SOLVING TWO DIMENSIONAL STEADY STATE CONDUCTION EQUATION WITH DIFFERENT BOUNDARY CONDITIONS USING MONTE CARLO METHOD

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ABSTRACT

During reactor thermal operation, the temperatures of the most doubted hot spots need to be estimated without solving the complete heat conduction equation in a two dimensional problem. A technique using finite difference method and Monte Carlo method is introduced for the evaluation of these temperatures. First, the finite difference method is used to represent the heat conduction equation with an arbitrary volumetric thermal source strength. Second, a discrete set of probabilities for both inner and boundary nodes are determined. A tally is used to follow up the temperatures of the most doubted hot spots. Although the method is time consuming on the computers, it is very powerful for complicated multi boundary conditions problems. A statistical study and error analysis are introduced to evaluate the degree of confidence in the resulting temperature values. The method is powerful if applied with supercomputers and multi-processing computers.

INTRODUCTION

Steady state conduction processes are of interest in the continuous operation of many systems such as furnaces, ovens, reactors, and buildings. Interest generally lies in the temperature distribution and in the energy losses that occur across the walls. These can then be linked with the proper control and operation of the system. The determination of the energy loss is also important in considerations related to thermal insulation and to the heat input needed for the system. In many cases of interest, complex boundary conditions, arbitrary geometry of the conduction region, and material property variation with temperature complicate the problem. Numerical methods then become a must to obtain the information needed for analysis and design.

The most popular techniques for solving such equations are,

(i) finite element method [1,2]
(ii) finite difference method [1,3,4]

(i) Finite element methods:

A finite element method is a mathematical procedure for satisfying a partial differential equation in an average sense over a finite element. All of finite element techniques require that an integral representation of a partial differential equation be constructed. The approaches include variational calculus, methods of weighted residuals, and moments of energy balance [1,2]. The solution requires a well defined sequential process. first, the domain is divided to discretized elements. The number, type, and allocation of elements are often arbitrary. Second, interpolation or shape functions are selected for the elements. Third, the matrix equations for an individual element are formulated using the integral statement for the element as a guide. Fourth, the matrix equations for the overall system consisting of all the elements are assembled. Fifth, the global equations are solved. For steady state problems, the system is solved for the nodal values of temperatures [1,2,3]. The flexibility of the finite element approach permits the development of general - purpose codes. Many such codes are available for direct usage. [2]

(ii) Finite difference methods:

The finite difference method has been one of the most widely used numerical methods for decades. Its popularity may be due to the fact that mathematical concept of its discretization is relatively simple. Discretization is defined as an approximation procedure in which a continuous domain is replaced by a network or mesh of discrete points, and the field of unknowns are sought only at these discrete points rather than every where in the domain [1,5]. First, the domain is divided into discretized nodes. Second a suitable finite difference scheme is chosen to represent the partial differential equation at each node. This procedure results in a set of linear algebraic simultaneous equations for the network. Third, solving this set of equations gives the temperature values at the nodal points. Many methods are used to solve the resulting set of equations like, iterative methods [5,7], and direct methods [1,5]. As the network nodes number increases, the solution needs a large computation memory and a massy computational CPU time.

Problem statement and method of solution

The steady state conduction equation in cartesian coordinates takes the form

$$\frac{\partial}{\partial x}(k\frac{\partial \phi}{\partial x})+\frac{\partial}{\partial y}(k\frac{\partial \varphi}{\partial y})+q^{///}=0$$

where ϕ is the temperature, q''' is the volumetric thermal source strength, and k is thermal conductivity of the material. Finite difference schemes are frequently used to approximate such equation. The result is a set of linear algebraic equations for nodal unknowns with information from a continuous medium replaced by information at discrete nodal points. The difference equations can often be solved under conditions when differential equations themselves cannot be solved by exact or closed form analytical procedure. The difficulty in solving finite difference equations arises in the application of complex geometric boundaries.

The general form of finite difference using control volume technique in an inner node is,

$$K_{i-1,j}(\phi_{i-1,j}-\phi_{i,j})+K_{i+1,j}(\phi_{i+1,j}-\phi_{i,j})$$

$$+K_{i,j-1}(\phi_{i,j-1}-\phi_{i,j})$$

$$+K_{i,j+1}(\phi_{i,j+1}-\phi_{i,j})+q'''\Delta x\Delta y=0$$

Defining

$$K_{i,j}=K_{i,j-1}+K_{i,j+1}+K_{i+1,j}+K_{i-1,j}$$

then,

$$\phi_{i,j}=\frac{K_{i-1,j}}{K_{i,j}}\phi_{i-1,j}+\frac{K_{i+1,j}}{K_{i,j}}\phi_{i+1,j}$$

$$+\frac{K_{i,j-1}}{K_{i,j}}\phi_{i,j}+\frac{K_{i,j+1}}{K_{i,j}}\phi_{i,j+1}$$

$$+S(i,j)$$

where

$$S(i,j)=\frac{q^{///}\Delta x\Delta y}{K_{i,j}}$$

$$K_{m,n}=\frac{1}{R[(m,n),(i,j)]}$$

Where

$K_{m,n}$ = the thermal conductance between nodes (m,n) and (i,j).
R[(m,n),(i,j)] = thermal resistance between node (m,n) and node (i,j).
(m,n) = one of the nodes surrounding node (i,j).
The conductance matrix is a symmetric dominant diagonal matrix [3]. It is needed only to generate half of the matrix elements and the reset is generated using symmetricity property.

Probability formulation

The problem turns to a set of linear equations to be solved numerically. These equations can be written in the form,

$$\phi ij=PD(i,j)\,\phi_{i-1,j}+PU(i,j)\,\phi_{i+1,j}$$

$$+ PL\ (i,j)\ \phi_{i,j-1} + PR\ (i,j)\ \phi_{i,j+1} + S\ (i,j) \qquad (3)$$

The coefficients of temperature can be viewed as discrete probability set for random walks of a fictitious (pseudo) particle.This is shown in Figure (1). These random walks start at the point of interest for which the temperature value is estimated. The random walks are terminated at specified temperature boundaries either for the medium or convective coolant at the boundary only. Steps in the walk from one node to an adjacent node in the lattice points are taken by random sampling techniques from the finite difference equations. A tally is made for each walk, from which the solution $\phi_{i,j}$ is estimated [6]. The tally depends on the transition probabilities between successive points of the random walk, the source term at each point, and the boundary condition of the problem. The discrete probabilities are

$$PL\ (i,j) = \frac{K_{i,j-1}}{K_{i,j}}$$

$$PR\ (i,j) = \frac{K_{i,j+1}}{K_{i,j}}$$

$$PD\ (i,j) = \frac{K_{i-1,j}}{K_{i,j}}$$

$$PU\ (i,j) = \frac{K_{i+1,j}}{K_{i,j}}$$

$$S\ (i,j) = \frac{q'''_{i,j}\ \Delta x \Delta y}{K_{i,j}} \text{(for inner node)}$$

But for specified heat flux boundary node, the source term is given as,

$$S(i,j) = \frac{q'''_{i,j}\Delta x \Delta y + \text{heat added throught the boundary}}{K_{i,j}}$$

An illustration for these probabilities for an inner node is given in Figure (1).

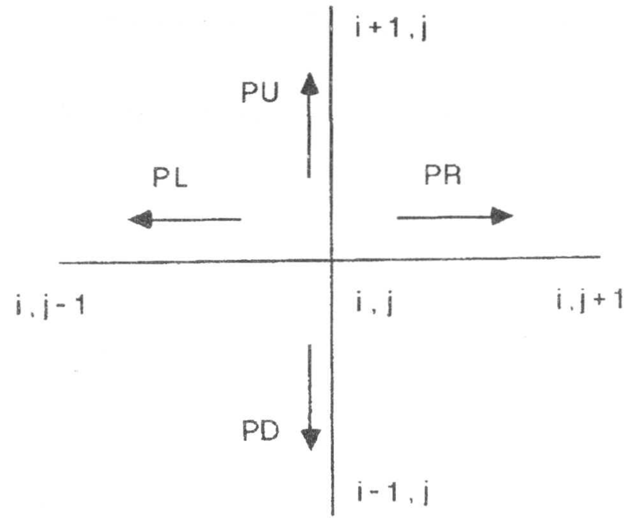


Figure 1. Probability distribution around node (i,j).

Tally and Temperature calculations

let a fictitious particle start a random walk at the point where the temperature is required to be estimated. The conditions of the walk are that if the particle is momentarily at the arbitrary point the probabilities of stepping to one of the surrounding adjacent nodes are PU, PD, PL, and PR respectively. When the particle moves to another node the source term of the node is added to the tally and the four probabilities of the new node are used for the next random walk. The walk is terminated at specified temperatures and convective boundary only. This procedure is considered as one history. If the procedure is repeated by generating more particles at the starting point and performing the random walks up to n-times, then the average value of the tally is considered as an estimation of the required temperature. A flow chart of the used program is shown in Figure (5).

Boundary conditions setting:

Spatial boundary conditions in heat transfer problems are of three types,

(i) Dirichlet function boundary condition,

$\phi = f_1\ (x,y)$ on S_1 (Specified temperature boundary)

(ii) Neumann gradient boundary condition,

$$\frac{\partial \phi}{\partial n} = f_2(x,y) \text{ on } S_2 \quad \text{(Specified heat flux)}$$

(iii) Mixed boundary condition,

$$a\ (x,y)\ \phi + b\ (x,y)\ \frac{\partial \phi}{\partial n} = f_3(x,y) \text{ on}$$

S_3(Convective boundary)

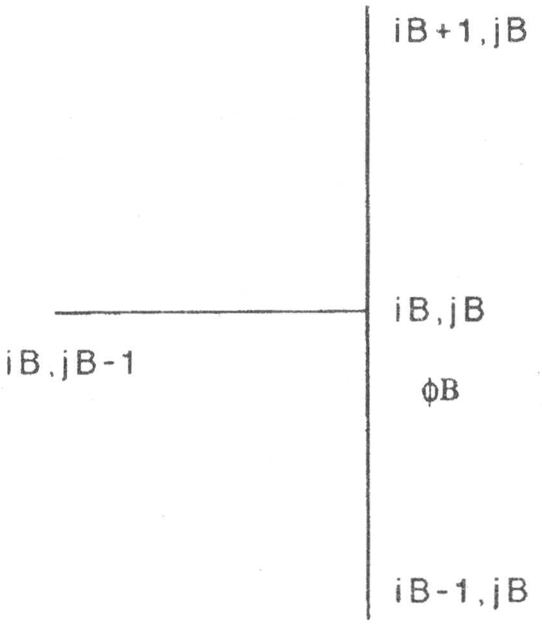


Figure 2. Specified temperature boundary node (iB, jB).

Where S_1, S_2, and S_3 denote three separate zones on the boundary surface S.

(i) Dirichlet function boundary condition:
This boundary condition is illustrated in Figure (2)

$$\phi_B = \phi_o$$

The random walk is terminated when reaching to a specified temperature without adding the source term at the boundary cell. The tally Z_i of the random fictitious particle i takes the form

$$Z_i = \sum S_m(i,j) + \phi_o$$

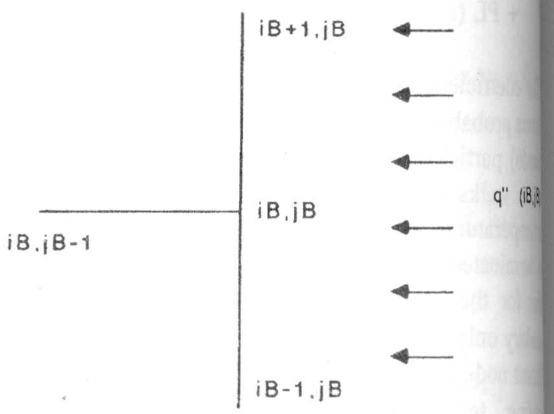


Figure 3. Specified heat flux boundary node (iB, j

where the summation is over the total random walks one particle till termination.

$$Z = \sum_{i=1}^{n} Z_i$$

where n = total number of particles generated at no (i,j) and m represents the steps moved in the history except for the boundary point. ϕ_o represent t boundary node temperature. Z is the summation of t tally for all histories. The temperature of the node (i where the fictitious particle is generated; is then giv by,

$$\phi_{i,j} = \frac{Z}{n}$$

The source term in Dirichlet boundary condition termination node is zero.

$$S\ (i_B, j_B) = 0$$

(ii) Neumann gradient boundary condition.
This boundary condition is illustrated in Figure (Assuming that the surface ,S_B , boundary has specified heat flux, q", at the node [iB, jB]. The fo of the finite difference equation for the node is,

$$\phi_{iB,jB} = PL(iB,jB)\ \phi_{iB,jB-1} + PR(iB,jB)\ \phi_{iB,jB+}$$

$$+ PU(iB,jB)\ \phi_{iB+1,jB}$$

$$+ PD(iB,jB)\ \phi_{iB-1,jB} + S\ (iB, jB)$$

Where PL,PU,PD, and PR have their usual meaning and

$$S(iB,jB) = \frac{q''' \frac{\Delta x}{2} \Delta y}{K_{iB,jB}} + \frac{q'' \Delta y}{K_{iB,jB}}$$

$K_{iB,jB}$ = sum of thermal conductance of surrounding nodes.

$K_{iB,jB-1}$ = thermal conductance between node (iB,jB-1) and (iB,jB)

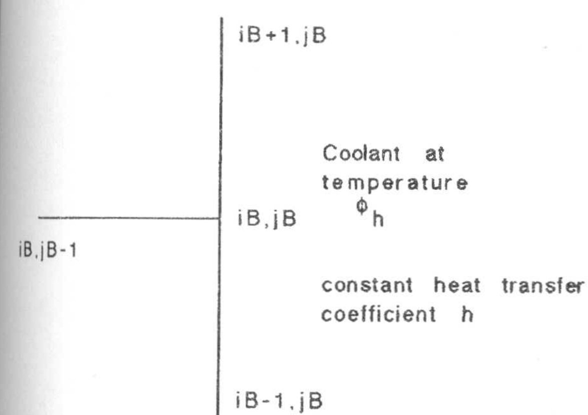


Figure 4. Convective boundary node (iB, jB).

So in Neumann gradient boundary condition the node source term is increased by the amount of heat flux in, and the probability distribution is evaluated, then the walk is continued. There is no history termination with this boundary condition. A special case of the specified heat flux boundary is the insulated boundary condition where the boundary heat flux is zero. For example, the source term of the Neumann boundary node for insulated boundary is similar to an inner node.

(iii) Mixed boundary condition

This boundary condition is illustrated in Figure (4). Assuming that the boundary is a convective boundary condition at the node (iB, jB). The average heat transfer coefficient is a constant h. and the coolant temperature is ϕ_h. The finite difference equation takes the form,

$$\phi_{iB,jB} = PU(iB,jB)\phi_{iB+1,jB} + PL(iB,jB)\phi_{iB,jB-1}$$
$$+ PR(iB,jB)\phi_h + PD(iB,jB)\phi_{iB-1,jB} + S(iB,jB)$$

For this boundary condition the source term of the boundary node is added to the tally, then a random number is generated and compared with the probabilities estimated. If the generated random number directs the fictitious particle to the coolant the tally is increased by an amount equal to the value of the temperature of the coolant, and the history is terminated. Otherwise the random walk procedure is continued for the same history by adding the source term of the new node in the random walk

DISCUSSION AND CONCLUSIONS

The method has been applied to a 10m by 10m two dimensional problem for the following cases,

(i) Four specified boundary temperatures with 50,100, and 200 generated particles.
(ii) Two specified temperatures, and two insulated boundaries with 50,100, and 200 generated particles.
(iii) Two specified temperatures and two convective boundaries with convective heat transfer coefficient ,h, of 100 W/m ^{2}.°C

In these cases the specified temperatures are taken as 100 °C, while the source term is taken as 100 W/Cu.M.

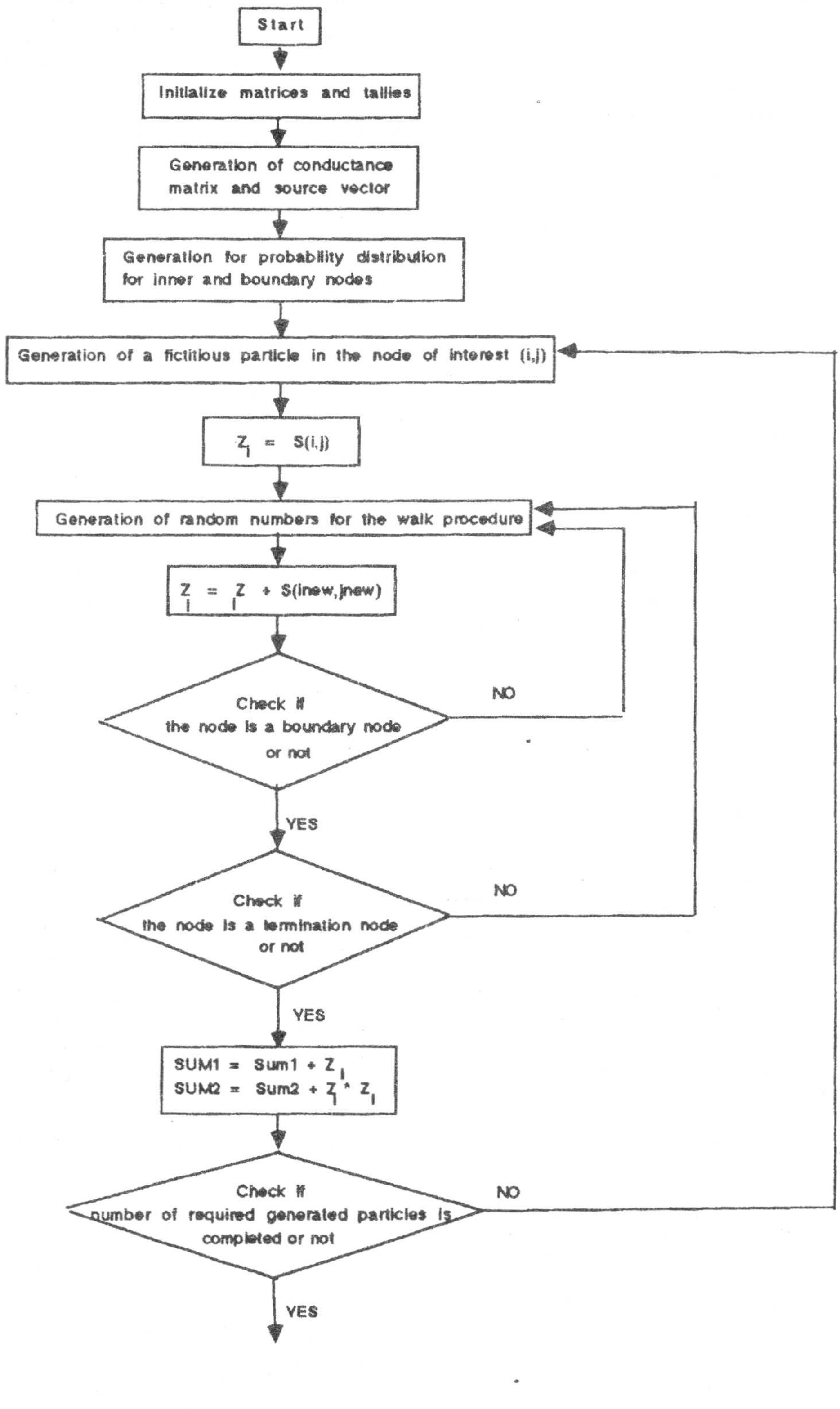
The results are compared with the corresponding finite difference solution. They show an error in Monte carlo results less than 5% when 200 generated particles are used.

The error decreases as the number of generated particles per node increases.

Figures (6),(7), and (8) show the temperature distribution versus X-position at a cross section y of y = 1m for different cases.

Figure (6) shows the temperature distribution for four specified temperature boundaries. The error is maximum for 50 generated particles per node. The error decreases as the number of generated particles increases. The maximum error appears at the central nodes of the cross section. It is less than 10% for 50 histories, and less than 5% when 200 histories are used. The percentage error drops as the number of generated histories per node increases.

Figure (7) shows the temperature distribution in the case of two insulated, and two specified temperature boundaries with different number of generated histories. Although the maximum error is still at the central nodes, the agreement with finite difference solution is excellent. The percentage error is less than 1% for 200 generated histories. This can be explained on the bases of Monte Carlo method by the effect of termination of the generated particles on the solution.


Start
Initialize matrices and tallies
Generation of conductance matrix and source vector
Generation for probability distribution for inner and boundary nodes
Generation of a fictitious particle in the node of interest (i,j)
Z_i = S(i,j)
Generation of random numbers for the walk procedure
Z_i = Z_i + S(inew,jnew)
Check if the node is a boundary node or not
NO
YES
Check if the node is a termination node or not
NO
YES
SUM1 = Sum1 + Z_i
SUM2 = Sum2 + Z_i * Z_i
Check if number of required generated particles is completed or not
NO
YES

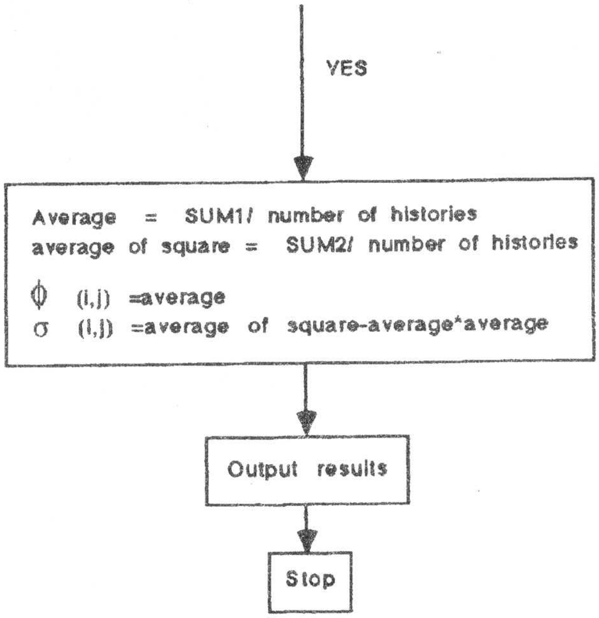
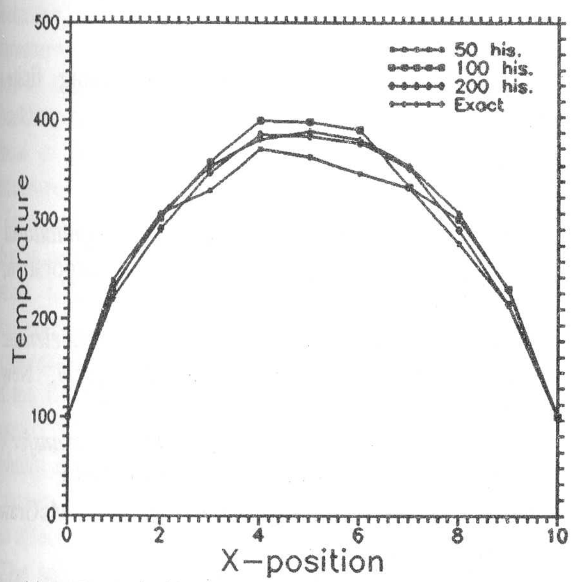
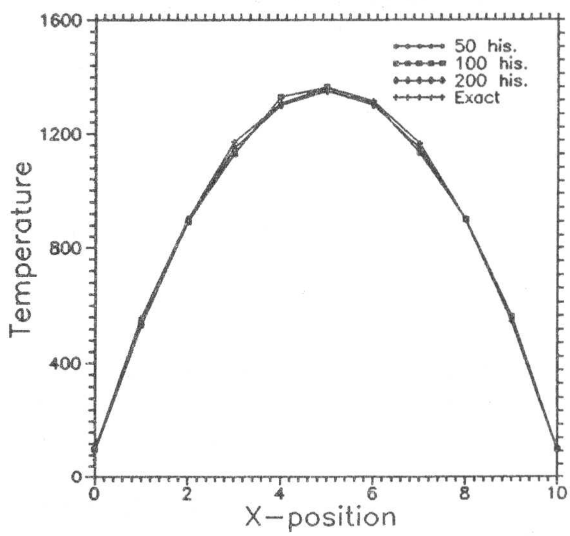


Figure 5. Flow chart of the Monte carlo procedure for temperature evaluation.



Figure(6) − Four specified boundary temperatures with 50,100 ,and 200 generated particles, and finite difference solution

The insulated boundary does not cause termination, while the specified temperature boundary causes termination of the history. With the same number of generated histories, the more the tally is, the more accurate the results are. If the same accuracy is required for four specified temperature boundaries, a higher number of generated particles should be used. This indicates that the accuracy is sensitive to boundary conditions. The faster the history termination is, the lower the accuracy is.



Figure(7) − Two specified temperatures and two insulated boundaries with 50,100,200 generated particles, and finite difference solution

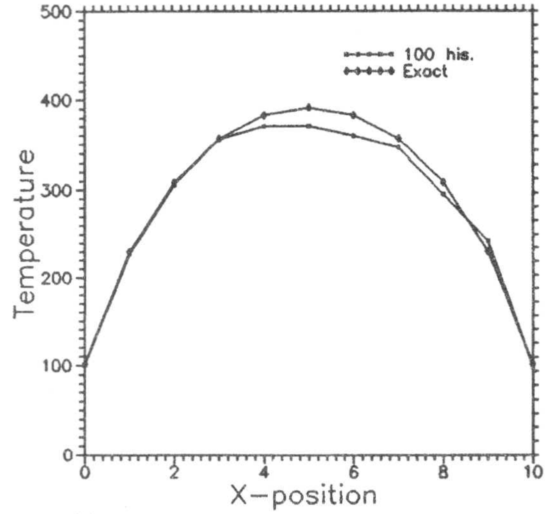
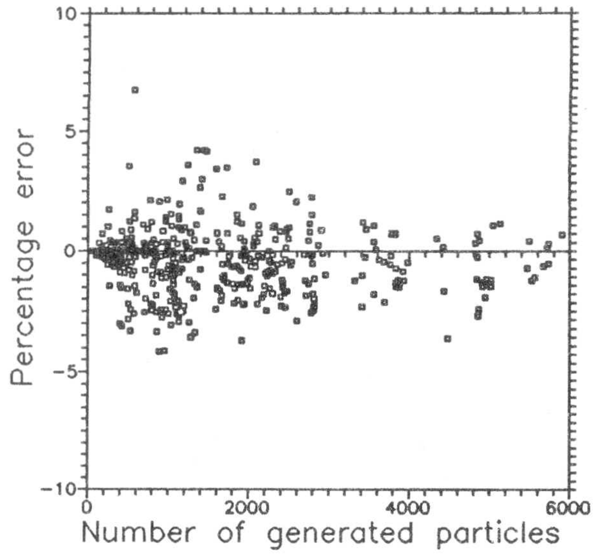


Figure (8)- Two convective and two specified temperature boundaries with 100 generated particles, and finite difference solution

Figure (8) shows the temperature distribution in the case of two specified temperature, and two convective boundaries with 100 generated histories. The inner nodes show maximum error less than 10%.



Figure(9) Percentage error versus number of generated particles.

Figure (9) shows the effect of increasing number of generated histories on the error. The percentage error decreases as the number of generated histories per node increases.

Figures (10), and (11) show the solution surfaces for both Monte Carlo and Finite Difference methods. They show a good agreement of overall behavior of both solutions.

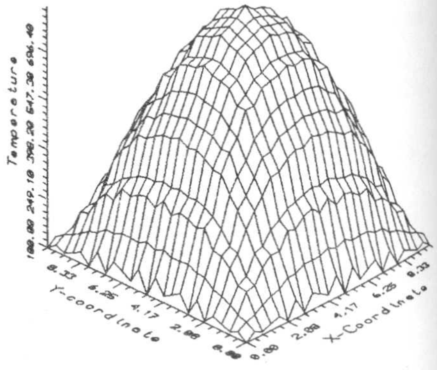


Figure 10. Temperature distribution using Monte Ca[rlo] method.

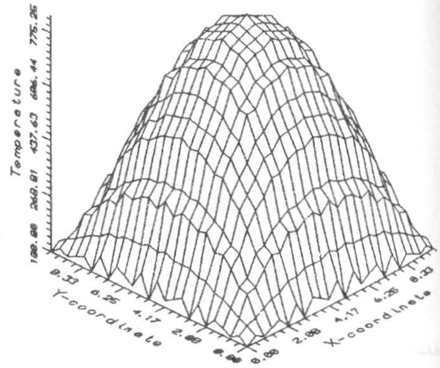


Figure 11. Temperature distribution using fi[nite] difference method.

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