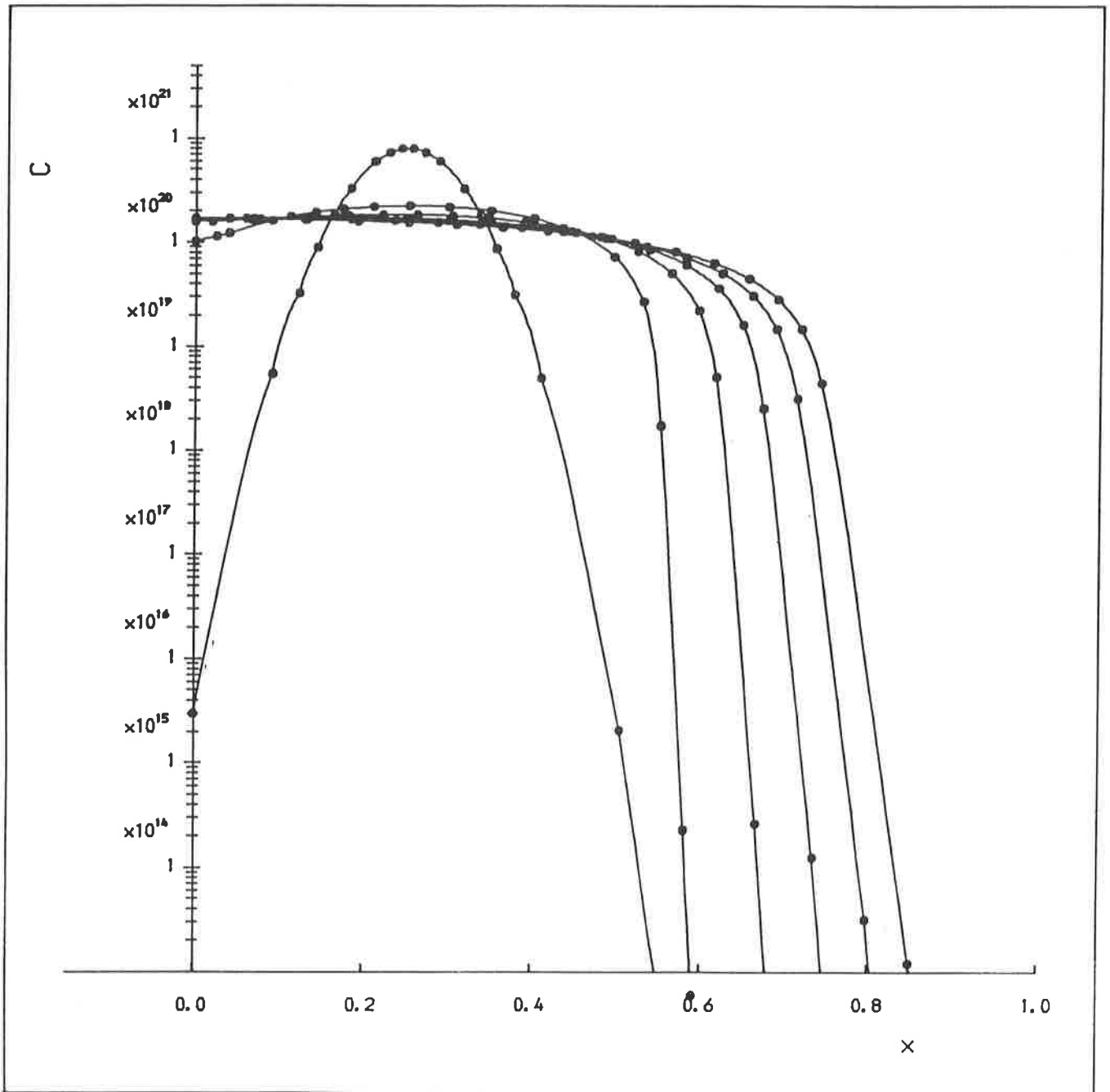


Figure 2: Calculations using the transformed variable.

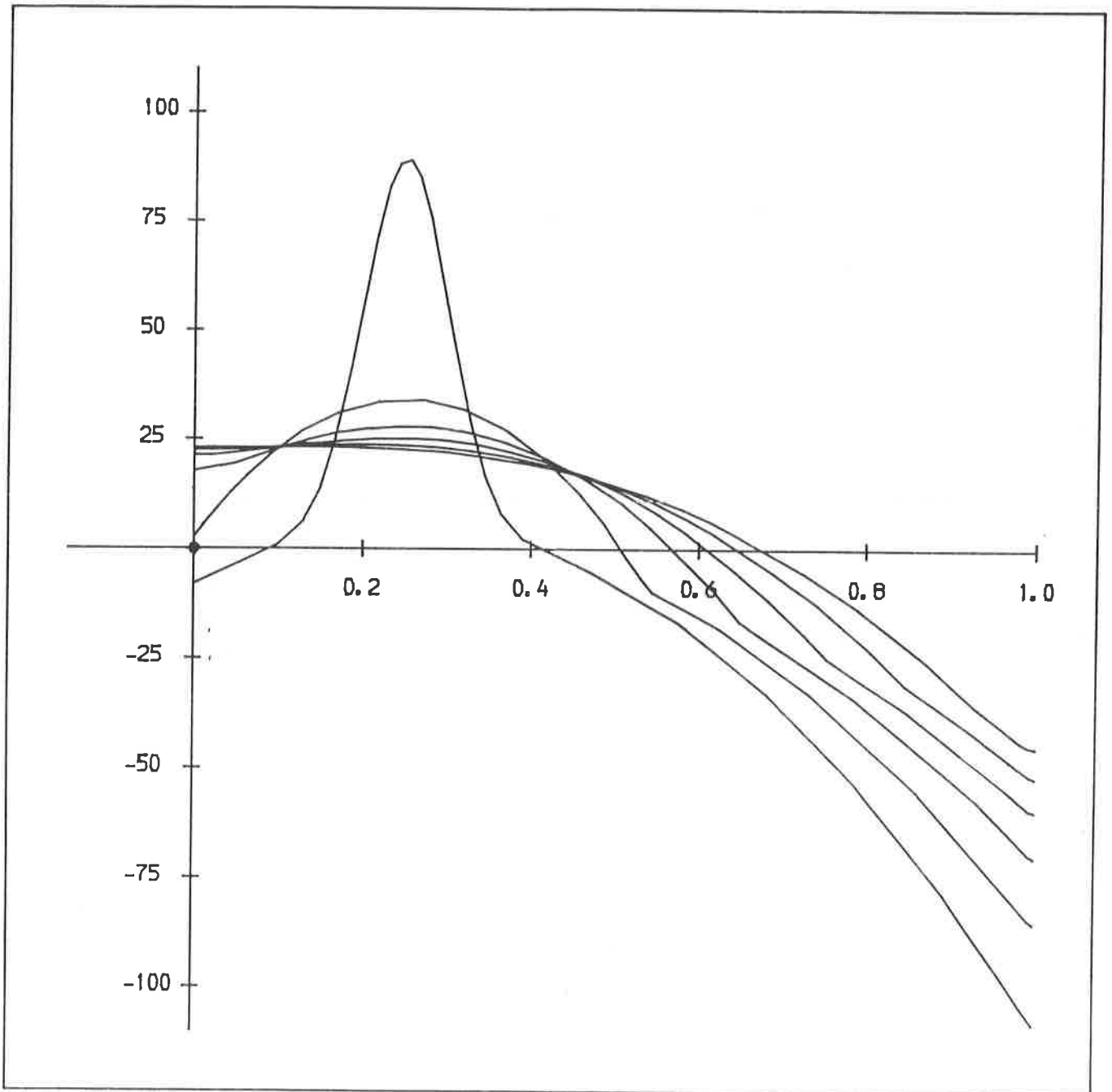


Figure 3: Solution plotted in the transformed variable.

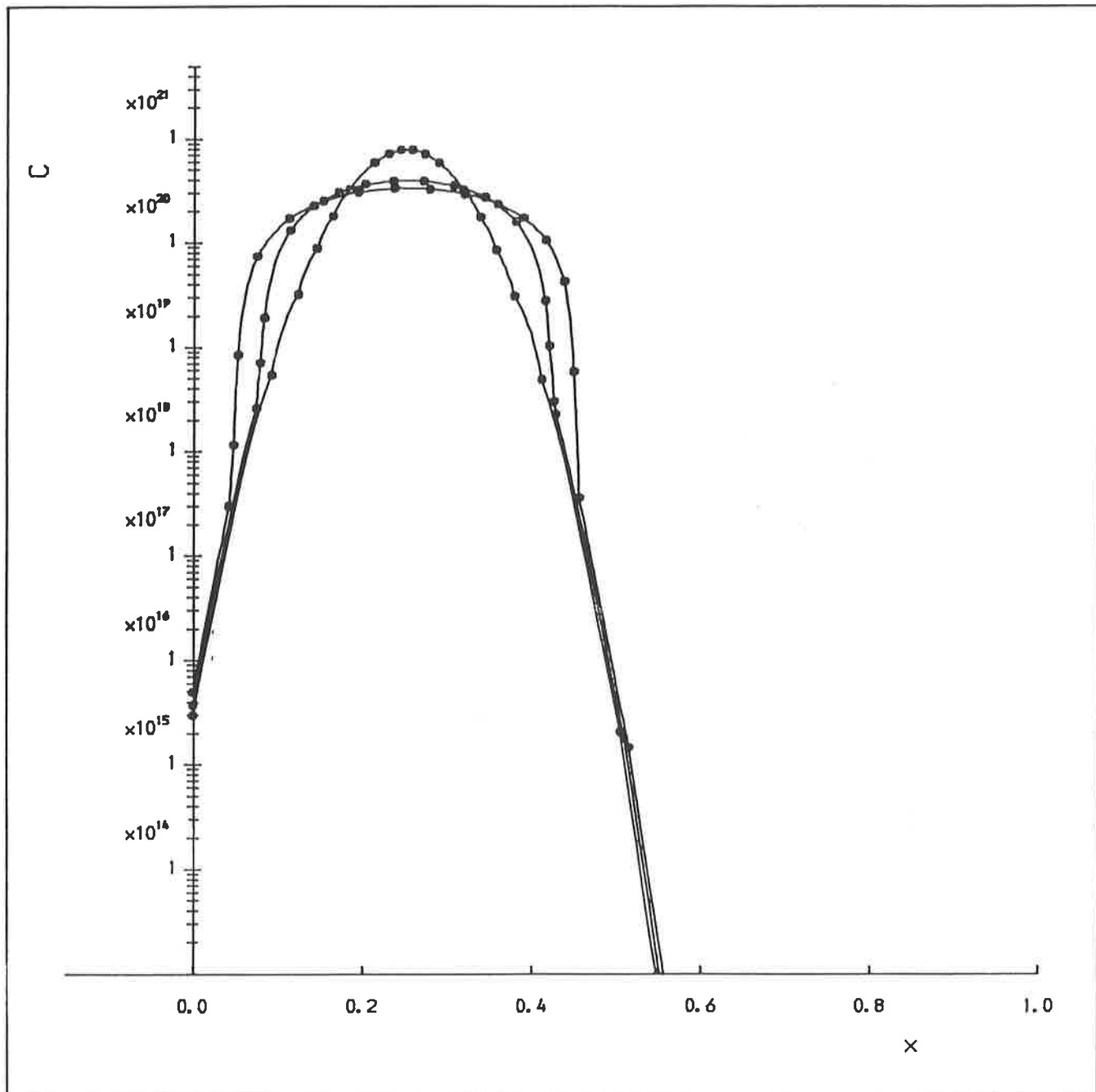


Figure 4: Calculations using the transformed variable.

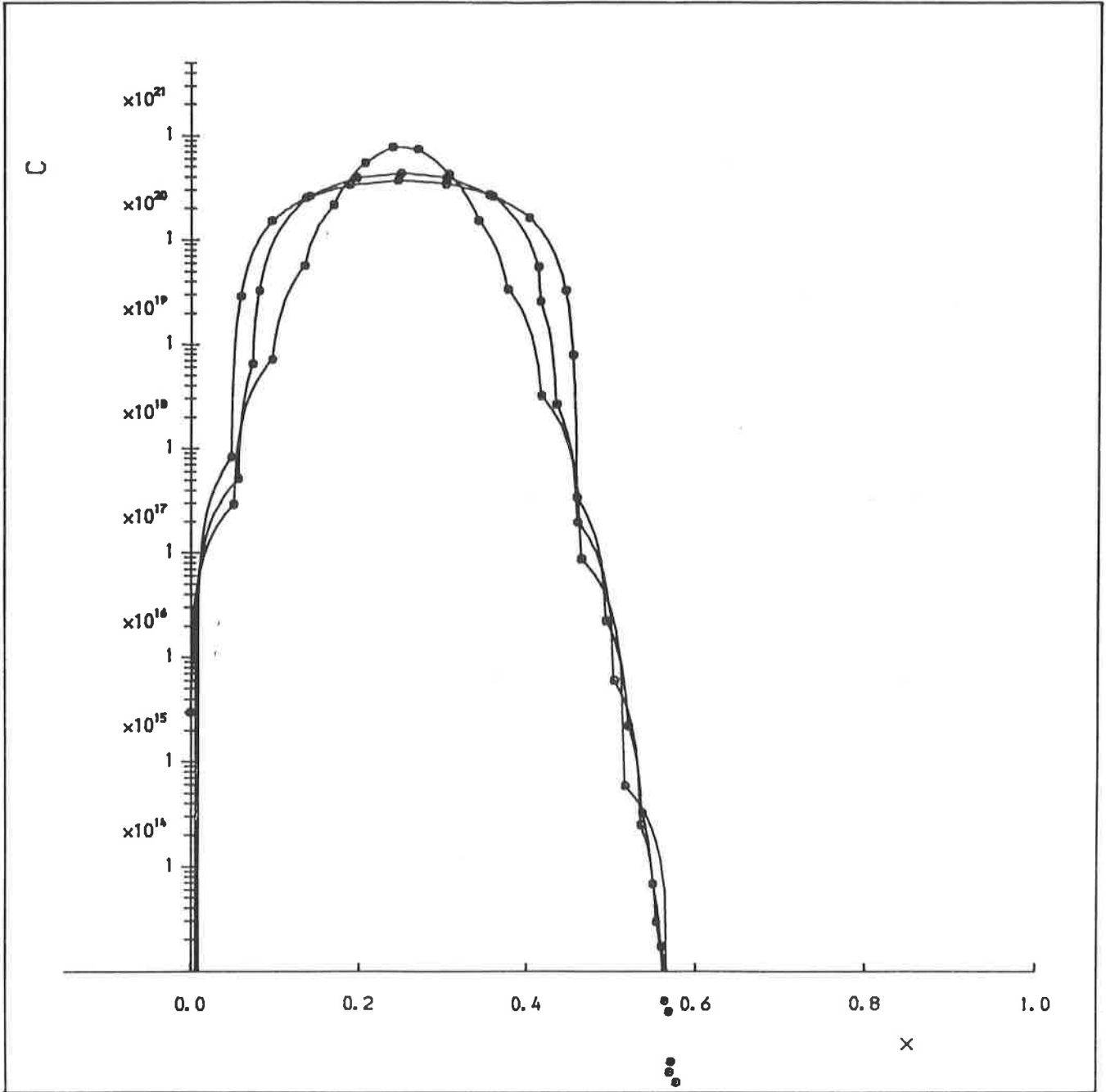


Figure 5: Calculations using the primitive variable.

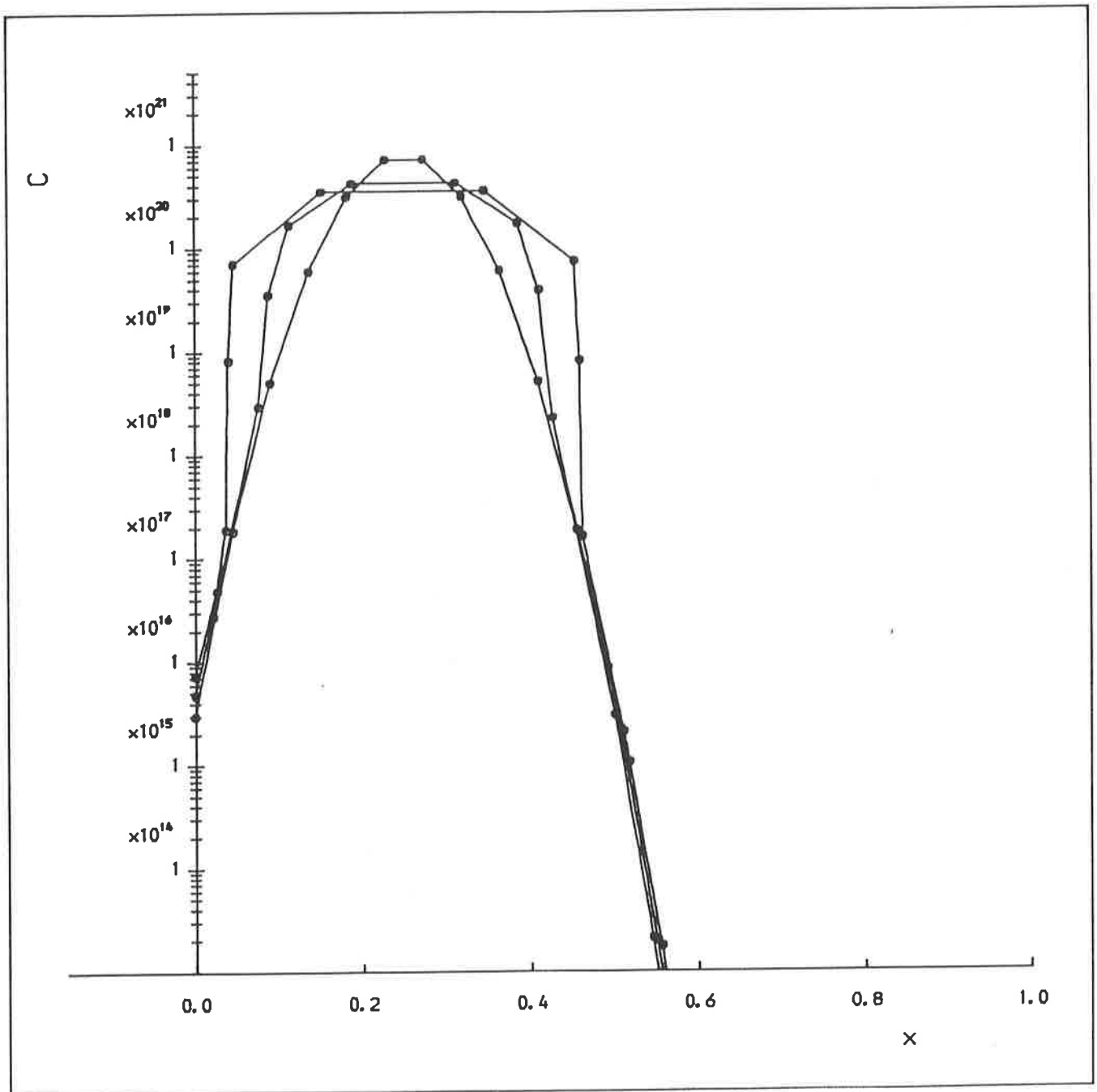


Figure 6: Calculations using ln variable.

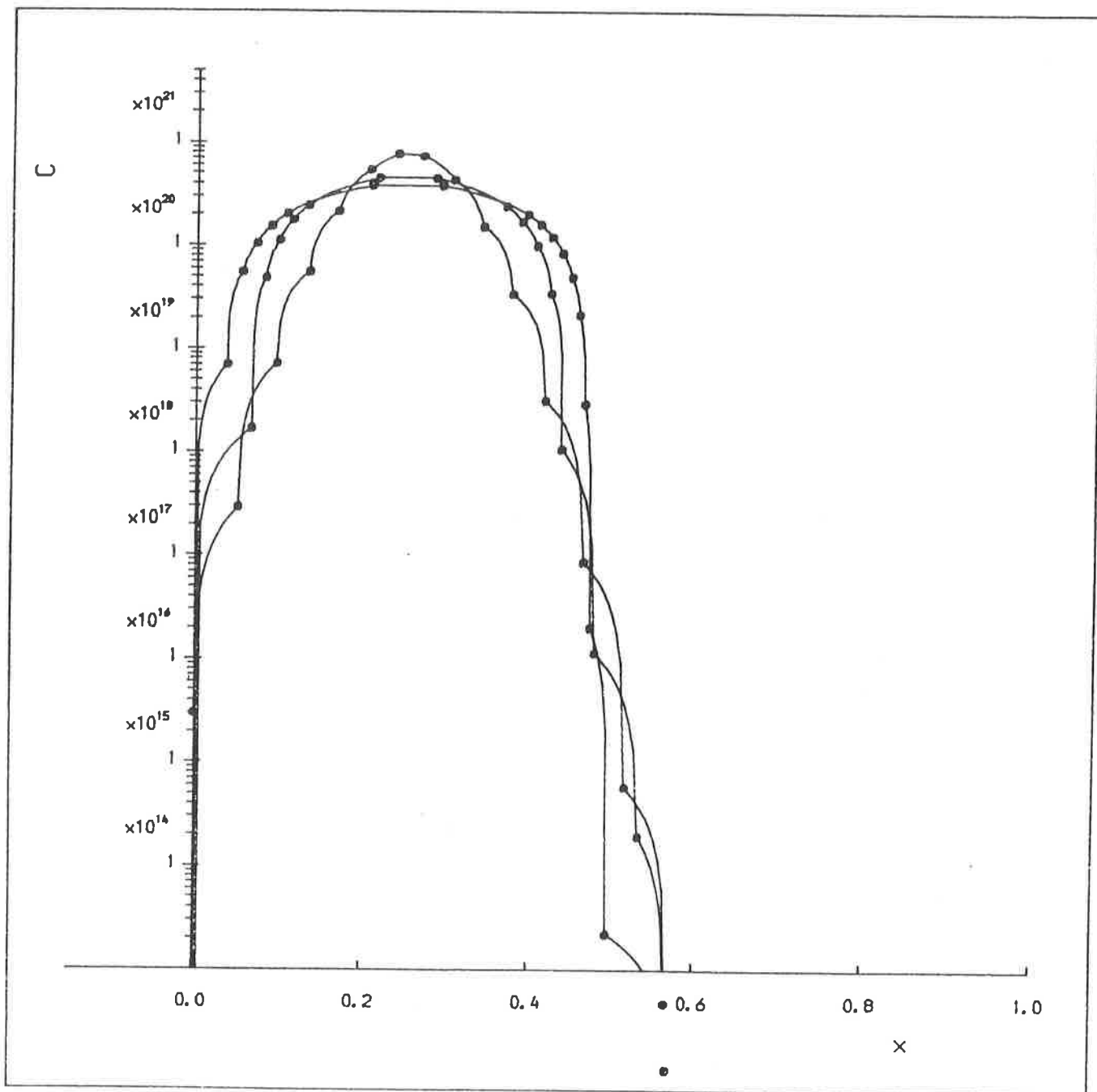


Figure 7: Calculations using the Kirchhoff transformation.