Fast and flexible gamma dose rate calculation for both three-dimensional fields and arbitrarily discrete positions with shielding effects of buildings[*]

2026-07-16

ChinaRxiv

Abstract

Rapid and accurate gamma dose assessment is crucial for radioactive environmental impact assessment and the optimization of nuclear emergency planning zones. However, existing methods lack the flexibility to perform rapid calculations at continuous and discrete locations and neglect the shielding effects of buildings. This study proposes an ultrafast method based on the fast multipole method (FMM) for calculating dose rates at discrete or continuous locations, with a theoretical computational complexity of O(N). A nested shielding matrix is proposed to account for the shielding effects of buildings, improving the accuracy and efficiency of FMM in multi-building scenarios. The method was validated using two benchmark cases and two complex dispersion cases, demonstrating high accuracy and high speed. In both cases, the deviation between the proposed method and the traditional three-dimensional integration method was less than 1%. In a flat dispersion case with 1000 monitoring points, the proposed method was ten times faster than the three-dimensional integration method, and the acceleration became more significant as the grid size increased. In multi-building scenarios, the nested FMM reduced the computation time by nearly half compared with the three-dimensional integration method, while maintaining high consistency with the traditional method and achieving perfect values (1.00) for the FAC2/5/10, MG, and VG metrics.

Full Text

Fast and flexible gamma dose rate calculation for both three-dimensional fields and arbitrarily discrete positions with shielding effects of buildings*

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Fast and accurate gamma dose evaluation is critical for radioactive environmental impact assessment and emergency planning zone optimization of nuclear energy. However, existing methods lack the flexibility of fast calculation for both continuous domain and discrete positions, and they omit the shielding effect of buildings. This paper proposes an ultra-fast method based on the Fast Multipole Method (FMM) to calculate the dose rates at discrete or continuous positions with a theoretical computational complexity of $O(N)$. A nested shielding matrix is proposed to handle the shielding effects of buildings, which

enhances the accuracy and efficiency of FMM in multi-building scenarios. The method is validated against two benchmark cases and two complex dispersion cases, demonstrating high accuracy and speed. In both cases, the deviation between the proposed and traditional 3D integral methods is less than 1%. In the flat dispersion case with 1000 monitoring points, the proposed method is ten times faster than the 3D integral method, with even greater acceleration as the number of grid sizes increased. In multi-building scenarios, the Nested FMM nearly halved the computation time compared to the 3D integral method while maintaining close agreement with traditional methods, achieving perfect metrics (1.00) for FAC2/5/10, MG, and VG.

Keywords: Fast 3D dose rate calculation; Radioactive environmental impact; Atmospheric radionuclide dispersion; Radiation shielding by buildings

I. INTRODUCTION

Nuclear energy is a safe and clean energy with significant potential to reduce coal consumption and greenhouse gas emissions, which is crucial in achieving carbon peak and neutrality goals [1-5]. However, its radioactive environmental impact [6, 7] is widely concerned as a hazard in both normal operation and accident emergency [8-10], despite the low probability of leakage and nuclear accidents [11-13]. The correspondingly environmental impact assessment requires repetitive and realistic calculation of gamma dose rate at irregular positions or surfaces. One typical example is the determination of Emergency planning zones (EPZ), which is an important technical basis for emergency planning [14, 15] and is critical for balancing environmental implication and economic benefit [16]. Optimizing EPZ requires several iterations. In each iteration, repetitive and realistic calculations of detailed dose rate field distributions and representative positions at the site boundary are performed for all 8760 hours a year [17]. Unfortunately, this is prohibitive in practice because the current realistic calculation of dose rates has to integrate the contributions from all radionuclides in a large three-dimensional (3D) volume for every single position on the site boundary, which is unacceptably time-consuming for 8760 calculations [18-20].

The acceleration of this 3D integral is the key to implementing realistic calculation of dose rates. This is particularly important for gamma dose rate calculation because the high mean free path of gamma rays in the air substantially increases the 3D integral volume. Therefore, numerous efforts have been devoted to developing fast and efficient methods for calculating the dose rate field.

Traditional dose rate calculation methods focus on 1D/2D ground-level dose rate calculations [21, 22]. They sacrifice accuracy and generality to enhance computational efficiency, thereby failing to evaluate 3D dose-rate fields. The most typical and widely used method, the semi-infinite cloud method, assumes homogeneous radionuclide distributions [23]. The more general methods assume Gaussian plume [24, 25] or spherical approximation [26], utilizing dimensionality reduction to achieve dose rate calculation efficiently. There is a method that assumes a Gaussian distribution to accelerate the calculation of 3D integrals on local scales [27]. The tabulated method, derived from a single spherical interpolation approach for calculating ground-level dose rate [26], cannot calculate dose rate above ground level and does not account for complex dispersion scenarios.

Unlike traditional methods, the convolution method is based on a fast Fourier transform [28] and has been developed recently. It can achieve fast and accurate calculation of 3D radiation dose rate fields without sacrificing either accuracy or generality. However, this method is limited to calculations on equispaced grids [28]. An augmented method for calculating the 3D dose rate on a non-equispaced grid with complex radionuclide distribution involves accelerating the 3D integral calculation using a non-uniform fast Fourier transform [29]. This method divides the 3D integral calculation for gamma dose rates into a 3D convolution with a regular smooth function and a correction term near the origin [29]. While this second method is more practical, it requires more computation

* This work was supported by the Beijing Natural Science Foundation [grant numbers JQ23011], the National Natural Science Foundations of China [grant number 12105103, 12275152], the Fundamental Research Funds for the Central Universities [grant number 2024MS045], and the LingChuang Research Project of China National Nuclear Corporation. Cunyou Wang1 and Sheng Fang2 contributed equally to this work.
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time. Furthermore, the above two methods have been verified through the air dispersion simulation in non-uniform terrain and the SCK-CEN field experiment, demonstrating their accuracy and versatility in fast 3D dose rate calculation.

However, the convolution and non-uniform fast Fourier transform are not flexible in calculating dose rates at discrete positions. Both need to calculate a 3D dose rate field first and interpolate on the specific positions. This feature leads to inefficiency in EPZ calculation, which requires calculating dose rates at irregular site boundaries multiple times. In addition, neither method considers the shielding effect and may overestimate the dose rates, potentially increasing the EPZ range and thus reducing the economy of NPP. This may also lead to sub-optimal evacuation routes and evacuation processes in emergency response [30, 31].

This study proposes a flexible and fast 3D dose rate field calculation method to address the above challenges. The proposed method is based on the FMM to accelerate the dose rate calculations [32–34]. The method divides the 3D dose rate field into subregions of different scales and uses multilevel expansion for distant sources and direct calculation for nearby sources [32], achieving a time complexity of $O(N)$ [34, 35]. To account for the shielding effects of buildings, an enhanced FMM approach with a nested shielding matrix (Nested FMM) is proposed, improving both accuracy and efficiency in multi-building scenarios. The proposed method has been validated using two benchmark cases and two dispersion cases. These include air dose conversion factor, ground deposition dose conversion factor, Lagrangian puff dispersion simulations in a flat domain with variable wind, and Lagrangian particle dispersion simulations for multi-building scenarios. The proposed method was coupled with various air dispersion models in these validations, demonstrating its versatility for fast 3D dose rate calculations. The performance of this approach was compared with the semi-infinite cloud method and the 3D integral method. Furthermore, the applicability of the Nested FMM method in multi-building scenarios was discussed and examined. This study highlights the potential of the FMM method to improve nuclear accident emergency responses by identifying low-dose evacuation routes and reducing radiation exposure for rescue and emergency personnel.

II. THEORY

2.1. 3D integral gamma dose rate model

The calculation equation of gamma dose rate at a calculation position $\vec{\alpha} = (x_0, y_0, z_0)$, which contributes from all incident photons of different energies, can be formulated as:

$$D_\gamma(\vec{\alpha}) = \sum_{E_\gamma} F(E_\gamma) \cdot \Phi(E_\gamma, \vec{\alpha}) \tag{1}$$

where D_γ is the gamma dose rate (Sv/s) and $\Phi(E_\gamma, \vec{\alpha})$ is the photon fluence rate of single-energy (E_γ) gamma rays at the calculated position ($\mathrm{m}^{-2} \cdot \mathrm{s}^{-1}$), which considers photons emitted from different position. And $F(E_\gamma)$ is a function of (E_γ):

$$F(E_\gamma) = \frac{\omega A \mu_e E_\gamma}{\rho} \cdot b^n(E_\gamma) \tag{2}$$

where ω is the ratio of the effective dose to the absorbed dose in air (Sv/Gy) [36], as defined under the isotropic geometry assumption, consistent with a previous study [27], $\rho = 1.293$ is the air density ($\mathrm{kg/m^3}$), $A = 1.60\mathrm{E}{-13}$ is a conversion factor (J/MeV), μ_e is the linear energy absorption coefficient (m^{-1}), E_γ is the gamma energy (MeV), $b^n(E_\gamma)$ is the branching ratio for radionuclide n to the specified energy E_γ [27].

Transport of photons with energy E_γ from source point $\vec{\beta} = (x, y, z)$ to the calculation point $\vec{\alpha} = (x_0, y_0, z_0)$ will be described by the quantity of photon fluence rate, which can be calculated as [18, 27, 37]:

$$\Phi(E_\gamma, \vec{\alpha}) = \sum_{\vec{\beta}} \frac{B\left(E_\gamma, \mu_a \cdot \left\|\vec{\alpha} - \vec{\beta}\right\|_2\right) \cdot \exp\left(-\mu_a \cdot \left\|\vec{\alpha} - \vec{\beta}\right\|_2\right)}{4\pi \left\|\vec{\alpha} - \vec{\beta}\right\|_2^2} \cdot \delta(\vec{\beta}) \tag{3}$$

where $\delta(\vec{\beta})$ (Bq/m^3) is an arbitrary 3D radionuclide distribution on an arbitrary grid, $B(E_\gamma, \mu_a \cdot \|\vec{\alpha}-\vec{\beta}\|_2)$ is the build-up factor that accounts for the flux of extra photons due to Compton scattering [24]. The most commonly used build-up factor is linear form or Berger' s formula [27], and the comparison of the two options can be found in literature of [38]. μ_a is the linear attenuation factor for air (m^{-1}), which depends on the photon energy. $\|\vec{\alpha}-\vec{\beta}\|_2$ is the Euclidean distance between the calculation point $\vec{\alpha} = (x_0, y_0, z_0)$ and a radionuclide source at $\vec{\beta} = (x, y, z)$; in this study, $\|\vec{\alpha}-\vec{\beta}\|_2 = \sqrt{(x_0-x)^2+(y_0-y)^2+(z_0-z)^2}$. Calculating the fluence rate is the most computationally time-consuming part of the 3D dose-rate field evaluations because it involves the 3D integral of every calculation position.

The build-up factor is a function of the photon energy, distance, and linear attenuation coefficient and has many different forms [39]. The linear form $B(E_\gamma, \mu_a \cdot \|\vec{\alpha}-\vec{\beta}\|_2) = 1 + k\mu_a\|\vec{\alpha}-\vec{\beta}\|_2$ is used in this study, where $k = (\mu_a - \mu_e)/\mu_e$ [24, 27].

Given a specific photon energy E_γ, the linear attenuation coefficient is constant because the air density is constant, and the right-hand side of Eq. (3) is essentially a function only of $\vec{\alpha}$ and $\vec{\beta}$. Therefore, Eq. (3) can be rearranged as:

$$\Phi(E_\gamma, \vec{\alpha}) = \sum_{\vec{\beta}} K_{E_\gamma}(\vec{\alpha}, \vec{\beta})\delta(\vec{\beta}) \tag{4}$$

where

$$K_{E_\gamma}(\vec{\alpha}, \vec{\beta}) = \frac{B(E_\gamma, \mu_a \cdot \|\vec{\alpha}-\vec{\beta}\|_2) \cdot \exp(-\mu_a \cdot \|\vec{\alpha}-\vec{\beta}\|_2)}{4\pi\|\vec{\alpha}-\vec{\beta}\|_2^2}.$$

2.2. FMM-based dose rate calculation method

Direct calculation of the sum in Eq. (4) has a complexity of $O(N^2)$ [35, 40]. When the number of calculation points and sources is enormous, directly computing the sum is laborious. Therefore, it is necessary to use a low-rank approximation of the kernel function to improve computational efficiency; this is also the core idea of the FMM algorithm [35]. In this study, the FMM algorithm and the corresponding code were used to accelerate the calculation [35, 41].

Following the FMM algorithm, the kernel function in Eq. (4) can be approximated as:

$$K_{E_\gamma}(\vec{\alpha}, \vec{\beta}) \approx \sum_{s=1}^{n} u_s(\vec{\alpha})v_s(\vec{\beta}) \tag{5}$$

where $u_s(\vec{\alpha})$ and $v_s(\vec{\beta})$ are the basis functions of $\vec{\alpha}$ and $\vec{\beta}$, respectively [42]. Then Eq. (4) can be expressed as:

$$\Phi(E_\gamma, \vec{\alpha}) \approx \sum_{s=1}^{n} u_s(\vec{\alpha}) \sum_{\vec{\beta}} v_s(\vec{\beta})\delta(\vec{\beta}) \tag{6}$$

The above framework for fast computation can be summarized as follows:

1. Transform the sources using the basis function v_s:

$$W_s = \sum_{\vec{\beta}} v_s(\vec{\beta})\delta(\vec{\beta}), \qquad s = 1, 2, 3, \dots, n. \tag{7}$$

2. Use the basis function u_s to calculate $\Phi(E_\gamma, \vec{\alpha})$ at each calculation point:

$$\Phi(E_\gamma, \vec{\alpha}) \approx \sum_{s=1}^{n} u_s(\vec{\alpha}) W_s \tag{8}$$

The computational complexity of these two steps is $O(nN)$. Therefore, the computational complexity of this fast algorithm is $O(2nN)$. When $n \ll N$ is satisfied, the computational complexity is greatly improved compared with the original algorithm.

The low-rank approximation of a matrix can be performed by interpolation. Consider the function $g(\vec{\alpha})$ on a closed interval, which can be represented by the n-point interpolation approximation:

$$p_{n-1}(\vec{\alpha}) = \sum_{s=1}^{n} g(\vec{\alpha}_s) w_s(\vec{\alpha}) \tag{9}$$

where $\vec{\alpha}_s$ is the different interpolated node, and $w_s(\vec{\alpha})$ is the interpolation function used.

The FMM algorithm uses matrix low-rank approximation to realize the calculation process. In the calculation, $\vec{\beta}$ is first fixed in the kernel function, and the kernel function is considered as a function of $\vec{\alpha}$:

$$K_{E_\gamma}(\vec{\alpha}, \vec{\beta}) \approx \sum_{s=1}^{n} K_{E_\gamma}(\vec{\alpha}_s, \vec{\beta}) w_s(\vec{\alpha}) \tag{10}$$

Applying the interpolation calculation to the variable $\vec{\beta}$, Eq. (10) can be expressed as:

$$K_{E_\gamma}(\vec{\alpha},\vec{\beta}) \approx \sum_{s=1}^{n}\sum_{m=1}^{n} K_{E_\gamma}(\vec{\alpha}_s,\vec{\beta}_m) w_s(\vec{\alpha}) w_m(\vec{\beta}) \tag{11}$$

Compared with Eq. (5), in Eq. (11),

$$u_s(\vec{\alpha}) = w_s(\vec{\alpha}), \qquad v_s(\vec{\beta}) = \sum_{m=1}^{n} K_{E_\gamma}(\vec{\alpha}_s,\vec{\beta}_m) w_m(\vec{\beta}).$$

2.3. Shielding matrix calculation method

To consider the shielding effect of the building, the shielding matrix $\mathbf{P}(\vec{\alpha})$ is introduced in Eq. (4), which can be expressed as follows:

$$\Phi(E_\gamma,\vec{\alpha}) = \mathbf{P}(\vec{\alpha}) \sum_{\vec{\beta}} K_{E_\gamma}(\vec{\alpha},\vec{\beta})\delta(\vec{\beta}) \tag{12}$$

where $\mathbf{P}(\vec{\alpha})$ is the shielding matrix representing the combination of the shielding factor $P(\vec{\alpha},\vec{\beta})$ of all source points $\vec{\beta}$ for a calculation point $\vec{\alpha}$. Thus, Eq. (4) can also be expressed as:

$$\Phi(E_\gamma,\vec{\alpha}) = \sum_{\vec{\beta}} K_{E_\gamma}(\vec{\alpha},\vec{\beta})\delta(\vec{\beta}) P(\vec{\alpha},\vec{\beta}) \tag{13}$$

Referring to the references [43–45], the shielding factors are determined by the geometric path length L_B of the gamma ray $\vec{R}(t)$ traveling through the building's concrete structures. The gamma ray $\vec{R}(t)$ is a semi-infinite ray arising from the source point $\vec{\beta}$ and passing through the calculation point $\vec{\alpha}$. To calculate L_B, each face of the building was first divided into non-coplanar triangles. Then the length L_B was calculated by intersecting the triangle with the ray $\vec{R}(t)$. The detailed process of this approach [46] is as follows:

The ray $\vec{R}(t)$ can be expressed as:

$$\vec{R}(t) = \vec{\beta} + t\vec{D} \qquad (t \geq 0) \tag{14}$$

where $\vec{D}$ is the direction vector of the gamma ray $\vec{R}(t)$, and t is the distance parameter along the ray. A point $\vec{T}(\mu,\nu)$ within a triangle can be represented as:

$$\vec{T} = (1-\mu-\nu)\vec{V}_0 + \mu\vec{V}_1 + \nu\vec{V}_2 \tag{15}$$

where $\vec{V}_0, \vec{V}_1, \vec{V}_2$ are the coordinates of the three vertices of the triangle. μ, ν are the coordinates of the center of gravity of $\vec{T}$ and satisfy $\mu \geq 0$, $\nu \geq 0$, $\mu + \nu \leq 1$.

If the ray intersects the triangle, then join Eq. (14) and Eq. (15) to obtain:

$$\vec{\beta} + t\vec{D} = (1 - \mu - \nu)\vec{V}_0 + \mu\vec{V}_1 + \nu\vec{V}_2 \tag{16}$$

Convert the above equation to matrix form:

$$\begin{bmatrix} -\vec{D} & \vec{V}_1 - \vec{V}_0 & \vec{V}_2 - \vec{V}_0 \end{bmatrix} \begin{bmatrix} t \\ \mu \\ \nu \end{bmatrix} = \vec{\beta} - \vec{V}_0 \tag{17}$$

Let $\vec{E}_1 = \vec{V}_1 - \vec{V}_0$, $\vec{E}_2 = \vec{V}_2 - \vec{V}_0$, $\vec{T} = \vec{\beta} - \vec{V}_0$, and use Kramer' s Law for Eq. (17), Eq. (17) can be expressed as:

$$\begin{bmatrix} t \\ \mu \\ \nu \end{bmatrix} = \frac{1}{\begin{vmatrix} -\vec{D} & \vec{E}_1 & \vec{E}_2 \end{vmatrix}} \begin{bmatrix} \begin{vmatrix} \vec{T} & \vec{E}_1 & \vec{E}_2 \end{vmatrix} \\ \begin{vmatrix} -\vec{D} & \vec{T} & \vec{E}_2 \end{vmatrix} \\ \begin{vmatrix} -\vec{D} & \vec{E}_1 & \vec{T} \end{vmatrix} \end{bmatrix} \tag{18}$$

Let $\vec{P} = (\vec{D} \times \vec{E}_2)$, $\vec{Q} = (\vec{T} \times \vec{E}_1)$, Eq. (18) can be expressed as:

$$\begin{bmatrix} t \\ \mu \\ \nu \end{bmatrix} = \frac{1}{(\vec{D} \times \vec{E}_2) \cdot \vec{E}_1} \begin{bmatrix} (\vec{T} \times \vec{E}_1) \cdot \vec{E}_2 \\ (\vec{D} \times \vec{E}_2) \cdot \vec{T} \\ (\vec{T} \times \vec{E}_1) \cdot \vec{D} \end{bmatrix} = \frac{1}{\vec{P} \cdot \vec{E}_1} \begin{bmatrix} \vec{Q} \cdot \vec{E}_2 \\ \vec{P} \cdot \vec{T} \\ \vec{Q} \cdot \vec{D} \end{bmatrix} \tag{19}$$

When a gamma ray passes through a building, it will intersect two triangles on the surface of the building. Assuming these two triangles are $\Delta V_0^{(1)} V_1^{(1)} V_2^{(1)}$ and $\Delta V_0^{(2)} V_1^{(2)} V_2^{(2)}$, and the distance $t^{(1)}$, $t^{(2)}$ from the source point to the intersection of the ray with these two triangles can be solved.

For a gamma ray passing through $\Delta V_0^{(1)} V_1^{(1)} V_2^{(1)}$, the value of $t^{(1)}$ obtained is:

$$t^{(1)} = \frac{(\vec{T}^{(1)} \times \vec{E}_1^{(1)}) \cdot \vec{E}_2^{(1)}}{(\vec{D} \times \vec{E}_2^{(1)}) \cdot \vec{E}_1^{(1)}} = \frac{\vec{Q}^{(1)} \cdot \vec{E}_2^{(1)}}{\vec{P}^{(1)} \cdot \vec{E}_1^{(1)}} \tag{20}$$

where $\vec{E}_1^{(1)} = \vec{V}_1^{(1)} - \vec{V}_0^{(1)}$, $\vec{E}_2^{(1)} = \vec{V}_2^{(1)} - \vec{V}_0^{(1)}$, $\vec{T}^{(1)} = \vec{\beta} - \vec{V}_0^{(1)}$, $\vec{P}^{(1)} = (\vec{D} \times \vec{E}_2^{(1)})$, $\vec{Q}^{(1)} = (\vec{T}^{(1)} \times \vec{E}_1^{(1)})$.

For a gamma ray passing through $\Delta V_0^{(2)} V_1^{(2)} V_2^{(2)}$, the value of $t^{(2)}$ obtained is:

$$t^{(2)} = \frac{(\vec{T}^{(2)} \times \vec{E}_1^{(2)}) \cdot \vec{E}_2^{(2)}}{(\vec{D} \times \vec{E}_2^{(2)}) \cdot \vec{E}_1^{(2)}} = \frac{\vec{Q}^{(2)} \cdot \vec{E}_2^{(2)}}{\vec{P}^{(2)} \cdot \vec{E}_1^{(2)}} \tag{21}$$

where $\vec{E}_1^{(2)} = \vec{V}_1^{(2)} - \vec{V}_0^{(2)}$, $\vec{E}_2^{(2)} = \vec{V}_2^{(2)} - \vec{V}_0^{(2)}$, $\vec{T}^{(2)} = \vec{\beta} - \vec{V}_0^{(2)}$, $\vec{P}^{(2)} = (\vec{D} \times \vec{E}_2^{(2)})$, $\vec{Q}^{(2)} = (\vec{T}^{(2)} \times \vec{E}_1^{(2)})$.

Combining Eq. (20) and Eq. (21), the length of L_B is:

$$L_B = \left| t^{(1)} - t^{(2)} \right| \tag{22}$$

In calculating the length L_B, it is assumed that the building is hollow and that the maximum length of L_B is 50 cm, which is the thickness of two concrete facades. This consideration is conservative.

2.4. Nested FMM

The Nested FMM is proposed to address the challenges of dose rate calculations in multi-building scenarios. Traditional FMM methods face limitations when applied to multi-building cases where each monitoring point requires a unique shielding matrix. This leads to inefficiencies that sometimes render the method slower than the conventional 3D integral method. The Nested FMM addresses these issues by introducing a hierarchical grid structure [47] that empirically divides the computational domain into three types of grids, based on parameters such as calculation range, building location and size, with varying resolutions based on their proximities to buildings (Fig. 1):

a) Fine grid (20 m resolution) for areas immediately surrounding buildings, where precise shielding effects are critical.

b) Medium grid (60 m resolution) for zones near but not directly adjacent to buildings.

c) Coarse grid (180 m resolution) for regions far from buildings, where shielding effects are less significant.

Within each grid, a single representative shielding factor, derived from the central point of the grid, is applied to all calculating points. This approximation maintains computational efficiency while ensuring the shielding effects are handled with reasonable accuracy.

Fig. 1. (Color online) Nested grids of the multi-building scenario.

2.5. Theoretical computational complexity

Figure 2 compares the computational complexity of the 3D integral, NFFT, FFT, and FMM, illustrating the acceleration effect of FMM compared to other methods as the number of grids increases. The results demonstrate that FMM provides significantly greater acceleration than the other three methods. When the number of grids reaches 1E10, the computational complexity of FMM is reduced by a factor of 1E10 compared to the 3D integral, by 1E8 compared to NFFT, and by nearly 1E2 compared to FFT. As for the Nested FMM, the acceleration effect depends on the nested strategies.

Fig. 2. (Color online) Computational complex of the 3D integral, NFFT, FFT and FMM.

III. MATERIALS AND METHODS

The FMM method was applied in various scenarios to validate its universality and accuracy in fast 3D dose rate field calculations. The validation of the scenarios in this section was carried out on a computer with an Intel (R) Xeon (R) Gold 6248R CPU @ 3.00GHz, 2 physical processors, 48 cores and 48 threads, and 256GB RAM. These scenarios include calculating gamma dose conversion factors (DCFs) for air submersion and ground surface, a Lagrangian puff dispersion simulation in a flat domain with variable wind, and Lagrangian particle dispersion simulations for simple multi-building scenarios. In these tests, the FMM method was compared with both the 3D integral method and the semi-infinite cloud method. Among them, the 3D integral method, which is equivalent to the convolution method, was validated against the SCK-CEN field experiment, demonstrating excellent agreement (FB: 2.14E−2, NMSE: 2.91E−1) [28]. Comparing the FMM method with the commonly used semi-infinite cloud method [37, 48, 49] highlights the reliability of applying the FMM method in real nuclear emergencies.

Fig. 3. (Color online) Lagrangian puff dispersion simulation scenario.

3.1. DCFs calculation

The DCFs were calculated for primary radionuclides expected to be released into the environment during a nuclear power plant accident. Both air submersion and ground surface DCFs were computed using the 3D integral and the FMM method. The effective dose factors from Federal Guidance Report No. 12 (FGR12) [50] were the gold standard. These factors primarily focus on gamma dose rates and do not include beta ones. Since beta rays are not included in the effective coefficient in FGR12 but are considered in the skin dose coefficient, we exclude the contribution of the skin dose rate in our calculations. The monitoring point was set at 1 m above the ground level for these calculations.

3.2. Lagrangian puff dispersion simulation in a flat domain

The dispersion of airborne radionuclide ^{41}Ar in a flat domain with the variable wind was simulated using the Risø Mesoscale PUFF model (RIMPUFF) [51]. The simulation domain covered 5 km × 5 km × 0.7 km with a grid resolution of 10 m × 10 m × 10 m (Fig. 3). The emission rate was set at 1.63E9 Bq/h with an effective release height of 60 m, and both wind speed and direction varied over time. Ground-level dose rates were calculated using the FMM, 3D integral, and semi-infinite cloud methods, with a grid resolution of 50 m, to evaluate the accuracy of the FMM method. Dose rate variations were further examined along four ground-level axes (X= 0.3 km, 0.6 km, and Y = −0.14 km, 0.41 km) to analyze regions with steep concentration gradients (Fig. 3). Additionally, to verify the universality of the acceleration effect and accuracy of the FMM method, different numbers of measuring points (10, 50, 100, 200, 500, and 1000 points) were randomly distributed within the domain, and the operation was

repeated 50 times to compare the average calculation time and results of the FMM and the 3D integral method.

3.3. Lagrangian particle dispersion simulations for multi-building scenario

A multi-building scenario was established to preliminarily verify the accuracy and speed of the proposed FMM method in complex building scenarios and to study the impact of building shielding on rapid dose calculation (Fig. 4). Quick Environmental Simulation (QES), including a Lagrangian particle dispersion model QES-plume, was used in this scenario [52]. QES is a fast-response model designed to rapidly generate high-resolution wind and concentration fields in complex environments. QES uses ^{41}Ar as the released radionuclide, with an emission rate of 0.83 g/s. The simulated domain is 2 km × 2 km × 0.8 km, containing seven buildings, each with a height of 75 m. The horizontal resolution is 5 m. For vertical resolution: 0 to 100 m at 5 m intervals, 100 to 200 m at 10 m intervals, 200 to 400 m at 40 m intervals, 400 to 700 m at 50 m intervals, and 700 to 800 m at 100 m intervals.

3.3.1. Dose rate calculation without building shielding Figure 5 shows the concentration distributions in two horizontal profiles (Z = 0.001 km and Z = 0.1 km) and two vertical profiles (Y = 1.15 km and X = 1.3 km) obtained from the QES model [52]. The influence of buildings results in a highly uneven distribution of pollutant concentration, particularly at the ground level (Z = 0.001 km). Based on these concentration distributions, the FMM, 3D integral, and semi-infinite cloud methods are used to calculate the dose rate in the horizontal and vertical profiles without building shielding.

3.3.2. Ground-level dose rate calculation with building shielding Nested grids and pre-computed shielding matrices were employed to enhance the speed of dose calculation while accounting for the shielding effect of buildings. The resolution of the nested grids is described in Section 2.4. Monitoring points were uniformly spaced with a 20 m resolution and positioned 1 m above the ground.

The dose rate results from the Nested FMM and the original FMM method were compared with the 3D integral method to assess the accuracy and speed of the Nested FMM and the original FMM method.

3.3.3. Axial dose rate with and without building shielding effect Monitoring points were set along two axes at $X = 1.25$ km and $Y = 1.14$ km (Fig. 4), which are significantly influenced by buildings to measure the accuracy of the proposed method and the impact of shielding effects. Monitoring points were spaced 100 m apart and 1 m above ground. Dose rate results of the FMM and 3D integral methods with and without building shielding were compared.

3.4. Calculation parameters

The following parameters were used for the dose rate calculations: $E_\gamma = 1.294$ MeV, $b^n(E_\gamma) = 99.2\%$, $\mu_a = 7.24\text{E}{-3}\ \text{m}^{-1}$, $\mu_e = 2.05\text{E}{-3}\ \text{m}^{-1}$ [28], and $\omega = 7.35\text{E}{-1}$ Sv/Gy [36] (linearly interpolated value).

3.5. Statistical evaluation

The following statistical measures were used to evaluate the accuracy of FMM calculations: the geometric mean bias (MG), the fractional mean bias (FB), the geometric variance (VG), normalized mean square error (NMSE), the fraction of predictions C_p within a factor of two/five/ten of the observations C_o (FAC2/5/10) [53-57]. The definitions of FAC2/5/10, FB, MG, VG, and NMSE are as follows:

$$\text{FB} = 2(\overline{C_o} - \overline{C_p})/(\overline{C_o} + \overline{C_p}) \tag{23}$$

$$\text{MG} = \exp\left((\overline{\ln C_o}) - (\overline{\ln C_p})\right) \tag{24}$$

$$\text{VG} = \exp\left(\overline{((\ln C_o - \ln C_p)^2)}\right) \tag{25}$$

$$\text{NMSE} = \overline{(C_o - C_p)^2}/\overline{(C_o \cdot C_p)} \tag{26}$$

$$\text{FAC2} = \text{fraction of data for which } 0.5 \leq \frac{C_p}{C_o} \leq 2.0 \tag{27}$$

$$\text{FAC5} = \text{fraction of data for which } 0.2 \leq \frac{C_p}{C_o} \leq 5.0 \tag{28}$$

$$\text{FAC10} = \text{fraction of data for which } 0.1 \leq \frac{C_p}{C_o} \leq 10.0 \tag{29}$$

where C_p is the calculation result of the FMM method, C_o is the calculation result of the 3D integral method, $\overline{C}$ is the average of the data set. It should be noted that a perfect model has MG, VG, FAC2, FAC5, FAC10 are 1 and FB, and NMSE are 0.

Fig. 4. (Color online) Multi-building scenario.

Visible labels: (a) Monitoring point; Building; axes: X (km), Y (km). (b) axes: X (km), Y (km), Z (km).

Fig. 5. (Color online) Horizontal and vertical profiles of the concentration distribution.

Visible panel labels: (a) Z=0.001 km; (b) Z=0.1 km; (c) Y=1.15 km; (d) X=1.3 km. Color scale: ln(Bq/m^3), 24-32.

IV. RESULTS AND DISCUSSION

4.1 DCFs comparison

The DCFs calculated using the FMM and 3D integral methods were compared with the standard values for 24 radionuclides (Fig. 6). The 3D integral method estimation results are very close to the standard values, achieving deviations within 5% for 79% of the total 24 calculated radionuclides. In comparison, the FMM method achieves deviations within 5% for 83% of the radionuclides. This finding shows that although the FMM method' s results differ slightly from the 3D integral method, its accuracy remains very high and may lead to better prediction results. Additionally, the FMM shows a minimum deviation of 0.2% relative to the standard value for ^{138}Cs and a maximum deviation of 47.4% for ^{131m}Xe. Therefore, for radionuclides like ^{131m}Xe, which have small gamma-ray energy

and significant deviations, targeted parameter adjustments should be made before using the FMM method for dose calculation.

Figure 7 shows the calculated DCFs for the ground surface. For all radionuclides, the FMM results are very close to those of the 2D integral method. Compared with the standard values, the FMM results show deviations of less than 4% for all 12 radionuclides. Specifically, in the 2D DCF calculations, the deviation of the FMM results from the standard value is at least 0.1% for ^{138}Cs and at most 6% for ^{88}Rb.

4.2. Lagrangian puff dispersion simulation in a flat domain

Figure 8 compares ground-level dose rates calculated using the FMM, 3D integral, and semi-infinite cloud methods; the computation time of the FMM method is approximately 1/9 of that of the 3D integral method (Table 1). The FMM and 3D integral methods show high agreement, with deviations below 0.5% across all regions. In contrast, the semi-infinite cloud method overestimates the dose rates (black arrows in Fig. 8) in high-concentration areas (Fig. 3). It underestimates them (red arrows in Fig. 8) in low-concentration areas

(Fig. 3) because it considers only local concentrations, neglecting contributions from surrounding regions.

Table 1. Calculation times for ground-level dose rate for different methods.

Method	Dose rate	Monitoring Point Number	Total time (s)
FMM	Ground-level	10 201	1404.5
3D integral	Ground-level	10 201	12 807.3

Figure 9 highlights dose rate discrepancies along four critical axes in steep concentration-gradient areas. The range of overestimation and underestimation for the semi-infinite cloud method is clearly shown, at about 30%-50% (black arrows in Fig. 9) and 55%-58% (red arrows in Fig. 9), respectively. These inaccuracies pose significant risks in nuclear emergencies, potentially leading to misjudged evacuation routes (underestimated areas) or unnecessary resource allocation (overestimated areas). In contrast, the FMM method accounts for contributions from surrounding points, delivering precise dose distributions essential for optimizing emergency evacuation plans and supporting decision-making.

In Fig. 10, the calculation time of the 3D integral and FMM methods increases linearly with the number of monitoring points, as the source number of radioactive pollutants remains unchanged while only the number of monitoring points varies. The acceleration effect of the FMM method becomes more pronounced with an increasing number of monitoring points. For example, with ten monitoring points, the 3D integral method requires approximately three times longer than the FMM method, while with 1000 monitoring points, the 3D integral method takes about ten times longer.

Table 2 presents the statistical metrics defined in Section 3.5 for the FMM method results. The FAC5 and FAC10 values remain consistently high for all results, indicating excellent agreement between the FMM and 3D integral methods. The FB is close to zero, and the NMSE is extremely small, suggesting negligible bias and variance in the FMM results. The relative error decreases as the number of monitoring points increases, dropping from 1.69E−4 at 10 points to 1.18E−4 at 1000 points. This demonstrates the FMM method's robust accuracy, even for large-scale calculations. The FMM method's ability to quickly and accurately calculate dose rates makes it highly suitable for nuclear accident scenarios, where timely and reliable information is critical for decision-making.

Table 2. Statistical metrics of different number of monitoring points.

Monitoring Point Number	FAC5	FAC10	FB	NMSE	Relative err
10	1.00	1.00	−1.93E−4	5.68E−8	1.69E−4
50	9.40E−1	9.40E−1	−2.54E−6	8.16E−9	1.92E−4
100	9.60E−1	9.80E−1	−3.53E−4	3.36E−7	1.64E−4

Monitoring Point Number	FAC5	FAC10	FB	NMSE	Relative err
200	9.30E−1	9.70E−1	−5.66E−5	1.49E−8	1.31E−4
500	9.20E−1	9.50E−1	−4.29E−5	1.37E−7	1.22E−4
1000	9.20E−1	9.50E−1	−8.68E−5	9.11E−8	1.18E−4

4.3. Comparison of different dose rate calculation methods in the multi-building scenario

The following subsections comprehensively summarize the dose rate comparisons using different calculation methods in the multi-building scenario.

4.3.1. Comparison of horizontal and vertical distribution of dose rates without building shielding for three methods

Figure 11 shows the horizontal and vertical profiles of the dose rate distribution calculated using the FMM, 3D integral, and semi-infinite cloud methods without considering building shielding. When the number of monitoring points is 4200, the computation time of the FMM method is approximately 2/5 of that of the 3D integral method. As the number increases to 10 000, the computation time of the FMM method becomes about 1/3 of that of the 3D integral method (Table 3). The dose rates calculated by the FMM method closely match those from the 3D integral method across all four profiles, with a deviation of less than 0.2%. The semi-infinite cloud method tends to overestimate (black arrows in Fig. 11) the dose rate in regions with higher concentration (Fig. 5) and underestimate it (red arrows in Fig. 11) in areas with zero concentration (Fig. 5), compared to the other two methods. This occurs because the semi-infinite cloud method considers only the concentration at a specific point, ignoring contributions from surrounding points to the overall dose rate. In a nuclear emergency, such inaccuracies can have significant consequences. The superior accuracy of the FMM methods highlights their reliability in providing reliable dose rate predictions for effective emergency response planning.

4.3.2. Comparison of ground-level dose rates with build-

Visible plot text (Fig. 6): y-axis labels: Rb-88; Ar-41; Ag-110m; Cs-138; Cs-137; Cs-134; Co-60; Co-58; I-135; I-134; I-133; I-132; I-131; Xe-138; Xe-135m; Xe-135; Xe-133m; Xe-133; Xe-131m; Kr-88; Kr-87; Kr-85m; Kr-85; Kr-83m. x-axis label: DCFs for air submersion ($Sv \cdot m^3/Bq/s$). Legend: FMM 3D; 3D integral; DCFs from FGR12.

Fig. 6. (Color online) Calculation of DCFs for air submersion.

Visible plot text (Fig. 7): y-axis labels: Rb-88; Ag-110m; Cs-138; Ba-137m; Cs-134; Co-60; Co-58; I-135; I-134; I-133; I-132; I-131. x-axis label: DCFs for ground surface ($Sv \cdot m^3/Bq/s$). Legend: FMM 2D; 2D integral; DCFs from FGR12.

Fig. 8: Ground-level dose rates for (a) FMM, (b) 3D integral, and (c) Semi-infinite cloud. Axes: X (km), Y (km); color scale: $\log_{10}$(Sv/s).

Figure 1: Fig. 8: Ground-level dose rates for (a) FMM, (b) 3D integral, and (c) Semi-infinite cloud. Axes: X (km), Y (km); color scale: $\log_{10}$(Sv/s).

Fig. 9: Comparison of dose rates along four critical axes in steep concentration gradient areas. Panels: (a) X = 0.3 km; (b) Y = −0.14 km; (c) X = 0.6 km; (d) Y = 0.41 km. Legend: FMM, 3D integral, Semi-infinite cloud. Axes include dose rate (Sv/s), X (km), and Y (km).

Figure 2: Fig. 9: Comparison of dose rates along four critical axes in steep concentration gradient areas. Panels: (a) X = 0.3 km; (b) Y = −0.14 km; (c) X = 0.6 km; (d) Y = 0.41 km. Legend: FMM, 3D integral, Semi-infinite cloud. Axes include dose rate (Sv/s), X (km), and Y (km).

Fig. 7. (Color online) Calculation of DCFs for ground surface.

Table 3. Calculation time for horizontal and vertical distribution of dose rates for different methods.

Method	Dose rate (km)	Monitoring Point Number	Total time (s)
FMM	Z=0.001	10000	1571.8
FMM	Z=0.1	10000	1591.2
FMM	Y=1.15	4200	733.8
FMM	X=1.3	4200	750.4
3D integral	Z=0.001	10000	4353.1
3D integral	Z=0.1	10000	4347.1
3D integral	Y=1.15	4200	1848.1
3D integral	X=1.3	4200	1846.7

ing shielding for different methods

Figure 12 illustrates the dose rates calculated by the 3D integral, original FMM, and Nested FMM methods for the ground surface, which is affected by the building shielding effect. The original FMM method exhibits nearly perfect agreement with the 3D integral method, with an error of less than 0.49% across all areas (Fig. 12a and Fig. 12b). A comparison of the ground-level dose rates between the original FMM

Fig. 8. (Color online) Ground-level dose rates for (a) FMM, (b) 3D integral, and (c) Semi-infinite cloud.

Fig. 9. (Color online) Comparison of dose rates along four critical axes in steep concentration gradient areas. (a): X = 0.3 km; (b): Y = −0.14 km; (c): X = 0.6 km; (d): Y = 0.41 km.

method with and without building shielding (Fig. 11a and Fig. 12b) reveals a significant reduction in dose rate within the area around buildings when shielding is considered (green arrows in Fig. 11a and Fig. 12b), In comparison, the dose rates in areas farther from the buildings show minimal variation (yellow arrows in Fig. 11a and Fig. 12b). This underscores the importance of considering building shielding in realistic dose rate calculations for nuclear emergencies. Figure 12c shows the ground-level dose rates calculated using the Nested FMM method. The original FMM and Nested FMM results are generally very similar, both showing small deviation occurring only in the area to the right of the building (indicated by the red circle in Fig. 12c). This difference is likely attributed to the coarse grid resolution, which becomes more pronounced in regions with high concentrations. It highlights the necessity for more refined shielding matrices for improved dose rate calculations within such areas.

In Table 4, the ground-level dose rate calculated by the 3D

Fig. 10. (Color online) Computational time of the 3D integral and FMM method.

integral is employed as the gold standard for evaluating the performance of the FMM and Nested FMM methods. The statistical metrics, perfect FAC2/5/10, MG, and VG, and extremely low FB and NMSE values show that the dose rate calculation results of both FMM methods are very close to the 3D integral calculation results. While the nested matrix introduces a slight bias (FB: 2.72E−3, NMSE: 2.42E−5), it is negligible in practical applications.

Table 4. Statistical metrics for FMM and Nested FMM.

Statistical metric	FMM	Nested FMM
FAC2	1.00	1.00
FAC5	1.00	1.00
FAC10	1.00	1.00
FB	−1.65E−4	2.72E−3
MG	1.00	1.00
VG	1.00	1.00
NMSE	1.70E−6	2.42E−5

Table 5 shows various mesh types used in the nested shielding matrix, including 421 grids with a resolution of 20 m, 55 grids with a resolution of 60 m, and 109 grids with a resolution of 180 m. It provides the average relative error of the dose rate calculated for each grid type compared to the dose rate calculated at a single point and the computation time for each grid type. The average relative error of the dose rate calculated using different grid types is less than 5% compared with the 3D integral method. The computation time of the Nested FMM is approximately 1/3 of the original FMM and about half of the 3D integral method' s computation time. This highlights that the Nested FMM method ensures computational accuracy and significantly improves efficiency, making it well-suited for timely dose rate assessments during nuclear emergencies in multi-building scenarios.

Table 5. Statistics of the results with different calculation methods.

Method	Resolution (m)	Grid number	Mean of relative errors	Time (s)
Nested FMM	20	421	0%	153.23
Nested FMM	60	55	3.06%	62.44
Nested FMM	180	109	3.92%	912.90
FMM	20	9745	0%	3546.85
3D integral	20	9745	0%	1912.84

4.3.3. Comparison of axial dose rate with and without building shielding effect

To quantitatively measure the accuracy of the proposed method and the impact of the shielding effect, the dose rate results from FMM and 3D integral methods with and without building shielding are compared for two axes (X = 1.25 km and Y = 1.14 km). Figure 13 shows that the results of the FMM method, both with and without building shielding, are highly consistent with the 3D integral, with a deviation of less than 0.01%. Besides, the shielding effect of buildings significantly reduces dose rates, particularly in areas close to the buildings (red arrows in Fig. 13). This is evident in Fig. 14, which depicts the ratio of axial dose rates with and without building shielding. For X = 1.25 km (Fig. 14a), the ratio reaches a minimum of 29% at Y = 1.2 km, showing a strong shielding effect near the building. For Y = 1.14 km (Fig. 14b), the ratio is 53% at X = 1.5 km in the area close to the building and a minimum of 29% at X = 2 km. The differences between the dose rate with and without building shielding emphasize the importance of considering shielding effects in dose calculations. This is essential for ensuring accurate evaluations, particularly when identifying evacuation routes that minimize radiation exposure.

V. CONCLUSION

This paper proposes a flexible and ultra-fast method for evaluating 3D dose rate fields at any specific point in the presence of extremely anisotropic radionuclide distribution. The method reformulates the most complex part of the 3D integral in dose rate calculation into a summation and reduces the computational complexity to $O(N)$ using the FMM. It also handles the building shielding effect by introducing nested shielding matrices. As the number of data points increases, the acceleration of FMM over the 3D integral becomes more pronounced. The proposed method was validated through two benchmark cases and two dispersion cases. The two benchmark cases include the calculation of gamma dose conversion factors for air submersion and ground surface. The two dispersion cases include Lagrangian puff dispersion simulations with variable wind fields and Lagrangian particle dispersion simulation of a multi-building scenario.

In the benchmark cases, the FMM method showed less than 5% deviation for 83% of radionuclides in air dose conversion coefficients and less than 4% for all radionuclides in ground deposition dose conversion coefficients. The dose rate calculation results of FMM, 3D integral, and semi-infinite cloud

Fig. 11. (Color online) Horizontal and vertical distribution of dose rates without building shielding for three methods.

Panel labels and visible annotations: (a) FMM; (b) 3D integral; (c) Semi-infinite; (d)-(l). Axes include X (km), Y (km), and Z (km), with slices labeled $Z = 0.001$ km, $Z = 0.1$ km, $Y = 1.15$ km, and $X = 1.3$ km. Color scale: ln(Sv/s), from -12 to 0.

Fig. 12. (Color online) Calculation of ground-level dose rates for (a) 3D integral, (b) original FMM, and (c) Nested FMM.

Panel labels and visible annotations: axes X (km) and Y (km). Color scale: ln(Sv/s), from -12 to 0.

methods were compared in two dispersion cases. The difference between the FMM and 3D integral method was very close, and the deviation was less than 1%. In contrast, the semi-infinite cloud method overestimated or underestimated the dose rates.

In the Lagrangian puff dispersion simulations scenario, FMM outperformed the 3D integral method, with the FMM achieving a calculation speed approximately ten times faster than that of the 3D integral method when the number of monitoring points was 1000. This efficiency improves further as the number of computational grids increases.

In the multi-building scenario, the deviation of the FMM from the 3D integral method is less than 0.2% for the horizontal and vertical profiles of dose rate calculations. The statistical metrics show that the results of the Nested FMM are very close to those of the 3D integral. Additionally, the Nested FMM method can reduce the calculation time to half of the 3D integral method while keeping the average relative error below 2.96%. These results demonstrate that the Nested FMM method can effectively handle the shielding ef-

Fig. 13. (Color online) Comparison of axial dose rate for FMM and 3D integral with and without building shielding effect.

Fig. 14. (Color online) Ratio of axial dose rate results with and without building shielding.

fect of buildings and can accelerate the calculation process in building scenarios. Moreover, the axial and ground-level dose rates of the FMM and 3D integral methods with and without building shielding were compared, revealing that considering buildings significantly improved the accuracy of dose rate calculations in multi-building scenarios. This feature provides more detailed support for emergency decision-making during accidents, especially evacuation. Due to its high efficiency, this method provides a promising solution to the longstanding challenge of rapid dose rate calculation in multi-building scenarios.

Acknowledgments

This work was financially supported by the Beijing Natural Science Foundation [grant numbers JQ23011], the National Natural Science Foundations of China [grant number 12105103, 12275152], the Fundamental Research Funds for the Central Universities [grant number 2024MS045], and the LingChuang Research Project of China National Nuclear Corporation. The authors would like to thank the BBFMM3D developed by Ruoxi Wang, Chao Chen, William Fong, and Eric Darve, which facilitated the completion of this research.

Data availability

The data that support the findings of this study are openly available in Science Data Bank at https://cstr.cn/31253.11.sciencedb.19957 and https://doi.org/10.57760/sciencedb.19957

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Note: Figure translations are in progress. See original paper for figures.