FINITE ELEMENT METHODS FOR THE CONVECTION DIFFUSION EQUATION

V. Nassehi
Department of Chemical Engineering
Loughborough University of Technology
Loughborough, Leicestershire, U.K.
S.A. King
Department of Mathematics and Statistics
Teesside Polytechnic
Middlesbrough, Cleveland, U.K.

Abstract This paper deals with the finite element solution of the convection diffusion equation in one and two dimensions. Two main techniques are adopted and compared. The first one includes Petrov-Galerkin based on Lagrangian tensor product elements in conjunction with streamlined upwinding. The second approach represents Bubnov/Petrov-Galerkin schemes based on a new group of exponential elements. It is shown that specially devised exponential elements can be very effective in finite element analysis of convection dominated phenomena.

چکیده دراین مقاله حل معادلات مربوط به پدیده انتقالی پخش به همراه کنوکسیون در حالات یک بعدی و دوبعدی توسط روش المانهای محدود مورد بحث قرار گرفته است. دو روش حل مختلف بررسی شده و نتایج آنها با همدیگر مقایسه گردیده است. این دو روش عبارتند از اولاً: پتروف گالرکین برمبنای المانهای لاگرانژی ضرب تانسوری با ضرایب وزنی برداری هم‌جهت با بردار سرعت انتقال و ثانیاً: بابنوف گالرکین برمبنای المانهای توانی با ضرایب وزنی اسکالر. نتیجه‌ای که از این بررسی گرفته می‌شود اینستکه المانهای توانی ابداعی ما راه حل بسیار مطمئن و قوی برای حل معادلات مربوط به پدیده های انتقالی که مؤثراً با مکانیسم کنوکسیون انجام می گیرند ارائه می دهند.

INTRODUCTION

The numerical solution of second order partial differential equations (arising in Convection Diffusion problems) whose first derivatives have large coefficients has long been known to present difficulties. The conventional way of overcoming the parasitic oscillations that result when finite differences or standard finite element methods are used, is to use upwinding techniques [1]. Traditional upwinding techniques tended to reduce the spurious oscillations but usually made the solution method first order accurate rather than second order accurate. An optimal scheme for upwinding in the finite element context was devised by Christie *et al.*[2]. This was achieved by adopting an essentially Petrov-Galerkin approach. In this method, in contrast to the standard Bubnov-Galerkin methods the weak variational (weighted residual functional) equivalent of convective diffusion equation is based on a group of weigh functions which are different from the used interpolation functions. Other approaches included adding artificial diffusivity to the second order term in the convection diffusion equation which was to have the effect of cancelling the negative diffusivity automatically generated by the finite element discretization. This can be interpreted as defining an upstream quadrature point. In one dimension all these approaches could be made nodally exact by adjusting the scheme to the correct amount of required numerical dissipation. When applied to two (or three) dimensional problems these techniques produced excessive crosswind diffusion. Hughes and Brooks overcame this problem to a large extent by "stream-lining" the artificial diffusivity term [3] or as they later presented it by stream-lining their modified weighting functions [4]. This stream-lined Petrov-Galerkin approach used discontinuous weighting functions and was applied quite successfully to a range of problems. In the present analysis we look at the basic convection diffusion equation in one and two dimensions. We outline the weighted residual finite element method in one dimension and present our approach which is essentially a Galerkin weighted residual technique based on exponential interpolation functions. This is compared with the modern polynomial based Petrov-Galerkin stream-lined upwind procedure. Then for a two-dimensional test problem, where an analytical solution is possible, we present our numerical solutions and evaluate their accuracy by comparison with the exact result. We aim to show that by adopting exponential functions, that is by tailoring the interpolation model to the problems rather than relying on simple polynomial functions for all eventualities, the finite element solution of convection diffusion equation can be significantly improved.

STATEMENT OF THE PROBLEM AND THE FINITE ELEMENT SOLUTION

We consider the differential equation:

$$\frac{d^2\phi(x)}{dx^2} - K(x)\frac{d\phi(x)}{dx} = S(x) \text{ in domain } x_1 \leq \Omega \leq x_2 \quad (1)$$

subject to essential boundary conditions. In order to develop a weighted residual finite element solution for equation (1) the domain Ω is discretized into a mesh of finite element. Within every elements. (Ω_e) a weak variational form of equation (1) is derived by integrating the functional which results from replacing $\phi(x)$ by a trial function $\phi^h(x)$ and weighting the generated residual:

$$\int_{\Omega_e} w(x)\left\{\frac{d^2\phi^h}{dx^2} - K(x)\frac{d\phi^h}{dx} - S(x)\right\} d\Omega_e = o \quad (2)$$

where w(x) is a weignt function and

$$\phi^h = \sum_{i=1}^{m} N_i \phi_i \quad (3)$$

N_i is the interpolation function associated with node i; m is the number of nodes per element and ϕ_i represents the nodal value of ϕ. In the standard Bubnov-Galerkin method the weigh function is taken to be identical to the interpolation function ($W_j = N_i$ for i= j). Integrating by parts equation (2) gives: (note that in one-dimensional case $d\Omega_e$ is simply dx).

$$-\int_{\Omega_e} \frac{dw}{dx}.\frac{d\phi^h}{dx}dx - \int_{\Omega_e} W.K.\frac{d\phi^h}{dx}dx - \int_{\Omega_e} W.S.dx + W\frac{d\phi^h}{dx}\Big|_{\Omega_e} = o \quad (4)$$

Thus by analogy to matrix forms, with summation over the repeated index i, the basic weighted residual finite element form of the original convection diffusion equation becomes:

$$\left[\int_{\Omega_e} \frac{dN_j}{dx}\cdot\frac{dN_i}{dx}dx + \int_{\Omega_e} K\,.\,N_j\,.\,\frac{dN_i}{dx}dx + \int_{\Omega_e} S\,.\,N_j dx\right]\{\phi_i\} = \left\{N_j\frac{d\Sigma N_i\phi_i}{dn}\Big|_{\Omega_e}\right\} \quad (5)$$

$$i, j = 1, \ldots, m$$

Using an isoparametric mapping of the form

$$x = \sum_{i=1}^{m} N_i(\xi)X_i \quad (6)$$

equation 5 is cast in a local natural co-ordinate system for a master element defined between $\xi = -1$ and $\xi = +1$ and the integrals in its left hand side are evaluated by Gaussian guadrature. This process is repeated for every element and finally all of the resulting elemental equations are assembled together [5]. The flux term in the right hand side of equation (5) vanishes for all inter-element boundaries and appears only on the exterior boundaries of the solution domain. Application of the boundary conditions renders the assembled global set of equations determinate and soluble. However, if the coefficient of the first order derivative (K) in equation (1) is large (convection dominated case) and the selected interpolation functions (N_i)

are polynomials (or for the multi-dimensional situations are the tensor products of polynomials) the solution of the obtained global set will yield oscillatory and useless result. In particular if linear interpolation functions are used the described Bubnov-Galerkin scheme will produce an oscillatory solution which is identical to the one obtained by a finite difference technique based on central differences. In the finite difference context the traditional way of overcoming this has been the use of less accurate forward (or backward) difference for the first order derivative term [6].

Upwinding

The stream-lined upwind Petrov-Galerkin modification of the described finite element procedures presented by Brooks and Hughes [4] is based on using a weighting function which is given by:

$$W_i(\xi) = N_i(\xi) + \left[\coth\frac{Kh}{2} - \frac{2}{Kh}\right]\frac{\partial N_i(\xi)}{\partial \xi} \tag{7}$$

where h is the element length. They have shown that using this weighting a nodally exact solution for the original equation can be obtained. Such a rigorous analysis is not possible for two or three dimensional problems and an analogous form for weight functions in two dimensions is given by:

$$W_i(\xi,\eta) = N_i(\xi,\eta) + K.d.\frac{\partial N_i(\xi,\eta)}{\partial \xi} + K.d.\frac{\partial N_i(\xi,\eta)}{\partial \eta} \tag{8}$$

where d is an upwinding constant which is a function of the so called nominal element length. The stream-lining concept arises from the idea of trying to define the upwinding constant d in a way which eliminates spurious diffusion in the crosswind direction [7].

Exponential Interpolation Functions

A differential equation of the form similar to equation (1) will have a solution consisting of two components-the particular integral and the complementary function (corresponding to the solution when S=O). The exponential interpolation functions are really designed to model the complementary function. In one dimension we discretize the solution domain into a mesh of binodal elements of length h_ξ. In terms of ξ (i.e the variable along the corresponding master element) we define the following interpolation functions:

$$N_{+1} = \frac{e^{Kh_\xi(\xi+1)/2} - 1}{e^{Kh_\xi} - 1}$$
$$N_{-1} = \frac{e^{Kh_\xi} - e^{Kh_\xi(\xi+1)/2}}{e^{Kh_\xi} - 1} \tag{9}$$

Firstly we note that these functions have correct local support i.e.:

$$N_{+1}(+1) = 1 \quad and \quad N_{+1}(-1) = o$$
$$N_{-1}(-1) = 1 \quad and \quad N_{-1}(+1) = o \tag{10}$$

Secondly they are square integrable (L_2) functions satisfying the necessary continuity, differentiability and smoothness, required for the finite element solution of equation (1) [8]. If we transform from our master element back to the global system we could write these interpolation functions as:

$$N_{+1} = \frac{e^{Kx} - 1}{e^{Kh} - 1}, \quad N_{-1} = \frac{e^{Kh} - e^{Kx}}{e^{Kh} - 1} \qquad o < x < h \tag{11}$$

It is easy then to see that these interpolation functions satisfy the homogeneous form of the equation (1) exactly if K is constant.

STABILITY ANALYSIS FOR EXPONENTIAL INTERPOLATION FUNCTIONS

Starting from the homogeneous form of equation (5) we construct a set of elemental equations based on exponential interpolation functions and isoparametric mapping. All of the required integrals in this case are evaluated analytically. In order to simulate a realistic two point boundary value problem we have to at least assemble two of the elemental equations. Combing two elemental equations at their common node we obtain:

$$\phi_{+1}(1/2-\alpha)+\phi_o(2\alpha)+\phi_{-1}(-1/2-\alpha)=o \qquad (12)$$

ϕ_{+1}, ϕ_o and ϕ_{-1} are the nodal values of Φ at three successive nodes and

$$\alpha = 1/2 \, . \frac{e^{Kh}+1}{e^{Kh}-1} \qquad (13)$$

Equation 12 represents a difference equation which using the shift operator E gives:

$$(1/2-\alpha)E^{+1}\phi_o + 2\alpha\,\phi_o + (-1/2-\alpha)E^{-1}\,\phi_o = o \qquad (14)$$

thus

$$(1/2-\alpha)E^2 + 2\alpha E - 1/2 - \alpha = o \qquad (15)$$

with solutions

$$E_1 = 1 \quad , \quad E_2 = \frac{\alpha+1/2}{\alpha-1/2}$$

Therefore by superimposition after substituting for α from equation (13):

$$\phi_o = A + B\, e^{Kh} \qquad (16)$$

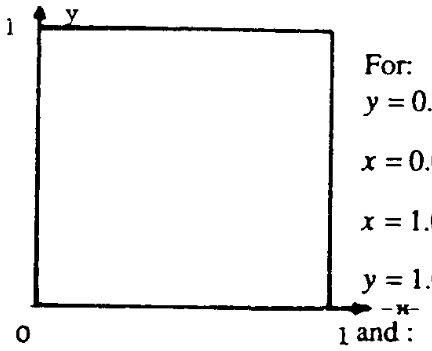
where A and B are constants. Clearly there is no chance of oscillations and equation (16) is the exact solution.

TWO DIMENSIONAL TEST PROBLEM

We consider the two dimensional convective diffusion equation represented by:

$$\frac{\partial^2\phi(x,y)}{\partial x^2} + \frac{\partial^2\phi(x,y)}{\partial y^2} - K_1\frac{\partial\phi(x,y)}{\partial x} - K_2\frac{\partial\phi(x,y)}{\partial y} = o \qquad (17)$$

in two dimensional smooth domain Ω with a closed boundary Γ. Unlike the one dimensional problems it is not very easy to invent a range of two dimensional problems whose analytical solutions can be readily derived. However, if we assume that the domain Ω is a square with the essential boundary conditions specified as is shown in Figure 1 we can obtain an analytical solution for equation (17) (for the case when K_1



For:
$y=0.0\,,0\leqslant x<1\,,\phi=1.0$
$x=0.0\,,0\leqslant y<1\,,\phi=1.0$
$x=1.0\,,0<y\leqslant 1\,,\phi=0.0$
$y=1.0\,,0<x\leqslant 1\,,\phi=0.0$
and:
$\phi(1,0)=0.5, \phi(0,1)=0.5$

Figure 1. Boundary conditious for two-dimensional problem.

and K_2 are constants) by the separation of variables.

This solution is given by:

$$\phi(x,y) = \sum_{n=1}^{\infty} \frac{8n\pi e^{\frac{K_1x+K_2y}{2}}}{\mathrm{Sinh}\left(\frac{\sqrt{A_n}}{2}\right)}$$

$$\left| \frac{1-(-1)^n e^{\frac{-K_1}{2}}}{K_1^2+4n^2\pi^2}\mathrm{Sin}(n\pi x)\,\mathrm{Sinh}\left(\frac{\sqrt{A_n}\,(1-y)}{2}\right)\right.$$

$$\left. + \frac{1-(-1)^n e^{\frac{-K_2}{2}}}{K_2^2+4n^2\pi^2}\mathrm{Sin}(n\pi y)\,\mathrm{Sinh}\left(\frac{\sqrt{A_n}(1-x)}{2}\right)\right| \qquad (18)$$

where

$$A_n = K_1^2 + K_2^2 + 4\,n^2\pi^2 > o \qquad (19)$$

In order to formulate a finitè element solution for equation (17) using exponential interpolation functions we construct a set of tensor product elements based on the one dimensional example. For a four noded master element we have:

$$\begin{Bmatrix} M_1(\xi,\eta) = N(\xi_{-1})\,.\,N(\eta_{-1}) \\ M_2(\xi,\eta) = N(\xi_{+1})\,.\,N(\eta_{-1}) \\ M_3(\xi,\eta) = N(\xi_{+1})\,.\,N(\eta_{+1}) \\ M_4(\xi,\eta) = N(\xi_{-1})\,.\,N(\eta_{+1}) \end{Bmatrix} \qquad (20)$$

where $N(\xi_{-1})$ and $N(\xi_{+1})$ are given in equation (9). Replacing h_ξ and ξ whit h_η and η in equation (9) we get $N(\eta_{-1})$ and $N(\eta_{+1})$. For Bubnov-Galerkin formulations we use exponential weight functions which are identical to interpolation functions. For Petrov-Galerkin (Upwind) formulations we use modified weight functions given either by:

$$W_i = M_i + \frac{K_1^2}{K_1^2+K_2^2}\left(\coth\frac{K_1 h_\xi}{2} - \frac{2}{K_1 h_\xi}\right)\frac{\partial M_i}{\partial \xi} + \frac{K_2^2}{K_1^2+K_2^2}\left(\coth\frac{K_2 h_\eta}{2} - \frac{2}{K_2 h_\eta}\right)\frac{\partial M_i}{\partial \eta} \quad (21)$$

(we refer to this scheme as exponential upwind scheme A); or by:

$$W_i = M_i + \frac{K_1 h_\xi}{2\sqrt{K_1^2+K_2^2}}\frac{\partial M_i}{\partial \xi} + \frac{K_2 h_\eta}{2\sqrt{K_1^2+K_2^2}}\frac{\partial M_i}{\partial \eta} \quad (22)$$

(we refer to this scheme as exponential upwind scheme B).

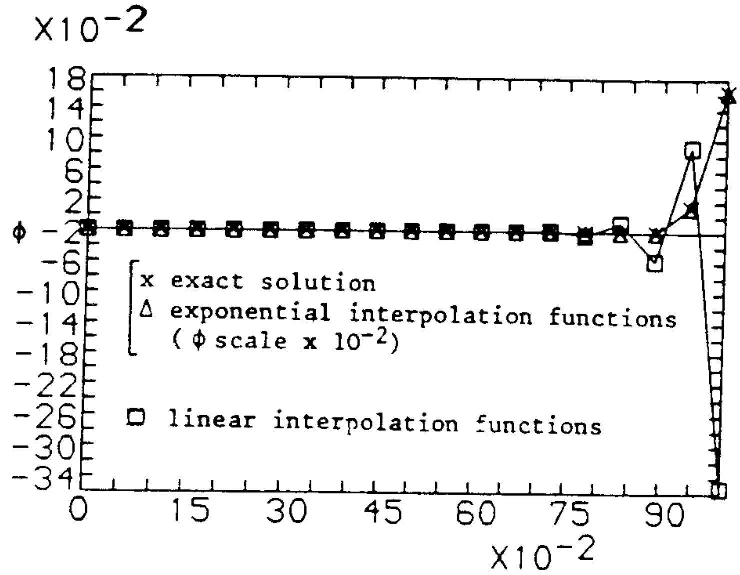


Figure 2. Results of numerical experiments for: K = 40.0, s = 0.0

NUMERICAL EXPERIMENTS: RESULTS AND DISCUSSION

In order to establish the validity and applicability of exponential interpolation functions an extensive set of numerical experiments has been carried out. The most important results are presented in this paper.

One Dimensional Problems

I) Bubnov - Galerkin formulations of equation (1).

1) Constant K with no source term. As expected the exponential functions give nodally exact solution for all value of K up to ±40. This is based on a six point Gaussian integration of the functions in the working equation. The departure from the exact solution for |K| above 40 is due to the inability of the integration scheme to cope with the exponential functions sufficiently accurately. The linear functions in general give inaccurate results for small K values and exhibit oscillatory behavior for large K (Figure 2).

2) Constant K with a source term. We look at relatively large K values with the constant or variable source terms. Exponential functions give much more accurate results in comparison with linear functions (Figure 3).

3) Variable K with or without a source term. Results for various cases are presented in Figure 4. They are in agreement with the general

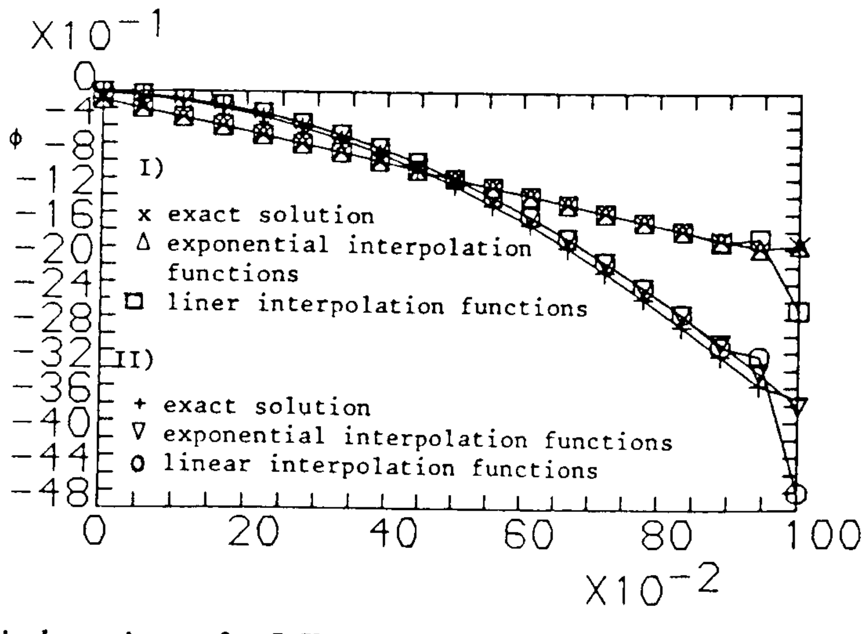


Figure 3. Results of numerical experiments for: I: K = 30.0, s = 30.0 II: K = 30.0, s = -2.0 + 60.0 X

conclusion which points to the superior accuracy of the exponential functions.

II) Petrov-Galerkin (upwind) formulations of equation (1).

1) Constant K with no source term. In all cases (even at K >> 40) upwinded solution give nodally exact results.

2) Constant K with source terms. The same upwinded weight function is used to multiply the source term. Accurate results are obtained using both types of interpolation functions.

3) Variable K with or without source terms. Both techniques produce accurate results.

Two-Dimensional Problems

Solution of the one-dimensional equation reveals that for larger values of K we need to use a higher order Gaussian quadrature in order to maintain the accuracy of the schemes based on exponential functions. This is computationally expensive. However, in the 2-D test problem K_1 or K_2 (coefficients of the first order derivatives) are constants and it is possible to evaluate the integrals in the elemental stiffness equation analytically. This is used to derive the working equation of the present solution scheme. We consider the results for various values of K_1 and K_2.

1) $K_1 = K_2$ 2.5 to 10. In this case the convection terms are comparatively small. Results for a 7 × 7 finite element mesh (Figure 5) for various cases are given in Figure 6. Bubnov-Galerkin schemes give acceptable results although for $K_1 = K_2 = 10$ those solutions which are based on linear interpolation function start to oscillate. Upwinded schemes in general produce overdamped solutions. The degree of overdamp is slight for consistant Petrol-Galerkin based on exponential functions and sever for biquadratic functions.

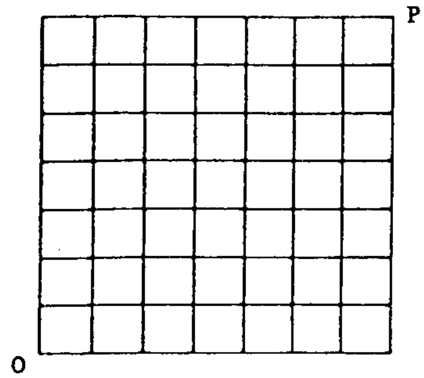


Figure 5. Finite elements mesh.

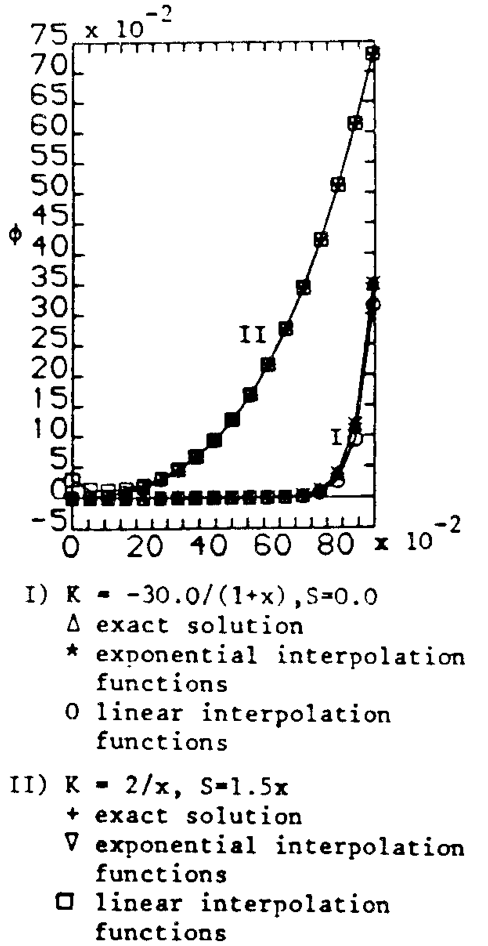


Figure 4. Results of numerical experiments for variable K.

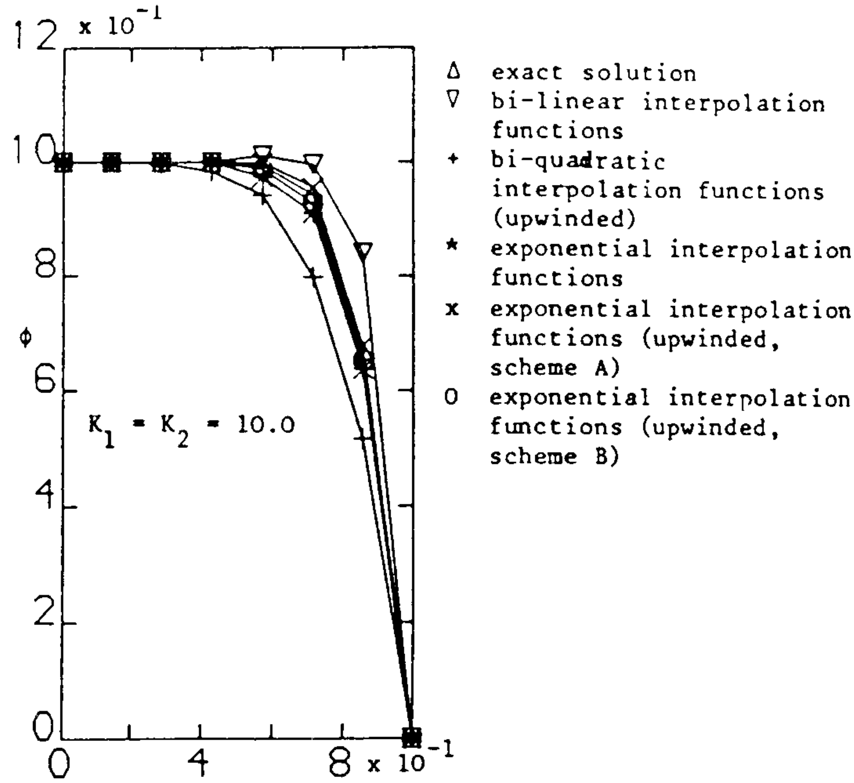
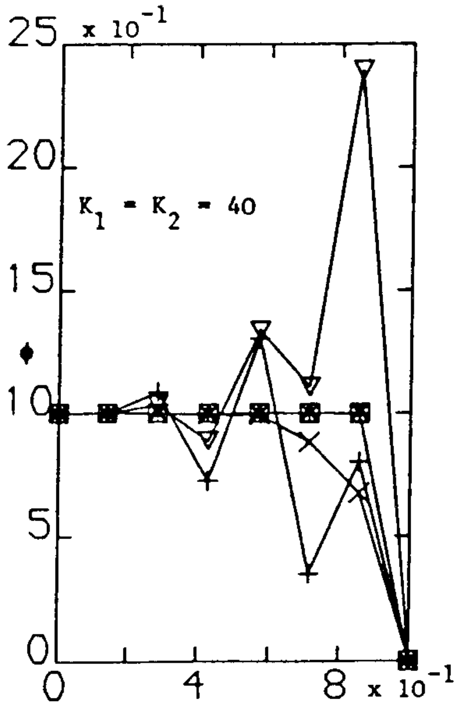


Figure 6. Solution along OP.

2) $K_1 = K_2 = 40$ to 160. The exact solution tends to be 1.0 for all interior nodes. The Bubnov-Galerkin formulations based on bilinear and biquadratic functions produce oscillatory and useless solutions. Upwinded Petrov-Galerkin schemes based on polynomial functions produce overdamped solution. Upwinded Petrov-Galerkin schemes A and B based on exponential functions produce accurate results with slight oscillations. The Bubnov-Galerkin scheme based on exponential functions produce the best result. These are shown in Figure 7.

3) Higher values of K_1 and K_2. As K_1 and K_2 increase (i.e. the convection terms become more dominant) the upwinded schemes (based on polynomial or exponential functions) become less effective. In fact they tend to produce very nearly the same nodal values irrespective of K_1 and K_2 values. In contrast the Bubnov-Galerkin scheme based on exponential functions produces more and more accurate results as K_1 and K_2 increase. With K = 90000 these results are accurate to 6 places of decimals.



Δ exact solution
∇ bi-linear interpolation functions
+ bi-quadratic interpolation functions
x bi-quadratic interpolation functions (upwinded)
* exponential interpolation functions
□ exponential interpolation functions (upwinded, scheme A)
O exponential interpolation functions (upwinded, scheme B)

Figure 7. Solution along OP.

CONCLUSION

The results for the one dimensional case show the expected oscillations for Bubnov-Galerkin solutions of the convection dominated phenomena when the scheme is based on linear or quadratic interpolation function. In contrast very accurate results are obtained if expónential interpolation functions are used. In general stream-lined upwind Petrov-Galerkin schemes also produce accurate results for one dimensional problems. In two dimensions the value of exponential functions becomes apparent in considering the solution of the convection diffusion equation where first order derivative terms are very large. Our study shows that Bubnov-Galerkin schemes based on exponential functions offer a very effective method to cope with convection dominated problems in two dimensions. We are now extending this approach to tackle convection dominated problems with an abrupt (discontinuous) upstream boundary condition. It seems that a combination of polynomials of low degree with exponential functions will produce the appropriate interpolation function to model such a complicated problem.

REFERENCES

1. M.B. Allen, Why Upwinding is Reasonable in: "Finite Elements in Water Resources", Laible J. P.(ed) pp 13-23, (1984).
2. L. Christie D.F. Griffiths, A. R. Mitchell, and O.C, Zienkiewicz "Finite Element Methods for Second Drder Differential Equations with Significant First Derivatives", *Int. J. Num. Meths, Engng,.* 10, 1389 (1979).
3. T.J.R. Hughes and A. Brooks, "Multi-Dimensional Upwind Scheme with No Crosswind Diffusion" in: "Finite Element Methods for Convection Dominated Flows". Hughes, T.J.R., (ed) pp 19-35, (1979)
4. A. Brooks and T.J.R. Hughes "Streamline-Upwind/

Petrov-Galerkin Methods for Advection Dominated Flows", Proc. 3rd Int. Conf. on Finite Element Methods in Fluid Flow, Banff., (1980).

5. O.C, Zienkiewicz, "Finite Element Method", McGraw-Hill, New York, (1977).

6. P.J. Roache "Computational Fluid Dynamics", Hermosa Publishers, Albuquerque, N.M., (1972).

7. S. Nakazawa, J.F.T. Pittman, and O.C., Zienkiewicz "Numerical Solution of Flow and Heat Transfer in polymer Melts", Chapter 13 in: Finite Elements in Fluids Gallagher, R.H., Norrie, D.H., Oden, J.T., and Zienkiewicz, O.C., (eds) John Wiley & Sons Ltd., (1982).

8. T.J.R.Hughes, "The Finite Element Method", Prentice-Hall, Inc., New Jersey, (1987).