Study on the Coupled Behavior of Coagulation-Gravitational Settling-Decay of Multicomponent Radioactive Aerosols Based on PBE-MC (Recommended Paper of the Second Annual Academic Conference of the Research Reactor and Advanced Reactor Branch of the Chinese Nuclear Society)

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Abstract

Aerosol coagulation affects the natural removal of aerosols in the containment under accident conditions by changing the particle size distribution (PSD), thereby exerting an important impact on accident source term assessment. Most existing studies either neglect coagulation and decay, or analyze single-component aerosols using deterministic methods, which limits the applicability of the models and makes it difficult to reflect realistic scenarios. To address this, this paper incorporates the linear chain method into the Monte Carlo method for population balance equation simulation (PBE-MC), and conducts coupled simulations of coagulation-deposition-decay for multicomponent, multinuclide aerosols, with the aim of revealing the post-accident behavior of aerosols and providing theoretical support for accident analysis. First, based on the analytical solution of coagulation for an initially monodisperse PSD, the accuracy of four advanced PBE-MC approaches is evaluated and compared with that of source-term codes to verify the correctness of decay calculations. Subsequently, taking as an example typical mixed aerosols of graphite and solid fission products in high-temperature gas-cooled reactors, coupled coagulation-deposition-decay simulations are carried out to assess the engineering applicability of PBE-MC and the influence of coagulation and decay on natural removal. The results show that SRMC has high theoretical accuracy; meanwhile, coagulation of solid fission products onto graphite promotes the migration of radioactive materials toward the large-size range dominated by gravitational settling, and this effect, together with decay, enhances the natural removal efficiency of the containment.

Full Text

Preamble

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Coupled Behavior of Multicomponent Radioactive Aerosols Involving Coagulation, Natural Deposition, and Decay Based on the PBE-MC

(Recommended Paper from the 2nd Academic Annual Conference of the Research Reactor and New Reactor Branch of the Chinese Nuclear Society)

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Abstract

[**Background**]: Aerosol coagulation modifies the particle size distribution (PSD) and thereby affects natural deposition processes in nuclear containment under accident conditions, playing an important role in source term assessment. However, many existing studies neglect coagulation or treat it using deterministic approaches for single-component aerosols, which limits model applicability and fidelity for realistic severe accident scenarios.

[**Purpose**]: The purpose of this study is to investigate the coupled behavior of multicomponent and multinuclide aerosol coagulation, natural deposition, and radioactive decay in containment under severe accident conditions, with the goal of revealing aerosol behavior characteristics and providing a robust basis for source term analysis.

[**Methods**]: This study incorporates the transmutation trajectory analysis into the particle-based Monte Carlo population balance approach (PBE-MC) to perform coupled simulations of coagulation, natural deposition, and radioactive decay for multicomponent and multinuclide aerosols. The computational performance of four advanced PBE-MC schemes—differentially weighted Monte Carlo (DWMC), weighted fractional Monte Carlo (WFMC), sorting algorithm-based merging Monte Carlo (SAMMC), and stochastic resolution Monte Carlo (SRMC)—was first evaluated using the analytical solution for an initially monodisperse PSD, and the decay calculation was further validated by comparison with results from a source term analysis code. Subsequently, coupled simulations were conducted using a bimodal lognormal PSD representing graphite and fission-product aerosols under HTGR accident conditions to assess the engineering applicability of the PBE-MC framework and analyze the impact of coagulation and decay on natural removal.

[**Results**]**:** The results show that the SRMC scheme achieves high theoretical accuracy. Graphite aerosols exhibit a pronounced coagulation-induced sweeping effect on fine solid fission-product particles, promoting the transfer of radioactive material toward larger particle sizes where gravitational settling dominates. This redistribution, together with radioactive decay, significantly enhances the natural removal efficiency of radioactive aerosols in containment.

[**Conclusions**]**:** Aerosol coagulation significantly enhances natural deposition in containment by shifting radioactivity from fine particles to size ranges with higher deposition efficiency. The PBE–MC framework is demonstrated to be suitable for multicomponent aerosol coagulation–deposition coupled analysis and provides an effective tool for improving source term evaluation in severe accident safety analysis.

Keywords: Radioactive aerosol, PBE-MC, Transmutation trajectory analysis, Coagulation, Natural deposition

Introduction

Nuclear energy is recognized as a clean energy source due to its significant low-carbon emission characteristics. However, the Fukushima accident demonstrated that nuclear power plants may release radioactive aerosols during accidents, which cause irreversible harm to the surrounding environment through deposition and affect human health via atmospheric dispersion. Effective containment of radioactivity is therefore a prerequisite for large-scale deployment of nuclear power plants. As the final barrier for radioactivity containment, the natural removal of radioactive aerosols within containment is critical for mitigating severe accident consequences. Accurate simulation of radioactive aerosol behavior within containment is essential to evaluate its removal rate.

Compared with ordinary aerosols, radioactive aerosol behavior is more complex. In addition to particle dynamic processes such as coagulation and natural deposition, it involves decay of complex nuclide systems within multicomponent particles. More importantly, these processes are highly coupled: coagulation and deposition affect each other by altering the particle size distribution (PSD); coagulation causes nuclide transfer among particles; deposition governs the activity distribution between the gas phase and containment walls; and ionization from decay radiation charges particles, which in turn affects coagulation and deposition through Coulomb forces. These mechanisms collectively determine the relationship between activity distribution and PSD in the system.

Traditional accident source term analysis typically neglects coagulation and decay, while treating deposition as a synergistic effect of thermophoresis, diffusiophoresis, Brownian diffusion, and gravitational settling. The removal rate of suspended aerosol mass in containment during accidents is then evaluated based on corresponding theoretical settling velocities. For instance, Tao et al. simulated the gravitational settling velocity and removal rate evolution of aerosols in the HPR1000 containment under loss-of-coolant accident conditions. Liu et al. further conducted simulations under the same conditions based on four traditional velocity models, concluding that gravitational settling is the dominant removal mechanism while diffusiophoresis and thermophoresis govern the removal of small particles. To improve traditional model accuracy, Li et al. introduced dynamic shape factors, momentum and energy accommodation coefficients, and scattering kernels for model correction, validating the modifications through AHMED, ABCOVE, and LACE experiments. In experimental research, Li et al. established the LSAB large-scale containment aerosol settling experimental platform to systematically analyze the influence of aerosol release patterns, timing, and rates on natural deposition. Results showed that coagulation significantly enhances removal under high-concentration aerosol conditions, indicating that neglecting coagulation may cause substantial errors in simulating natural deposition during the initial phase of large PWR accidents or throughout small modular reactor accident sequences. Although some severe accident analysis codes (e.g., MELCOR, PISAA) consider coagulation–deposition coupling based on the MAEROS model, this model is only applicable to mass removal analysis of single-component aerosols. Overall, the nuclear engineering field still lacks coupled coagulation–deposition–decay simulation studies for multicomponent, multinuclide aerosols.

In aerosol science, modeling these complex behaviors falls under multivariate population balance modeling (PBM). Some exploratory work exists on coagulation–deposition and coagulation–decay coupling for single- and two-component aerosols. For example, Burd et al. solved the single-variable population balance equation (PBE) using a sectional model and combined it with a nuclide tracer model to analyze coagulation' s effect on the settling flux of particulate organic carbon (POC) in the upper ocean, finding that coagulation enhanced the settling of tracer ^{234}Th with POC. However, this tracer model is difficult to extend to multinuclide systems in containment and can only describe the evolution of total activity of a single nuclide in different size intervals, failing to obtain the two-dimensional particle size–activity distribution required for accident analysis. Clement et al. analyzed charging and coagulation of aerosols containing a single nuclide in containment environments through experimental research and model development, discovering that decay-induced particle charging significantly affects coagulation, with the effect magnitude closely related to particle size, decay type, and ion mobility. Building on this, Kim et al. employed the fixed pivot technique to solve the two-variable PBE and further investigated the effect of single-nuclide decay on charging and coagulation of two-component aerosols. However, this model still cannot meet the requirements of accident source term analysis for characterizing multicomponent, multinuclide aerosol behavior.

In summary, while aerosol science has made important progress in simulating coagulation of single- and two-component aerosols coupled with single-nuclide decay and in studying charging mechanisms, and has clearly identified the necessity of simultaneously coupling decay, coagulation, and deposition in radioactive aerosol behavior analysis, existing models are still not directly applicable to source term analysis. First, most studies do not incorporate natural deposition into the coupling and thus cannot describe the evolution of activity distribution between the gas phase and containment walls during accidents. Second, deterministic methods commonly employed require multiple integrals in high-dimensional space when solving multivariate PBEs, resulting in high computational complexity. Related research has been limited to two-variable cases and cannot capture the dynamic evolution of multicomponent, multinuclide aerosols. Third, the radioactive decay models employed are highly specific with poor generality and cannot cover the hundreds of nuclides involved in accident source terms. Therefore, there is an urgent need to develop a simulation method that can comprehensively couple aerosol dynamic processes and support multicomponent, multinuclide analysis to meet the requirements of accident source term analysis.

$$\frac{\partial n(\vec{q},t)}{\partial t} = \frac{1}{2}\int_0^{\vec{q}} \beta(\vec{q}-\vec{s},\vec{s},t)n(\vec{q}-\vec{s},t)n(\vec{s},t)d\vec{s} - n(\vec{q},t)\int_0^{\infty} \beta(\vec{q},\vec{s},t)n(\vec{s},t)d\vec{s} - n(\vec{q},t)R_{\text{dep}}$$

where R_{dep} is the deposition rate.

Compared with deterministic methods, the particle-based Monte Carlo population balance method (PBE-MC) naturally aligns with the discrete nature of particle systems by tracking individual particle dynamics, offering flexibility in handling multivariate problems and directly obtaining detailed information within particles. The fundamental concept of PBE-MC is that a single simulation particle represents a cluster of real particles with identical properties, with its quantity characterized by the simulation particle' s weight (w). In this framework, coagulation corresponds to particle merging, deposition removes particles from the system, and decay directly alters the nuclide composition within particles.

Early PBE-MC employed equal-weight strategies, causing the number of simulation particles to continuously decrease during coagulation and deposition, introducing significant statistical noise in low-concentration regions. Conversely, breakage and nucleation processes increase the number of simulation particles, leading to computational expansion. To maintain a constant number of simulation particles, Matsoukas et al. proposed a constant-number equal-weight method: after each dynamic event, simulation particles are randomly added or deleted with corresponding scaling of the simulation volume to conserve system statistical properties. However, simulation volume scaling limits its applicability in practical engineering.

Recent advances in computational capabilities have alleviated the computational burden of PBE-MC, and related algorithms have continued to evolve. Zhao et al. proposed differentially weighted Monte Carlo (DWMC), allowing different simulation particles to have different weights, thereby balancing the number of simulation particles across the entire PSD and effectively suppressing statistical noise in low-concentration regions. Subsequently, Jiang et al. introduced weighted fraction Monte Carlo (WFMC), which employs a weight-splitting function varying with particle size to address the limited weight distribution adjustment in DWMC and uses random particle removal to maintain a constant number of simulation particles. However, this strategy introduces additional statistical fluctuations in the PSD. To address this issue, Wang et al. combined sorting algorithms with neighboring particle merging to replace the random removal in WFMC, developing sorting-merging Monte Carlo (SAMMC) to further improve PSD stability. Parallel to these weight regulation strategies, Kotalczyk et al. proposed stochastic resolution Monte Carlo (SRMC). This method introduces a random resolution s in each dynamic event processing, splitting weighted particles into multiple equal-weight particles and executing the event on only one of them, thereby improving simulation accuracy in a more intuitive manner.

These proposed methods overcome the limitations of original PBE-MC regarding statistical noise and computational efficiency, demonstrating excellent performance in multivariate PBM and being applied to engineering simulations such as fluidized bed particle preparation and atmospheric pollutant particle control. Although radioactive aerosol behavior shares similarities with these application scenarios, applying PBE-MC to complex decay chains faces computational challenges, and no studies in aerosol science have yet applied PBE-MC to source term analysis in nuclear engineering.

Given these advantages of PBE-MC, this study incorporates the linear transmutation trajectory analysis (TTA) method for decay calculations into PBE-MC to conduct coupled coagulation–deposition–decay simulations for multicomponent, multinuclide radioactive aerosols in nuclear accidents. Specifically, the computational accuracy of four advanced PBE-MC schemes (DWMC, WFMC, SAMMC, and SRMC) is first evaluated based on analytical solutions for coagulation with an initially monodisperse PSD. The Np-237 complex decay chain is then used as a test case for comparison with source term analysis code results to validate decay calculation accuracy. Finally, typical graphite–solid fission product multicomponent aerosols in high-temperature gas-cooled reactor (HTGR) accidents are used as a case study for coupled multi-mechanism simulations to evaluate the engineering applicability of PBE-MC and the impact of decay and coagulation on natural removal. The results of this study not only help improve the accuracy of accident source term analysis, ensuring the development and environmental safety of nuclear energy, but also deepen the understanding of radioactive aerosol behavior and lay the foundation for further coupling mechanisms such as particle charging within the PBE-MC framework.

1 Simulation Methods

PBE-MC discretizes simulation time into a series of time steps to advance system evolution. Based on how the time step is determined, PBE-MC can be classi-

Figure 1

Figure 1: Figure 1

fied as time-driven or event-driven. In time-driven mode, the waiting times for various dynamic events for each simulation particle in the system are first calculated, and the time step is determined based on the minimum value. Within this time step, all particles are traversed and probability sampling is performed for various events to determine whether they occur. Event-driven mode determines the time step based on the average waiting time for any event in the system. Subsequently, the event type to occur is sampled according to the total occurrence rate of various events, and simulation particles are further sampled to execute the event. PBE-MC is used to handle aerosol dynamic events, and decay models must be further embedded within this framework to account for changes in nuclide content within particles.

This chapter details the decay-coupled PBE-MC. Sections 1.1, 1.2, and 1.3 describe the driving modes, particle sampling rules, and processing of dynamic events, respectively. Section 1.4 focuses on the method for rapidly updating particle nuclide composition using TTA to construct normalized decay transition matrices.

illustrates the main computational flow.

Fig.1 Flowchart of the decay-coupled PBE-MC (event driven).

1.1 Driving Modes

Both time-driven and event-driven modes require calculating the waiting time for dynamic events of simulation particles. Taking coagulation as an example, the coagulation rate between real particles with volumes v_i and v_j can be expressed by the coagulation kernel as:

$$R_{ij} = \beta_{ij} n_i n_j$$

where n_i is the number concentration of particles with size v_i (m^{-3}), β_{ij} is the coagulation kernel between particles of sizes v_i and v_j ($\mathrm{m}^3 \cdot \mathrm{s}^{-1}$), and R_{ij} represents the corresponding coagulation rate ($\mathrm{m}^{-3} \cdot \mathrm{s}^{-1}$).

Whether for coagulation of real particles or coagulation between groups of real particles represented by simulation particles, the coagulation behavior should be identical as long as the physical properties of the described particles are consistent. If the equivalent coagulation rate between simulation particles is denoted as R_{ij}^{MC}, then:

$$R_{ij}^{\mathrm{MC}} = \beta_{ij} \Omega_{ij}^{\mathrm{MC}}$$

where $\Omega_{ij}^{\mathrm{MC}}$ is the number of real particle pairs from the real particle groups represented by the two simulation particles that actually participate in coagulation when one coagulation event occurs between the simulation particles. Different PBE-MC methods adopt different values for $\Omega_{ij}^{\mathrm{MC}}$. DWMC assumes that real particles from simulation particles i and j participate in actual coagulation with probabilities $\min(w_i, w_j)/w_i$ and $\min(w_i, w_j)/w_j$, respectively, yielding $\Omega_{ij}^{\mathrm{MC}} = \min(w_i, w_j)$. This leads to the coagulation rate between particles i and j:

$$R_{ij}^{\mathrm{MC}} = \frac{2\beta_{ij} w_i w_j}{\max(w_i, w_j)}$$

SAMMC and WFMC assume that only a fraction α_{ij} (a weight-splitting function between 0 and 1) of real particles undergo coagulation, thus taking $\Omega_{ij}^{\mathrm{MC}} = \alpha_{ij} \cdot \min(w_i, w_j)$, corresponding to a coagulation rate:

$$R_{ij}^{\mathrm{MC}} = \frac{\max(w_i, w_j)\beta_{ij}}{w_i + w_j}$$

SRMC takes $\Omega_{ij}^{\mathrm{MC}} = s$, meaning particles i and j are first split into several equal-weight simulation particles with weight s, and then one pair of equal-weight particles undergoes complete coagulation. This yields the coagulation rate:

$$R_{ij}^{\mathrm{MC}} = \frac{s \cdot \beta_{ij}}{w_i + w_j}$$

The total occurrence rate of coagulation in the system equals the sum of coagulation rates for all simulation particle pairs. Since each particle pair is counted twice in the summation, the result must be divided by 2:

$$R_{\mathrm{coag}} = \frac{1}{2} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} R_{ij}$$

where R_{coag} is the total coagulation rate in the system ($\mathrm{m}^{-3} \cdot \mathrm{s}^{-1}$) and N_p is the total number of simulation particles.

Deposition involves only single-particle evolution. The deposition rate of particle i can be expressed by settling velocities contributed by different physical mechanisms:

$$R_{\mathrm{dep},i} = \frac{1}{V} \left[v_{\mathrm{th},i} + v_{\mathrm{di},i} + v_{\mathrm{br},i} + v_{\mathrm{gr},i}\right] \cdot A_s \cdot \mathrm{sgn}(v_{\mathrm{th},i} + v_{\mathrm{di},i} + v_{\mathrm{br},i} - v_{\mathrm{gr},i}) + \frac{1}{V} \cdot \left[v_{\mathrm{th},i} + v_{\mathrm{di},i} + v_{\mathrm{br},i} - v_{\mathrm{gr},i}\right] \cdot A_c$$

where $R_{\text{dep},i}$ is the deposition rate of particle i ($\mathrm{m}^{-3} \cdot \mathrm{s}^{-1}$), $v_{\text{th},i}$, $v_{\text{di},i}$, $v_{\text{br},i}$, and $v_{\text{gr},i}$ are thermophoretic velocity ($\mathrm{m} \cdot \mathrm{s}^{-1}$), diffusiophoretic velocity ($\mathrm{m} \cdot \mathrm{s}^{-1}$), Brownian diffusion velocity ($\mathrm{m} \cdot \mathrm{s}^{-1}$), and gravitational settling velocity ($\mathrm{m} \cdot \mathrm{s}^{-1}$), respectively, V is the containment volume (m^3), A_s is the surface area of structures (m^2), A_c is the containment floor area (m^2), and sgn is the sign function.

The time step for event-driven PBE-MC is determined by the inverse of the total event occurrence rate:

$$\Delta t_{\text{event}} = \frac{-\ln r_1}{R_{\text{coag}} + R_{\text{dep}}}$$

where Δt_{event} is the time step for event-driven PBE-MC (s) and r_1 is a uniformly distributed random number between 0 and 1.

For time-driven mode, to minimize decoupling errors, the time step must be smaller than the minimum characteristic timescale for any event occurring for any particle:

$$\Delta t_{\text{time}} = \min\left(\frac{C}{R_{\text{coag}} + R_{\text{dep}}}\right)$$

where the expression is $\Delta t_{\text{time}} = \min_i\left(\frac{C}{R_{\text{coag},i} + R_{\text{dep},i}}\right)$.

After determining the event type, specific simulation particles participating in the event must be sampled. During sampling, candidate particles (or particle pairs) and corresponding random numbers are generated repeatedly until the judgment condition is satisfied, thereby determining the simulation particles involved in the event. If the event is deposition, a single particle i is sampled according to the deposition rate; if the event is coagulation, a particle pair (i, j) is sampled according to the coagulation rate.

Fig.7 presents the evolution characteristics of the two-dimensional activity-particle size distribution of I-131 in graphite dust-solid fission product aerosols at different time nodes. At the initial moment, the two-dimensional distribution exhibits two clearly separated structures: a high-activity band extending diagonally upward along the particle size direction corresponds to solid fission product particles containing only I-131, while a horizontal distribution at zero activity reflects the initial particle size distribution of graphite dust without radionuclides. As time progresses, non-zero activity particles gradually appear between the fission product high-activity band and the graphite dust distribution, indicating that Brownian coagulation promotes the transfer of I-131 from the original fission product size range to larger graphite dust particles. This process significantly alters the distribution pattern of radioactive nuclides in particle size space, making I-131 more likely to accumulate in large particles where gravitational settling efficiency is high. Simultaneously, the overall high-activity region shifts toward lower activity, reflecting the continuous reduction of activity per particle due to I-131 decay, while the gradual decrease in the number of large particles demonstrates that gravitational settling becomes an important removal pathway for radionuclides after coagulation promotes activity migration to the large size end. By 48 h, the high-activity region has significantly contracted, with residual I-131 in the system mainly concentrated in the small-to-medium size range, whose subsequent removal is dominated by decay. Overall, Fig.7 clearly reveals the coupling effects among coagulation, decay, and settling in multicomponent aerosol systems: coagulation indirectly enhances the natural removal efficiency of radioactive aerosols by altering the particle size distribution of radionuclide carriers, exerting an important influence on accident source term evolution.

Fig.8 more intuitively shows the evolution of the one-dimensional particle size distribution over time, where the size space is discretized using logarithmic binning and N represents the number of particles in logarithmic size intervals starting at $2 \times 10^{-4} \mu m$ with a spacing of $0.02 \mu m$. As time progresses, the amplitude of the graphite dust peak at the large-size end of the initial bimodal lognormal PSD decreases significantly, indicating stronger removal of large particles by gravitational settling. Meanwhile, the overall distribution shows a slow migration toward larger sizes, demonstrating that coagulation continuously plays a role in system evolution. This coagulation occurs not only between solid fission products and graphite dust but also within each component group, gradually weakening the initial bimodal structure and making the PSD smoother and more concentrated. It should be noted that coagulation and settling exhibit a competitive relationship in PSD evolution: coagulation promotes particle growth toward larger sizes, while gravitational settling preferentially removes large particles. The coupled effect of these two mechanisms jointly determines the characteristic of PSD gradually converging in the middle-to-late stages.

Fig.9 illustrates the effects of components, coagulation, and decay on gravitational settling. Due to decay, the suspended fraction of I-131 decreases more rapidly than the aerosol mass suspended fraction, indicating that using aerosol mass removal rate to evaluate removal efficiency of short-lived nuclides in previous studies tends to be conservative. Homogeneous coagulation among fission product particles has a relatively limited effect on natural deposition, while heterogeneous coagulation between graphite dust and fission products promotes the transfer of I-131 to larger size ranges, thereby significantly enhancing its removal efficiency by gravitational settling.

Conclusion

This study embedded the transmutation trajectory analysis (TTA) method into the PBE-MC framework to conduct coupled coagulation–deposition–decay simulations for multicomponent, multinuclide aerosols in nuclear accidents. Using analytical solutions for coagulation with an initially monodisperse distribution and constant coagulation kernel, the computational accuracy of four advanced PBE-MC schemes was compared, and the accuracy of multinuclide decay calculations was validated using a source term code. Coupled simulations were then performed for typical graphite dust–fission product two-component aerosols in HTGR accidents. The results demonstrate that SRMC achieves high theoretical accuracy. Aerosol coagulation can significantly enhance the natural removal efficiency of radioactive aerosols in containment by altering the PSD. Coagulation of small radioactive particles by large graphite dust particles promotes the migration of radioactive material toward the large size range where gravitational settling dominates. Additionally, decay of short-lived nuclides causes the suspended activity fraction to decrease faster than the mass fraction, indicating that evaluating removal efficiency of such nuclides based solely on aerosol mass removal rate is conservative. This study proves that decay-coupled PBE-MC is suitable for coupled analysis of multicomponent, multinuclide radioactive aerosol behavior, providing theoretical support for severe accident source term assessment and deepening the understanding of radioactive aerosol behavior characteristics. Future work may further incorporate aerosol charging mechanisms to improve the model.

Author Contributions

Cao Chenghao: Methodology, Software, Original draft preparation
Chen Junyi: Data curation
Li Ruihan: Review and editing
Shen Shaoning: Methodology investigation
Liang Jingang: Methodology, Software, Original draft preparation
Cao Jianzhu: Project supervision

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Figure 2

Figure 2: Figure 2

Figure 3

Figure 3: Figure 3

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Figures

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