

## A NEW METHOD FOR NUMERICAL TREATMENT OF DIFFUSION COEFFICIENTS AT CONTROL-VOLUME SURFACES

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*Diffusion coefficients at control-volume surfaces are required for numerical simulation of  
convection-diffusion equations. Various interpolation methods for these diffusion coeffi-  
cients are briefly discussed and compared with the analytical solutions of both pure diffusion  
and convection-diffusion problems. It is found that the harmonic mean method is not as  
accurate and reliable as is supposed. A new method is thus developed. Extensive numerical  
comparisons are given for both the harmonic mean and the present method, and the results  
show that the method proposed is accurate, reliable, and easy to use.*

### INTRODUCTION

Many numerical methods can be used for solving convection-diffusion equations. Among them, the finite-volume or control-volume method is perhaps the most widely used in handling heat and fluid flow problems [1]. The method is still popular due to its great success in formulating convection terms and its wide applicability. The basic idea of the method is to integrate the convection-diffusion equations over so-called control volumes that are actually subdomains of the discretized computation domain and surround the grid nodes [2, 3]. The resulting discretization equations contain the unknown values of dependent or unknown variables of a group of grid nodes and several constants that are functions of diffusion coefficients that pertain to the boundaries or control surfaces of neighboring control volumes. Since the boundaries or control surfaces of these neighboring control volumes are in between and not at the grid nodes, the dependent variables at these control surfaces are not

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## NOMENCLATURE

$a$	coefficients in discrete equations	<b>Subscripts</b>	
$F$	convection parameter in Eq. (9)	$e$	right control surface
$x$	space coordinate	$E$	right neighboring grid node of node $P$
$\delta x$	distance between grid nodes	$P$	grid node under consideration
$\Delta x$	volume of control volume	$w$	left control surface
$\Gamma$	diffusion coefficient	$W$	left neighboring grid node of node $P$
$\phi$	dependent or unknown variable		
$\Phi$	Kirchhoff transformation		

known even after the solution process is completed. Unless the diffusion coefficient is independent of the dependent variables and is uniformly distributed in the entire computation domain, a situation that is rarely true in practical engineering problems, a method should be constructed for determining the values of these diffusion coefficients at the control surfaces. 30

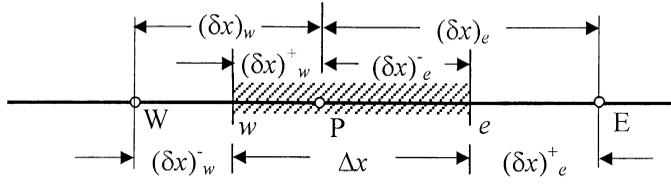
The most straightforward method to determine the control-surface diffusion coefficients is to interpolate linearly from the diffusion coefficient values of the two neighboring nodes of a control surface, which is usually called the arithmetic average method in the literature [2, 4]. A possible alternative to this method is to take a harmonic mean of the nodal diffusion coefficients. Patankar seems to have been the first to suggest the harmonic mean method. In 1978 he examined a conduction problem in composite materials and compared the arithmetic method with the harmonic mean method. He obtained a better result with the harmonic mean method and thus the method was recommended [5]. Since then the method has been so popular, perhaps due to Patankar's famous book [3], that it is almost accepted as a standard interpolation method and prevails in the literature [2, 6, 7]. Later, Chang and Payne reexamined the method [6]. Their work again approved Patankar's conclusion, with a suggestion that the abrupt change interface of the diffusion coefficient should be superposed with a grid node. More recently, Voller and Swaminathan [4, 8] discussed different treatment methods that can possibly be used to handle discontinuities in the thermal properties at the phase-change boundary. They developed a new method based on the Kirchhoff transformation, and a very good result was obtained compared with that of the harmonic mean method. 40 45 50

In this article, we will reexamine the problem, and a more direct and more effective approximation method for the control surface diffusion coefficients will be developed. The new method is almost as effective as the Kirchhoff transformation method and is very simple to use. 55

## THE APPROXIMATION METHODS

In order to introduce and demonstrate the various methods for the control-surface diffusivity approximation, the following one-dimensional steady-state diffusion-type problem, defined by

$$\frac{d}{dx} \left( \Gamma \frac{d\phi}{dx} \right) = 0 \quad (1)$$



**Figure 1** Control-volume discretization showing the nodes and the control surfaces for one-dimensional problems.

was considered. Based on the finite-difference control-volume grid as shown in Figure 1, the above equation is discretized by the finite-volume method, which gives the following discrete equation for an internal node  $P$ :

$$a_P \phi_P = a_W \phi_W + a_E \phi_E \quad (2)$$

where

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$$\left. \begin{aligned} a_W &= \left( \frac{\Gamma}{\delta x} \right)_w & a_E &= \left( \frac{\Gamma}{\delta x} \right)_e \\ a_P &= a_W + a_E \end{aligned} \right\} \quad (3)$$

The variables in the above equations with a lowercase subscript should be determined at the corresponding control surface, and the variables with an uppercase subscript are to be calculated at the corresponding node point. Since the diffusivity in Eq. (1) is supposed to be a function of both the dependent variable  $\phi$  and space coordinate  $x$  and the value of the dependent variable is unknown at the control surface, therefore, the control surface diffusion coefficients cannot be calculated directly even during an iteration process. Hence it is essential to propose an effective method to determine these control-surface parameters. 70

As we have discussed, there are a number of possible methods to calculate these control-surface parameters. Among them the harmonic mean is perhaps the most widely used [2, 6, 7]. The Kirchhoff approximation [4, 8] is perhaps the newest as far as the present authors know. In order to simplify discussion and comparison with the method suggested in the later part of this article, the arithmetic mean method and both of these two newer methods are described here. 80

### The Arithmetic Mean Method

In the arithmetic mean method, a linear distribution of diffusion coefficient is supposed over the region of two neighboring grid nodes, and thus the control-surface diffusion coefficient can be calculated by

$$\Gamma_w = \Gamma_W + (\Gamma_P - \Gamma_W) \frac{(\delta x)_w^-}{(\delta x)_W} \quad (4)$$

with similar expressions for the other control surfaces. This method, as has been

repeatedly proved, is not a very good approach due to its inability to handle a discontinuity of diffusion coefficient, and is now very rarely used [2, 4, 6].

### The Harmonic Mean Method

The harmonic mean method basically reflects the requirement that diffusion flux should be the same even when calculated by different representative portions of the region concerned. For example, the diffusion flux should be the same at the control surface  $w$  no matter whether it is calculated by considering the portion  $W-w$  or  $w-P$  or  $W-P$ . This leads to the following expression for the control-surface coefficient: 95

$$\Gamma_w = \frac{\Gamma_W \Gamma_P}{\Gamma_P - (\Gamma_P - \Gamma_W) [(\delta x)_w^+ / (\delta x)_w]} \quad (5)$$

with similar equations for the other control surfaces.

This method, as we have pointed out in the Introduction, is the most widely used approach in numerical heat transfer because it gives a reasonable result when it is used to simulate those problems with discontinuity of diffusion coefficient. However, as we shall prove, this method is not very effective and even could not produce a physically true result under some special conditions due to its very large error in approximating control-surface diffusion coefficients. 100

### The Kirchhoff Approximation

The Kirchhoff approximation method, as its name indicates, is based on the Kirchhoff transformation for variable-property problems. The Kirchhoff transformation is defined by 105

$$\tilde{\phi} = \int_{\phi_{\text{ref}}}^{\phi} \Gamma(\phi) d\phi \quad (6)$$

which transforms a diffusion-type differential equation with a variable diffusivity into an equation with a constant “diffusivity” [9]. By using this transformation, Voller and Swaminathan [4, 8] were able to define the following approximation for the control-surface diffusion coefficient: 110

$$\Gamma_w = \frac{1}{\phi_P - \phi_W} \int_{\phi_W}^{\phi_P} \Gamma(\phi) d\phi \quad (7)$$

with similar definitions for the other control surfaces. From Eq. (7) one can find that this approximation method actually sets the diffusion coefficients at the control surfaces equal to the integral mean values of diffusion coefficients between the values of the dependent variables at the neighboring grid points. 115

The Kirchhoff approximation is the most accurate approach to the control-surface diffusivities. It will give an accurate prediction of the control-surface diffusion coefficients since the Kirchhoff transformation can change the variable-property problems into constant ones under some conditions. However, as one can understand, it will lose its veracity for more general problems. Furthermore, it is inconvenient to use because of the need to complete the integral in Eq. (7), though Voller and Swaminathan [4] argued that the additional computation in using Eq. (7) over the harmonic or arithmetic-average approach is relatively small and sometimes can be offset by its rapid convergence. Therefore, though the method is accurate, it has not been widely used yet.

### The Proposed Method

From the derivation of the discrete equation of the finite-volume method, one can see that it is the true value of the diffusion coefficient at the control surface, not its average value over the neighboring nodes, that is needed in order to make the solution of the discrete equations possible. This means that a better method can be developed if one can find a way to approximate the value of the dependent variable at the control surfaces. This because once a good approximate value of the dependent variable is obtained, this value can be used to determine the corresponding diffusion coefficient. Recalling that a linear distribution is actually proposed within the neighboring nodes in the discretization of Eq. (1) by the finite-volume method, it is quite natural to use a linear interpolation to determine the control-surface value of the dependent variable and use this value to calculate the control-surface diffusion coefficient. Hence we propose the following approximation method for the control-surface diffusion coefficients:

$$\left. \begin{aligned} \Gamma_w &= \Gamma(\phi_w) \\ \phi_w &= \phi_W + (\phi_P - \phi_W) \frac{(\delta x)_w^-}{(\delta x)_W} \end{aligned} \right\} \quad (8)$$

with similar expressions for the other control-surface diffusion coefficient.

One should find no difficulty in using the above approximation if the diffusion coefficient is a continuous function of dependent variables and space coordinates. However, if the diffusion coefficient has a discontinuity with dependent variable or space coordinate (for example, in the case of composite materials), the discretization grid should be arranged in such a way that the abrupt-change interface should not be superposed with the control surface. This sometimes may make us feel uncomfortable, since we have become used to the harmonic mean method, which usually requires that no nodes should be placed on the abrupt interface. However, more recent work [6] has proved that if the nodes are set to the position of abrupt-change interfaces with a finer modification in calculating the node values of the diffusion coefficient, then a better result can be obtained with the harmonic mean method. Hence it is suggested that the abrupt-change interfaces should not be used as control-volume surfaces to avoid unnecessary troubles.

## NUMERICAL VERIFICATION

Since we are concerned mainly with the numerical treatment of diffusion terms in diffusion-convection equations, several diffusion-type problems that can be solved analytically were designed. In order to simplify the numerical procedure and to express the results more clearly, most of the problems that are used here to verify the effectiveness of the proposed method are one-dimensional. Two-dimensional results are also presented to prove the applicability to multidimensional problems of the proposed method. 160

### One-Dimensional Problems

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The one-dimensional problems were designed based on the following steady-state convection-diffusion model:

$$\left. \begin{aligned} F \frac{d\phi}{dx} &= \frac{d}{dx} \left( \Gamma \frac{d\phi}{dx} \right) \\ \phi|_{x=0} &= \phi_0 \\ \phi|_{x=2} &= 1.0 \end{aligned} \right\} \quad (9)$$

With Eq. (9) and different values of  $F$ ,  $\Gamma$ , and  $\phi_0$ , eight different problems were designed and are listed in Table 1 for quick reference. All these problems can be solved easily by analytical methods, and their solutions are omitted here to save space. 170

**Table 1** Values of  $F$ ,  $\Gamma$ , and  $\phi_0$  in Eq. (1) for the designed problems

Problem	$\Gamma$	$\phi_0$	$F$
A	$\Gamma = \phi^3 \quad 0 \leq x \leq 2$	0.2	0
B	$\Gamma = \begin{cases} \phi^3 & 0 \leq x < 1 \\ 100\phi^3 & 1 \leq x \leq 2 \end{cases}$	0.2	0
C	$\Gamma = \begin{cases} \phi^3 & 0 \leq x < 1.0075 \\ 100\phi^3 & 1.0075 \leq x \leq 2 \end{cases}$	0.2	0
D	$\Gamma = \begin{cases} 1 & 0 \leq x < 1 \\ 100 & 1 \leq x \leq 2 \end{cases}$	0.2	0
E	$\Gamma = \begin{cases} 1 & 0 \leq x < 1.0555 \\ 100 & 1.0555 \leq x \leq 2 \end{cases}$	0.2	0
F	$\Gamma = \begin{cases} \phi^3 & 0 \leq x < 1 \\ 100\phi^3 & 1 \leq x \leq 2 \end{cases}$	0.2	1
G	$\Gamma = \phi^3 \quad 0 \leq x \leq 2$	0.0	0
H	$\Gamma = \begin{cases} \phi^3 & 0 \leq x < 1 \\ 100\phi^3 & 1 \leq x \leq 2 \end{cases}$	0.0	0

**Two-Dimensional Problems**

The two-dimensional problems are used to prove that the conclusions drawn from the one-dimensional problems are also correct for multidimensional problems. 175 Hence the following very simple problem was designed:

$$\frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma \frac{\partial \phi}{\partial y} \right) = 0 \tag{10}$$

$$\phi|_{x=0} = \phi|_{y=0} = 0.2 \tag{11}$$

$$\phi|_{x=1} = \phi|_{y=1} = 1.0 \tag{12}$$

with 180

$$\Gamma = \phi^3 \quad \text{for Problem (I)} \tag{13}$$

or

$$\Gamma = \begin{cases} \phi^3 & 0 \leq x < 0.5 \\ 100\phi^3 & 0.5 \leq x \leq 1 \end{cases} \quad \text{for Problem (J)} \tag{14}$$

**Numerical Calculation** 185

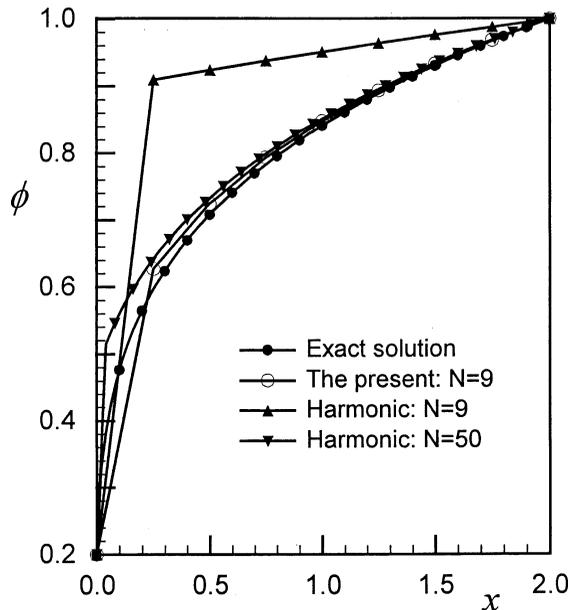
There are two basic methods of discretization of the computational domain in the finite-volume method. One is so-called method A [3] or the cell vertex scheme [10], in which a certain number of nodal points are positioned over the computational domain first and then the control-volume surfaces are set at the midpoint of the neighboring nodes. Another is method B [3] or the cell-centered scheme 190 [10], in which the whole computational domain is divided into a certain number of control volumes and then the nodal points are placed at the center of each control volume. Since method A is more convenient to use than method B for the problems with first-kind boundary conditions, as in our example problems, all the following results are based on the cell vertex scheme. 195

Both Eqs. (9) and (10) are discretized by the finite-volume method. The diffusion terms are formulated with the second-order central difference scheme, and the convection terms are discretized with the second-order upwind scheme [2]. The resulting nodal equations are solved by the tridiagonal matrix algorithm (TDMA) method for the one-dimensional problems and by the alternating direction implicit 200 (ADI) line iteration method for the two-dimensional problems. All the results are obtained with an accuracy requirement such that the largest absolute deviation between two successive iterations is smaller than  $0.5 \times 10^{-6}$ . As mentioned earlier, the arithmetic mean method is not effective in dealing with abrupt-change problems and the Kirchhoff approximation method is inconvenient to use, and therefore the 205 present method is compared only with the harmonic mean method.

## RESULTS AND DISCUSSION

Problem A and Problem B were designed to examine the ability of the various methods to treat variable-property diffusion problems. Problem A is of one material and its diffusion coefficient is a continuous function of dependent variable  $\phi$  and thus of space coordinate  $x$ , while Problem B is of two different materials and has an abrupt change at the interface of the two materials. Figures 2 and 3 present the comparisons of the present method with the harmonic mean method. The number of nodes that are used to carry out each calculation are indicated in these figures with capital  $N$ . It should be pointed out that an even number of the grid nodes is used to ensure that the abrupt-change interface of the composite materials coincides with a control surface in the case of the harmonic mean method, while an odd number of the grid nodes is used to make the abrupt-change interface be located at a grid node in the case of the present method. As one can see from Figures 2 and 3, the results of these comparisons show clearly that the present method works much better than the harmonic mean method. It should also be mentioned that these problems have also been computed with the Kirchhoff approximation, and slightly better results than those using the present method are obtained. These results of the Kirchhoff approximation are omitted in these figures for clarity.

One may argue that the results of the present method and the harmonic mean for Problem B are not obtained on completely the same basis, since the interface is placed at a control surface in the harmonic mean method and at a grid node in the present method. Hence Problem C is designed. Problem C is the same as Problem B except that the abrupt-change interface position is shifted from  $x = 1$  to  $x = 1.0075$ . This ensures that the abrupt interface position will not coincide with



**Figure 2** Comparisons of the present method with the harmonic mean: Problem A.

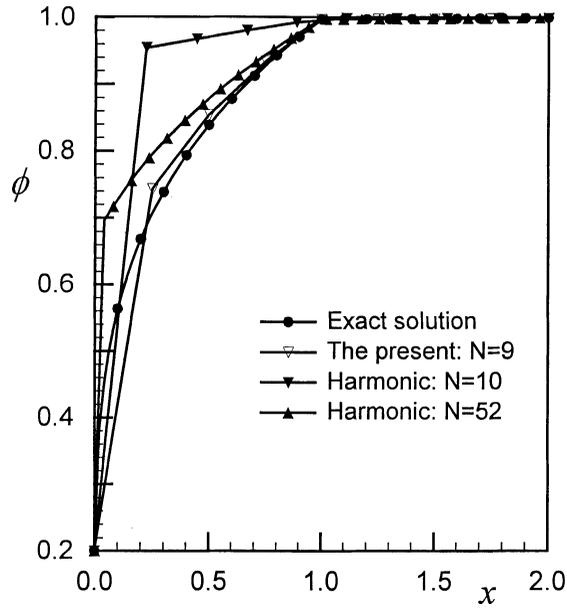


Figure 3 Comparisons of the present method with the harmonic mean: Problem B.

a grid node or a control surface. The abrupt interface is in between a grid node and a control surface. Figure 4 depicts the results of both the present and the harmonic mean method. It clearly shows that the present method is much better than the harmonic mean method.

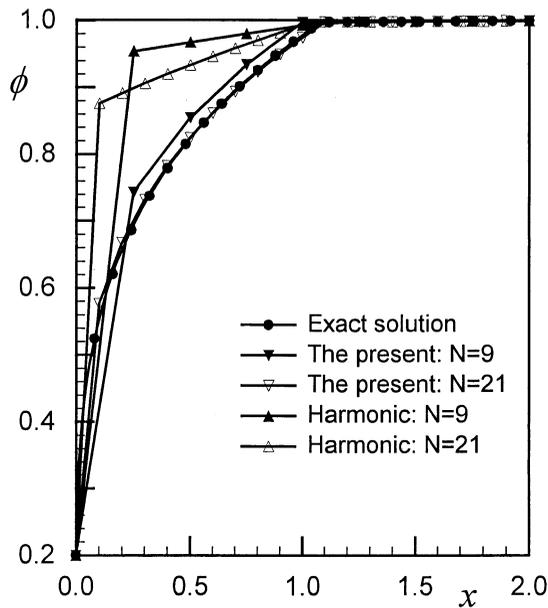


Figure 4 Comparisons of the present method with the harmonic mean: Problem C.

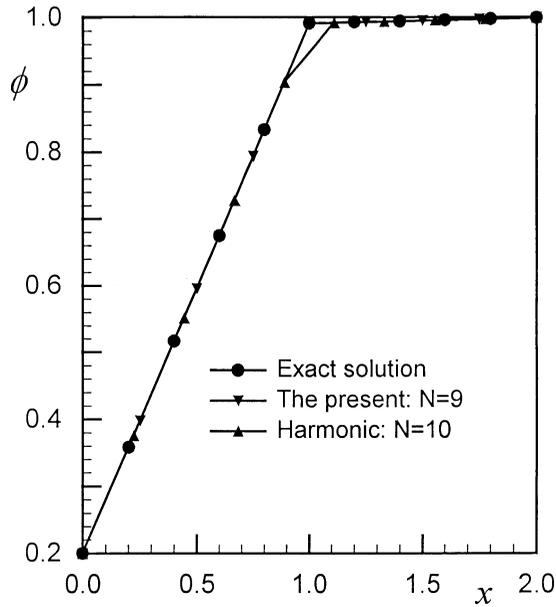


Figure 5 Comparisons of the present method with the harmonic mean: Problem D.

Since the original harmonic mean method was developed for composite materials with a constant diffusion coefficient for each, it will be helpful if the present and the harmonic mean method are compared on such a basis. It is for this purpose that

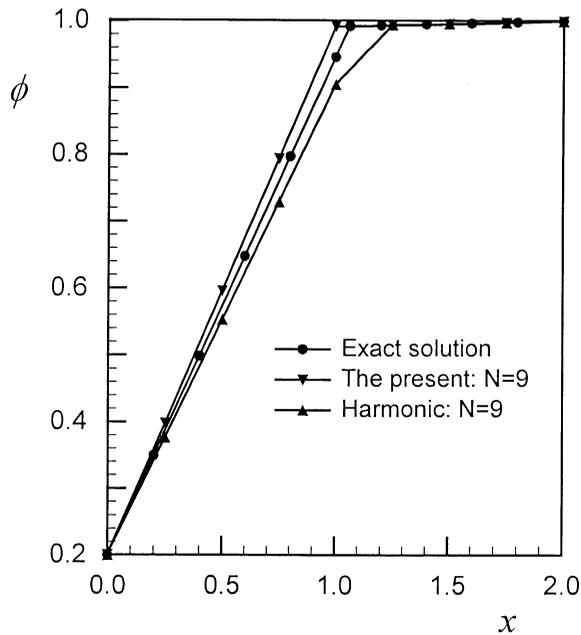


Figure 6 Comparisons of the present method with the harmonic mean: Problem E.

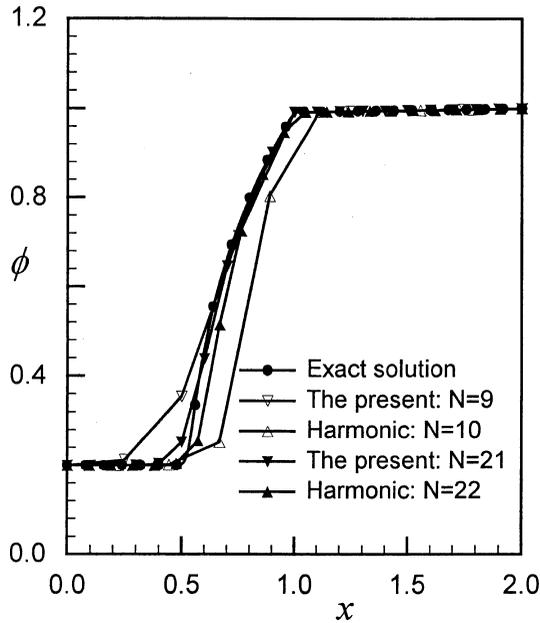


Figure 7 Comparisons of the present method with the harmonic mean: Problem F.

Problems D and E were designed and solved with the present and the harmonic mean method. Again, similar to Problem C, Problem E is used to shift the abrupt-change interface to a position in between a grid node and a control surface. Figures 5 and 6 show again that the present method is superior to the harmonic mean method.

The method is tested against a convection-diffusion problem (Problem F) and the results are shown in Figure 7. Since the method we proposed here can only improve the treatment of diffusion terms, one can expect that the improvement of the present method over the harmonic mean method will be less significant for convection-diffusion problems. The convection effect will certainly suppress the diffusion effect to a less significant position. Nevertheless, the present method still presents a significant improvement over the harmonic mean method as shown in Figure 7. It should be noted that grid Peclet numbers in this calculation are not very small: the largest is equal to 31.5.

The above results prove that the present method is much better than the harmonic mean method. The reason for this, as we have discussed earlier in this article, is due to the fact that what we really need is the true value of the diffusion coefficient at the control surface, not the average value within the neighboring nodes. Therefore the harmonic mean is not so effective if the diffusion coefficient is a strong function of the dependent variable or space coordinates. Actually, by scrutinizing Eq. (5) one can find that the harmonic mean method can produce completely wrong information about boundary conditions: suppose that node  $W$  is a point on a first-kind boundary, and the diffusion coefficient at this point is zero, i.e.,  $\Gamma_w = 0$ ; then Eq. (5) predicts that the diffusion coefficient is also zero at the control surface  $w$ , i.e.,  $\Gamma_w = 0$ . This means that the boundary in discussion is of the second kind, not the first kind,

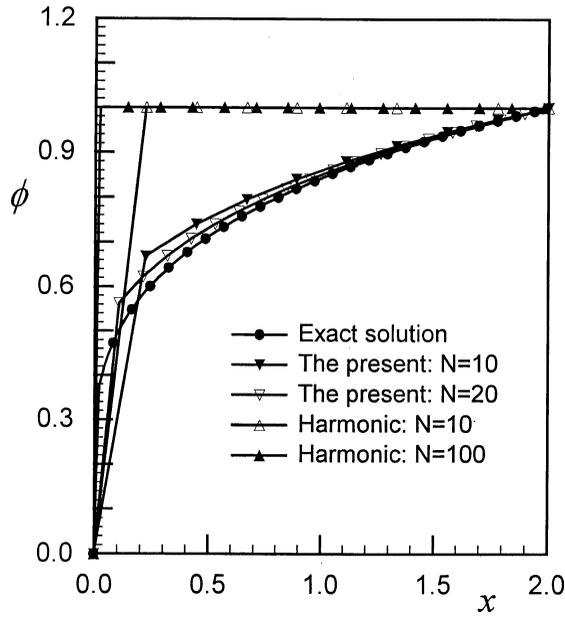


Figure 8 Comparisons of the present method with the harmonic mean: Problem G.

which is entirely wrong. In order to prove this, Problems G and H were designed. These two problems are the same as Problem A and Problem B, respectively, except that the boundary value at  $x = 0$  is set to 0 instead of 0.2, which results in a zero

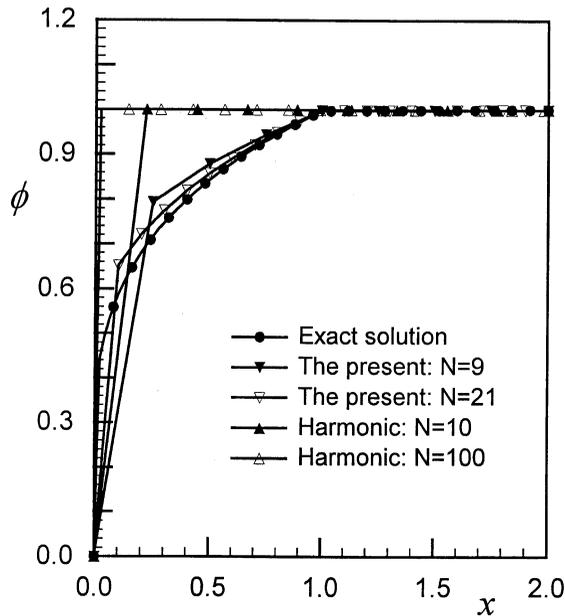


Figure 9 Comparisons of the present method with the harmonic mean: Problem H.

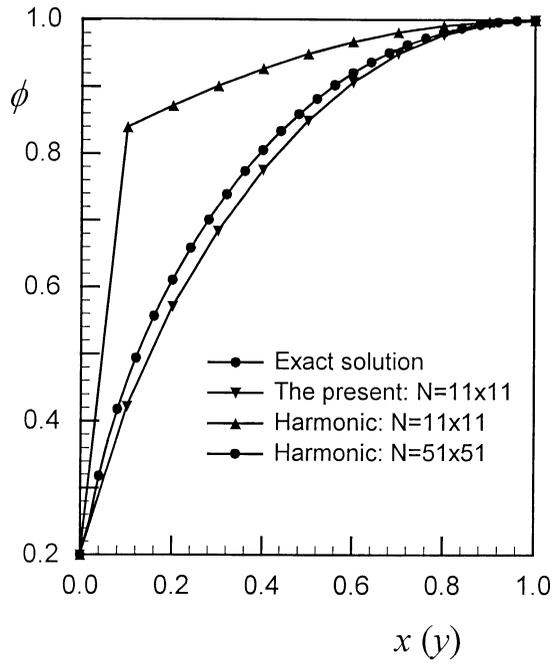


Figure 10 Comparisons of the present method with the harmonic mean: Problem I.

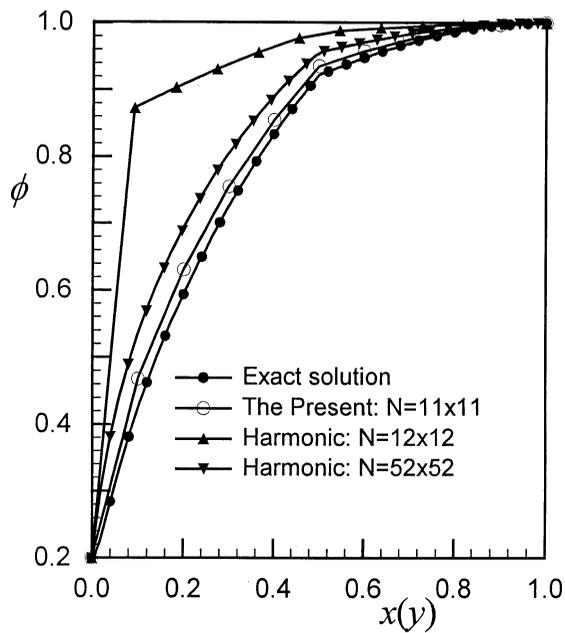


Figure 11 Comparisons of the present method with the harmonic mean: Problem J.

value of diffusion coefficient at  $x = 0$ . The results are shown in Figures 8 and 9, from 265  
 which one can see that although the present method works very well, the harmonic  
 mean method just could not produce physically true results!

The same conclusion can be drawn from the results of the two-dimensional  
 problems (Problem I and Problem J). For conciseness, only the distributions of  
 the dependent variable  $\phi$  along the  $x = y$  diagonal line are depicted in Figures 10 270  
 and 11, which show again that the proposed method can give a much better result  
 than the harmonic mean method.

## CONCLUSION

The main contribution of this study has been the development of a more direct  
 and more effective method for the approximation of diffusion coefficients at control- 275  
 volume surfaces. The extensive numerical examples in this article prove that the pro-  
 posed method, Eq. (8), is much more effective than the widely used harmonic mean  
 method for diffusion-convection problems that incorporate continuous and/or dis-  
 continuous changes of diffusion coefficients. Even for those situations in which 280  
 the harmonic mean method fails to work and could not produce physically true  
 results, the proposed method can still give a very satisfactory prediction. The above  
 conclusion about the method developed in this article is independent of the grid  
 arrangement; i.e., the present method always works better than the harmonic mean  
 method, no matter how grid nodes are arranged. The abrupt-change interface or  
 the discontinuity position of diffusion coefficients can be placed at a grid node or 285  
 between a grid node and a control-volume surface.

In order to avoid unnecessary difficulties in computer programming with the  
 present method, it is recommended that the abrupt-change interface not be placed  
 at a control-volume surface; that is, the abrupt-change interface and the control  
 surface should not be superposed. If such an arrangement is inevitable, then it 290  
 is necessary to identify to which control volume a specific control surface in ques-  
 tion belongs. For example, referring to Figure 1, if the control-volume surface  $w$   
 is also the abrupt-change interface (suppose that the diffusion coefficient at the  
 left side of the interface is  $\Gamma_A$ , and at the right side of the interface it is  $\Gamma_B$ ), then  
 the control-surface diffusion coefficient  $\Gamma_w$  should be set to  $\Gamma_A$  if the control vol- 295  
 ume  $W$  is concerned, and  $\Gamma_w$  should be set to  $\Gamma_B$  if the control volume  $P$  is con-  
 cerned. In this way one can obtain as satisfactory results as with the other grid  
 arrangement.

It should be noted that the Kirchhoff approximation developed by Voller and  
 Swaminathan can produce a slightly better result than the present method for pure 300  
 diffusion problems and a similar result to the present method for the convection-  
 diffusion problem tested in this article. As one can expect for more complex  
 problems, the Kirchhoff approximation will not be able to produce the exact  
 solutions (one should recall that the Kirchhoff transformation can transform a  
 variable-property pure diffusion problem into a constant-property problem, with 305  
 certain limitations). Besides, the Kirchhoff approximation involves an integral calcu-  
 lation and an increase in computation compared with the present method, so it is not  
 recommended compared with the simplicity and effectiveness of the present method.  
 Of course it is the reader's choice which method to use, the present or the Kirchhoff

approximation, since both methods can produce very good results compared with the harmonic mean method. 310

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