Chapter 2. Monte Carlo Ray-Trace Formulation

Many heat transfer problems require the definition of the radiative exchange among surfaces in an enclosure. Even though the formulation of radiation exchange problems is not particularly difficult, the result is usually a set of tedious integral equations or their algebraic equivalent, a large system of coupled linear algebraic equations. Some simplifying assumptions and approximations usually have to be made in order to resolve the inherent mathematical difficulties. For example, the workload may be reduced tremendously by assuming that the medium filling the cavity does not participate in the radiative exchange and that the surfaces behave only as diffuse and gray emitters, absorbers, and reflectors of radiation. These assumptions lead to the definition of configuration factors that account for the geometrical effects. However, since no surface is purely diffuse, the validity of using configuration factors is limited. In 1962 Seban, in a written discussion of a paper by Sparrow *et al.* suggested that the reflectivity of many surfaces of practical engineering interest could be expressed as the sum of a diffuse and a specular component. Using this approximation the reflectivity can be written

$$\rho = \rho^d + \rho^s \tag{2.1}$$

Based on this idea, Mahan and Eskin [1981, 1984] introduced the concept of the *radiation distribution factor*. In his book, Mahan [2002] defines the *total radiation distribution factor* D_{ij} as “the fraction of the total radiation emitted from surface element i that is absorbed by surface element j, due both to direct radiation and to all possible reflections within the enclosure.” This definition includes directional emission and absorption and bidirectional reflection. The model developed in this thesis assumes only diffuse emission and absorption and diffuse-specular reflection and so the *total, diffuse-*

specular distribution factor D'_{ij} is used. This simplifying assumption is often justified in the design and modeling of radiometric instruments by the judicious choice of coatings to be used in the fabrication of the instrument. In other words, the instruments are designed to be amenable to accurate thermal radiative analysis using the total, diffuse-specular radiation distribution factor.

2.1 The Total, Diffuse-Specular Radiation Distribution Factor

The total, diffuse-specular radiation distribution factor D'_{ij} is defined as the fraction of total thermal radiation emitted diffusely from surface element i that is absorbed by surface element j, due to direct radiation and to all possible diffuse and specular reflections within the enclosure. Using this distribution factor, the radiative energy emitted by surface i that is absorbed by surface j may be written as

$$Q_{ij} = \varepsilon_i A_i \sigma T_i^4 D'_{ij} \qquad \text{(W)} \tag{2.2}$$

where ε_i is the hemispherical, total emissivity of surface i, A_i is the area of surface i (m^2), σ is the Stefan-Boltzman constant ($5.6696 \times 10^{-8}\ Wm^{-2}K^{-4}$), and T (K) is the temperature of surface i. Equation 2.2 may be taken as the definition of D'_{ij}. The distribution factor has three useful properties [Mahan, 2002]:

1. Conservation of energy

$$\sum_{j=1}^{n} D'_{ij} = 1.0\,, \quad 1 \le i \le n \tag{2.3}$$

2. Reciprocity

$$\varepsilon_i A_i D'_{ij} = \varepsilon_j A_j D'_{ji}\,, \qquad 1 \le i \le n,\ 1 \le j \le n \tag{2.4}$$

3. Combination of reciprocity and conservation of energy

$$\sum_{i=1}^{n} \varepsilon_i A_i D'_{ij} = \varepsilon_j A_j \qquad 1 \leq j \leq n. \tag{2.5}$$

In Equations 2.3, 2.4 and 2.5, n is the number of surface elements into which the enclosure has been divided, ε is the hemispherical, total emissivity of a given surface element, and A is its surface area.

The conservation of energy relation and the reciprocity relation may be used to detect and eliminate errors made during the estimation of distribution factors or to find unknown distribution factors from known distribution factors (but not both).

It is noted that it is possible to define other distribution factors; for example, if the enclosure has an opening through which radiation may pass, the opening can be treated as a black membrane that absorbs all radiation incident from the interior and through which a power Q_o passes into the enclosure with a specified angular distribution. Then the distribution factor

$$D'_{oj} = Q_{oj}/Q_o \qquad 1 \leq j \leq n \tag{2.6}$$

can be defined where Q_{oj} is the power (W) entering the enclosure through opening o that is absorbed by surface element j.

The value of the distribution factor does not depend solely on geometry but also on the radiative characteristics of the surfaces making up the cavity. This means that it is not possible to use the traditional methods for finding configuration factors to estimate distribution factors. Distribution factors are estimated using the Monte Carlo ray-trace (MCRT) method.

2.2 The Monte Carlo Ray-Trace (MCRT) Method

The discussion in this section is liberally adapted from Mahan [2002].

The Monte Carlo ray-trace (MCRT) method solves radiation heat transfer problems by performing statistical sampling experiments on a computer using random numbers. The method is named after the capital of the principality of Monaco, famous for its casino, because the random numbers could be obtained by dropping a ball in a spinning roulette wheel [Anon, 2002].

The MCRT method is sometimes described as a statistical approach where a "game", or model, with the same behavior of the physical process being modeled replaces the specific problem, producing the same outcome as the physical process but with the advantage that the "game" is easier to play.

In this approach radiation energy emitted from a given surface is divided into a large number N_i of discrete and uniform energy bundles. Thus, solving a thermal radiation problem by the MCRT method implies tracing the history of these bundles from their emission by surface element i, through a series of reflections on other surface elements, to their absorption by one of the surface elements j of the enclosure. Using the properties of the enclosure and the laws of probability it is possible to determine the number of energy bundles N_{ij} emitted by surface i and absorbed by surface j. Then the distribution factors may be estimated as

$$D'_{ij} \cong \frac{N_{ij}}{N_i} \tag{2.7}$$

As N_i becomes increasingly large, the accuracy of the estimate increases. In practice the distribution factor D'_{ij} can be estimated to an arbitrary degree of accuracy using a finite but large value of N_i.

Once all the properties of the surfaces are defined, the MCRT method can be used to determine the value of the distribution factor. The logic flow chart for applying the MCRT method to obtain total, diffuse-specular radiation distribution factors is shown in Figure 2.1. The standard technique is to release a large number of energy bundles from randomly selected locations on a given surface element and then to trace their paths through a series of reflections until they are absorbed by another (or the same) surface element. The number of energy bundles used depends on the required accuracy and on the availability of computer resources. Normally, 100,000 bundles is considered a minimum number to release from each surface of the enclosure for statistically significant results, with one million being common. The normal steps in numerical implementation of the MCRT method are described below. The step numbers refer to the block numbers in the logic flow chart, Figure 2.1

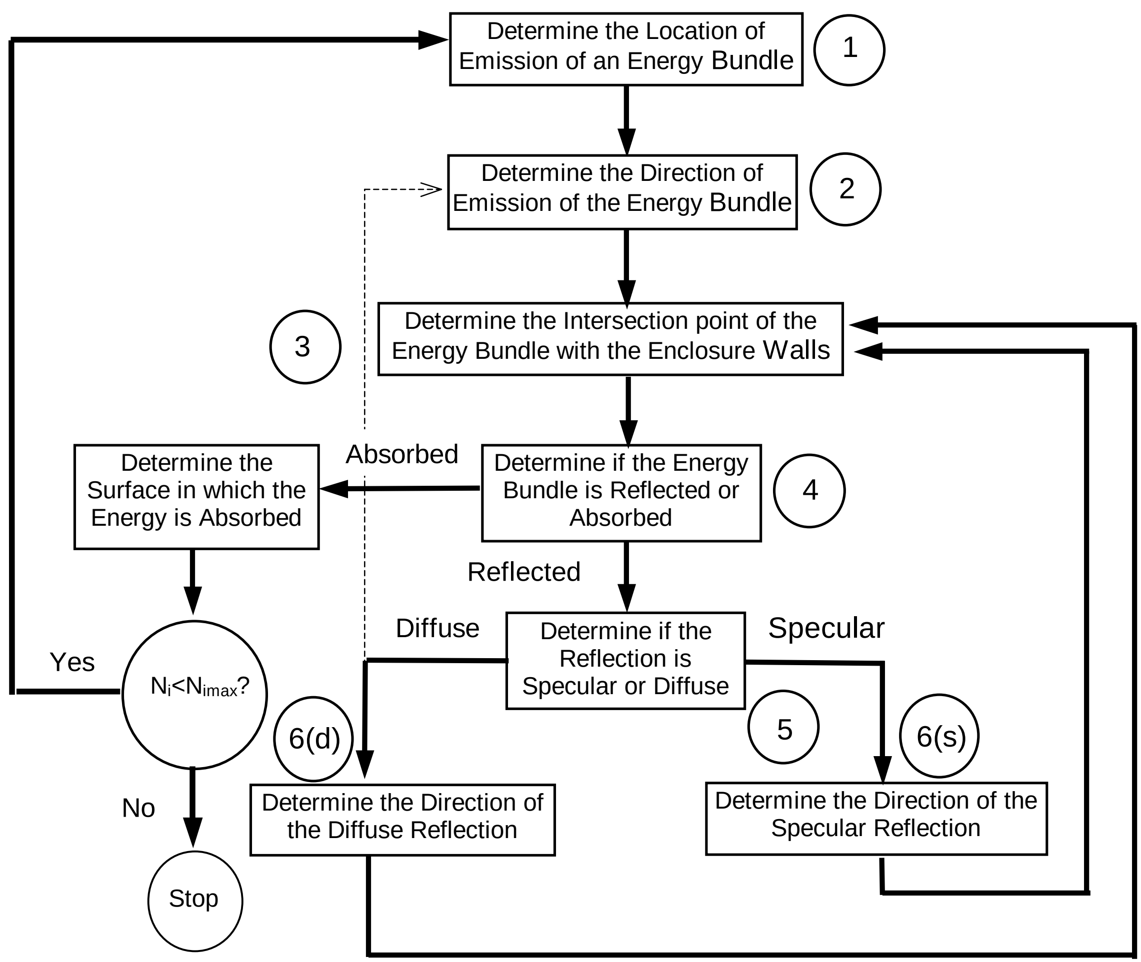

Figure 2.1 Logic flow chart for implementing the Monte Carlo ray-trace method for a given source surface in a diffuse-specular, gray enclosure

1. Determine the location of emission of an energy bundle

In the typical application to radiometric instruments the energy bundle is often not really emitted from a surface element but rather enters the cavity through an opening, the aperture. A pseudo-random number generator is used to generate a very long sequence, usually tens of millions, of highly uncorrelated random numbers uniformly distributed between zero and unity. For further information about pseudo-random number generators the reader is referred to Appendix D in Mahan [2002]. Three random numbers, R_x, R_y, R_z, are drawn sequentially from a population of previously generated random numbers. Then for example in the particular case of a planar rectangular surface, the location of emission is in principle defined by

$$x = x_{min} + (x_{max} - x_{min})R_x \tag{2.8}$$

$$y = y_{min} + (y_{max} - y_{min})R_y \tag{2.9}$$

$$z = z_{min} + (z_{max} - z_{min})R_z \tag{2.10}$$

In Equations 2.8 through 2.10, the subscripts *min* and *max* denote, respectively, the minimum and maximum value of the appropriate coordinate on the surface element. Note that in practice only two of these equations are actually needed to determine the coordinates (x, y, z) of the point of "emission" of the energy bundle, because the third coordinate can be calculated using the equation of the plane,

$$n_x(x - x_0) + n_y(y - y_0) + n_z(z - z_0) = 0 \tag{2.11}$$

In Equation 2.11, n_x, n_y, and n_z are the components of the unit vector normal to the plane, and x_0, y_0, and z_0 are the coordinates of any point on the surface.

2. Determine the direction of emission of the energy bundle.

Sparrow and Cess [1966] give expressions for the direction of diffuse emission as a function of two independent coordinates: the circumferential angle ϕ in the plane of the surface with respect to a local unit surface tangent $\vec{t}$, and the azimuth angle θ with respect to the local unit surface normal $\vec{n}$. These two angles are given by

$$\phi = 2\pi R_\phi \tag{2.12}$$

and

$$\theta = \sin^{-1}\sqrt{R_\theta} \tag{2.13}$$

where R_ϕ and R_θ are two consecutive random numbers uniformly distributed between zero and unity. The angles ϕ and θ and the normal and tangent vectors are used together to determine the direction cosines (l, m, n) of the path along which the emitted energy bundle travels in the global coordinate systems. The direction cosines are defined as

$$l = \cos\alpha \tag{2.14}$$

$$m = \cos\beta \tag{2.15}$$

$$n = \cos\gamma \tag{2.16}$$

where α, β, and γ are the angles that a directed line makes with respect to the coordinate axes x, y, and z, respectively, as shown in the Figure 2.2. Angles ϕ and θ are defined with respect to the local coordinates $(\vec{t}, \vec{n})$, which must be transformed to global coordinates (x, y, z). The relation between the local and global coordinates is shown in Figure 2.3. Vector manipulation and/or coordinate transformation are required to relate $(\vec{t}, \vec{n})$ and (x, y, z), and thus the angles ϕ and θ to the direction cosines (l, m, n). The details of this process are given in Mahan [2002].

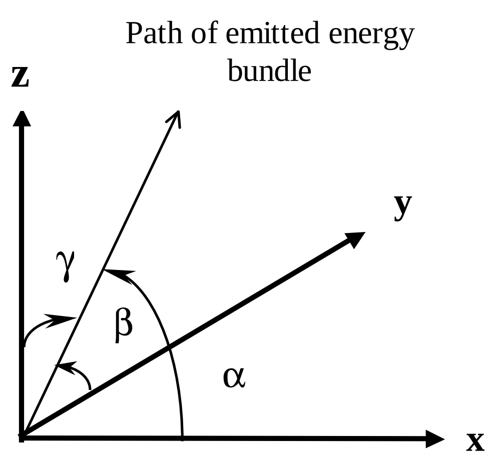

Figure 2.2 Illustration of the direction cosines

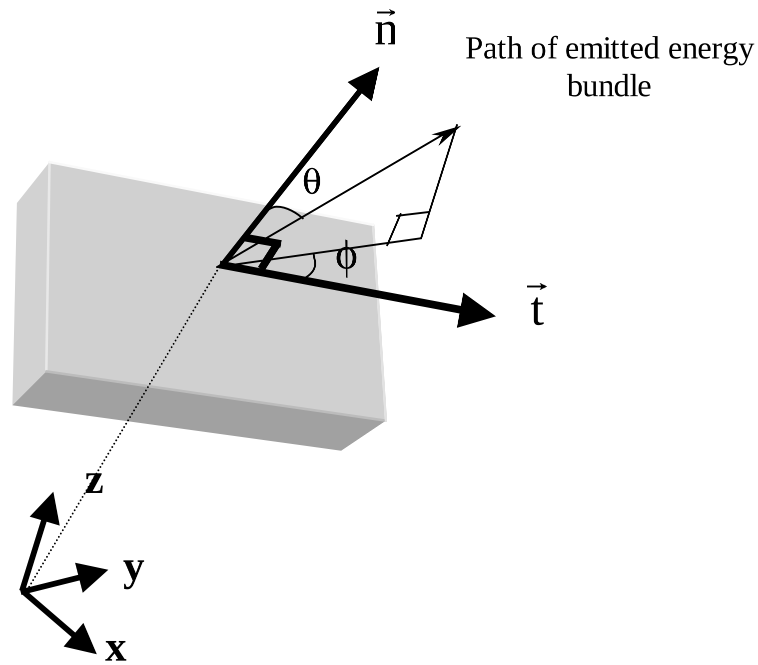

Figure 2.3 Relationship between local and global coordinates

3. Determine the point of intersection of the emitted energy bundle with the enclosure walls

Using the equations of the surfaces that make up the enclosure and the equations of the line for the path along which the energy bundle travels (the “ray”), all the possible points of intersection of the energy bundle with the walls can be found. Because the equations of a line describe an infinitely long line and, in the case of enclosures consisting of planar surfaces, the equations of the surfaces describe planes infinite in extent, many candidate points of interaction will generally be found. Therefore it is necessary to eliminate all of the points of intersection except the one corresponding to the actual intersection of the path of the energy bundle and the enclosure wall. This problem is illustrated in Figure 2.4.

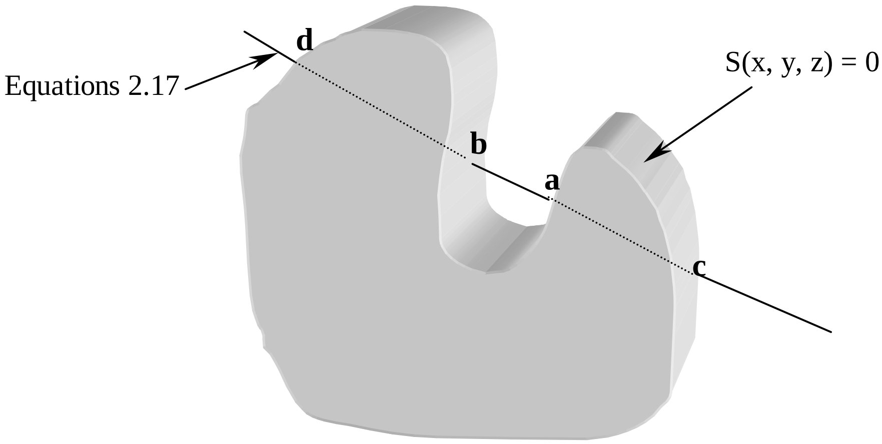

Figure 2.4 Intersections of a straight line with the surfaces of an arbitrary enclosure

In the situation depicted in Figure 2.4, an energy bundle is emitted from Point a in the direction of Point b. The equations of the line are given by

$$T = \frac{x - x_a}{l} = \frac{y - y_a}{m} = \frac{z - z_a}{n} \tag{2.17}$$

where T is the length of the line connecting x_a, y_a, z_a with x, y, z. Equations 2.17 and the equation of each surface of the enclosure, S(x,y,z) = 0, constitute sets of four equations in the four unknowns x, y, z, and T. In the example of Figure 2.4 when Equations 2.17 are solved with the equations of the surfaces, four points are obtained: a, b, c, d. From the figure, it is clear that Point b is the desired point. However, ensuring that the computer "selects" the correct point is a task accomplished through the following three-step process:

1. First, eliminate the point of origin (Point a). This point will always emerge as a candidate. One way to do this is to compare the coordinates of candidate points of intersection between the line and the surface with the coordinates of the emission

point. If these coordinates are the same, within some specified tolerance, this point is rejected.

2. Next, eliminate the "back" candidate (Point c). This may be accomplished by forming the dot product of the outward-directed surface normal $\nabla S(x, y, z)$ with the vector

$$(x_c - x_a)\vec{i} + (y_c - y_a)\vec{j} + (z_c - z_a)\vec{k}$$

directed from the source point toward the candidate point. A positive value of this dot product indicates that the candidate lies in front of the source, while a negative value indicates that the candidate lies behind the source and therefore must be rejected.

3. Finally, choose the nearest candidate from among all the candidates that lie in front of the source. In order to do this, it is necessary to compare the distances from the source to all the candidates in front of it, and then to choose the shortest one. Equation 2.17 gives the distance T between any two points.

Equations 2.17 may be written in the form

$$x = x_a + lT \tag{2.18}$$

$$y = y_a + mT \tag{2.19}$$

$$z = z_a + nT \tag{2.20}$$

The form of Equations 2.18 through 2.20 avoids the possibility of division by zero that could occur if one or two of the direction cosines have values of zero (which occurs whenever the path of an energy bundle is normal to a given coordinate axis).

4. Determine whether the energy bundle is absorbed or reflected

Using the assumption that all surfaces are opaque diffuse-specular, gray reflectors, it is possible to write that

$$\alpha = 1 - \rho = 1 - \rho^d - \rho^s \tag{2.21}$$

where ρ^d is the diffuse component of reflectivity and ρ^s is the specular component.

The absorptivity may be interpreted as the probability that an incident energy bundle will be absorbed. Then each time that an energy bundle intercepts a surface, the next available random number R_α, uniformly distributed between zero and unity, is drawn and compared with the absorptivity. If the random number is less than or equal to the absorptivity, the energy bundle is absorbed; otherwise, it is reflected. If the energy bundle is absorbed, the value of N_{ij} is incremented and control returns to Step 1 with the emission of a new energy bundle. If the energy bundle is reflected, the logic continues to the next step.

5. Determine if the reflection is diffuse or specular

The *specularity ratio* r_s is a surface property, defined as the ratio of the specular component of reflectivity to the reflectivity,

$$r_s \equiv \frac{\rho^s}{\rho} = \frac{\rho^s}{\rho^s + \rho^d} \tag{2.22}$$

This ratio can be interpreted as the probability that a reflection from the surface in question is specular. A random number R_s, uniformly distributed between zero and unity, is drawn and compared with r_s. If R_s is less than or equal to r_s, the reflection is specular; otherwise it is diffuse. If the reflection is specular, the logic branches to Step 6(s), whereas if the reflection is diffuse, the logic branches to Step 6(d).

6(s) Determine the direction of the specular reflection

A reflection is said to be specular when the paths of the incident and reflected energy bundles and the surface normal all lie in the same plane, and the angle between the reflected energy bundle and the surface normal is equal to the angle between the incident energy bundle and the surface normal. These relationships are illustrated in Figure 2.5. The rules illustrated in this figure may be combined to yield

$$\vec{V}_r = \vec{V}_i - 2(\vec{V}_i \cdot \vec{n})\vec{n} = \vec{V}_i + 2\left|\vec{V}_i\right| \cos\theta\, \vec{n} \tag{2.23}$$

where

$$\vec{V}_i = (x_b - x_a)\vec{i} + (y_b - y_a)\vec{j} + (z_b - z_a)\vec{k} \tag{2.24}$$

In Equation 2.24, (x_b, y_b, z_b) are the coordinates of the point where the energy bundle intersects the receiving surface and (x_a, y_a, z_a) are the coordinates of the source point.

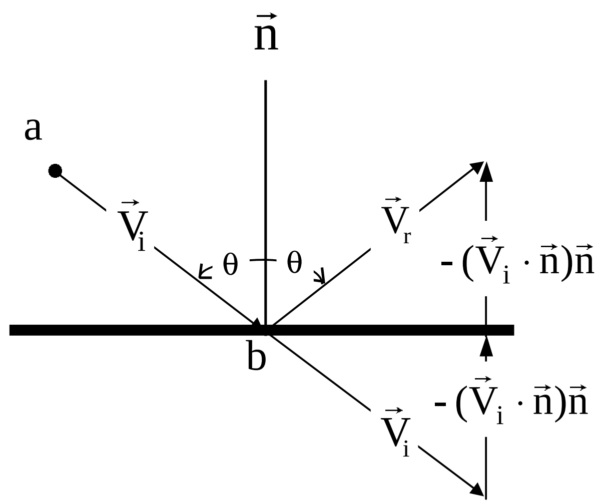

Figure 2.5 Relationship between incident and specularly reflected rays

The result given by Equation 2.23 may be interpreted in terms of the direction cosines. Knowing that the magnitude of the reflected vector is given by

$$T_r = \sqrt{(V_{r,x})^2 + (V_{r,y})^2 + (V_{r,z})^2} \tag{2.25}$$

then

$$l_r = \frac{V_{r,x}}{T_r} \tag{2.26}$$

$$m_r = \frac{V_{r,y}}{T_r} \tag{2.27}$$

and

$$n_r = \frac{V_{r,z}}{T_r} \tag{2.25}$$

6(d) Determine the direction of the diffuse reflection

When an energy bundle is reflected diffusely, it retains no knowledge of its history before suffering the reflection. That is, the energy bundle has been reborn as a newly emitted energy bundle. This means that a diffuse reflection is exactly like a diffuse emission. Then the current logic step would be identical to Step 2, as the dashed line in the block diagram of Figure 2.1 indicates.

The steps described above are repeated for a large number of energy bundles, leading to as a final result the distribution factor estimated by

$$D'_{ij} \cong \frac{N_{ij}}{N_i} \tag{2.29}$$

where N_{ij} is the number of energy bundles emitted by surface i and absorbed by surface j, and N_i is the total number of energy bundles emitted by surface i.

2.3 MCRT in FELIX (**F**unctional **E**nvironment for **L**ongwave **I**nfrared e**X**change)

The majority of the numerical experiments done in this research were carried out using the program FELIX developed by Félix Nevárez-Ayala [2002]. The program receives the geometries from a CAD-based software such as AutoCad© and divides every surface into facets. Each facet is a triangle located in space whose position and orientation are defined by its three vertices and the normal to the facet. Using this approach the intersection point between an energy bundle and a facet can be found by solving simultaneously the equations of the path followed by the energy bundle and the plane that contains the facet. The reader is referred to Nevárez-Ayala [2002] for a more detailed discussion of FELIX.

In this chapter an overview of the Monte Carlo ray-trace method was presented. The theoretical foundations of this method along with the methodology for applying the MCRT method to radiation heat transfer problems were discussed. In the next chapter a statistical protocol for determining the uncertainty associated with estimates of the distribution factors using from the MCRT method is presented.