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Study on variational assimilation in chemical hazard leakage accidents

Jinli Jiang[1,a],Chaoshuai Han[1,2],Xuezheng Zhu[1,*]andJin Gu[1]

Jinli Jiang and Chaoshuai Han contributed equally to this paper.

[1]Institute of NBC-Defense, Beijing, 102205,China

[2]State Key Laboratory of NBC ProTection for Civilian, Beijing, 102205,China

[a]1801210580@pku.edu.cn

[*]Corresponding author's e-mail: 493371839@qq.com

Abstract. In this paper, the problem is studied and analyzed by introducing variational assimilation method and combining with the gaussian plume model.Through the analysis and study of background error covariance, observation error covariance and diffusion parameters, the variational assimilation scheme of chemical hazards was designed and the mathematical modeling was carried out.Then, through Matlab platform programming, numerical experiments are carried out on the established model and an example analysis is made. The results show that the concentration prediction field after assimilation can effectively reduce the prediction error and achieve convergence.

1.Introduction

At present, the world is facing serious environmental hazards, especially the developed regions and the regions with high level of industrialization. Whether it's a chemical leak, a chemical explosion or a chemical attack on a battlefield, the damage to human health and the environment can be enormous.Whatever the form of chemical hazard, when an accident occurs, the toxic substances are dispersed as vapors and aerosols into the atmosphere, forming toxic clouds. It will move along with the airflow and spread around at the same time, forming a chemical hazard zone [1]. Highly effective chemical protection is the premise of the chemical hazard area accurately defined, detection and prediction.Only grasp the hazard substances concentration of space distribution and time distribution, accurately described the harm of poison cloud area, to predict the future for a period of time the concentration distribution inside the window, and then analyze the toxic effect of this time. Currently, for chemical hazard prediction ,it almost through atmospheric diffusion theory to deduce a lethal concentration distribution of the future for a period of time, the development trend of chemical hazard assessment.However, just based on the atmospheric diffusion model of chemical concentration prediction of clouds has a certain deviation, and the volatile weather, terrain conditions, the results tend to have larger error.

In fact, even if the model is accurate, there are many complex factors in the whole diffusion process, so any diffusion model cannot completely accurately describe the diffusion law and reflect the concentration distribution.

Data assimilation has been successfully used to predict concentrations of atmospheric hazards.In the field of chemical hazard prediction, data assimilation algorithm is introduced to obtain the concentration trend and distribution diagram of hazard field in a period of time in the future with faster speed and higher accuracy, so as to provide accurate decision basis for protection and rescue as far as possible while ensuring the speed.At present, there are mainly stepwise iteration method [2], optimal interpolation method [3], Kalman filter method [4], set Kalman filter method [5], and genetic algorithm [6] on pollutant diffusion data assimilation. However, stepwise iteration method and optimal interpolation method are of low accuracy and belong to the early assimilation algorithm. Kalman filtering algorithm has a high requirement on the number of sets and is difficult to be quickly applied to the environment. Genetic algorithm is a new intelligent optimization algorithm, which is still in the early stage of exploration in the field of data assimilation. Therefore, the variational assimilation [7, 8] method is adopted in this paper, which not only avoids the problem of insufficient accuracy, but also does not have such a high requirement for data samples as set Kalman filtering.

Therefore, in this paper, the method of variable fraction data assimilation, combined with the classical chemical diffusion model, is mainly used to construct and analyze the diffusion prediction problem after chemical hazard leakage.

2. Chemical hazard diffusion model

Gaussian diffusion model[9] is a classical pollutant diffusion model. In the atmosphere, turbulence movement of different scales exists almost everywhere all the time. The common turbulence theories mainly include gradient transport theory and statistical theory. But no matter from which theory, the Gaussian diffusion model can be deduced. The diffusion equation established by the theory of turbulent diffusion gradient transport, when the diffusion coefficient is constant, the solution of normal distribution can be obtained. When the airflow is smooth and uniform, the particle distribution of diffusing material also follows the normal distribution. Although the relevant conditions cannot be strictly satisfied in the actual atmosphere, the Gaussian distribution is at least a good approximation without knowing the actual concentration distribution of substances. In practice, the Gaussian diffusion model requires less meteorological conditions and is fast in calculation, and it can better reflect the spatial and temporal distribution of concentration.

Gaussian diffusion model is mainly divided into Gaussian smoke cluster model and Gaussian smoke plume model, the former is mainly suitable for diffusion under instantaneous release condition, the latter is suitable for hazardous substance leakage in chemical warehouse, chimney and discharge pipe. As the research object of this paper is chemical hazard leakage under the condition of continuous release, the Gaussian plume model is selected [11].

2.1.Gaussian plume model

Point source diffusion is one of the main research objects of Gaussian diffusion model. It refers to the diffusion under the condition that the diffusion lasts for a period of time and the weather condition is stable (the wind direction is constant).In this process, we take the location of the release source as the origin of coordinates, and the source releases toxic gases or aerosols in a strong continuous and balanced way, and the released gas continuously diffuses along the wind direction. If a coordinate system is established with the direction of the wind as the X-axis and the vertical direction as the Y-axis, it is not difficult to foresee that toxic gas will form a conical cloud in the downwind direction, and conform to a two-dimensional normal distribution at any section of the X-axis.

On the premise that the law of conservation of mass is satisfied, the general solution of the differential equation is:

$$C(x,y,z) = Kx^{-1}\exp\left[-(\frac{y^2}{K_y}+\frac{z^2}{K_z})\frac{u}{4x}\right] \quad (1)$$

Where : u- the wind speed; C- concentration; K-Diffusion parameters.

In the process of diffusion, when the toxic agent settles to the ground, it is reflected back to the atmosphere or does not settle to the ground. The mathematical expression is to satisfy the integral:

$$Q = \int_0^{+\infty}\int_{-\infty}^{+\infty} u \bullet C dydz \quad (2)$$

Substituting Equation (1) into Equation (2):

$$C(x,y,z,h)=\frac{Q_p}{2\pi u\sigma_y\sigma_z}e^{-\frac{y^2}{2\sigma^2_y}\left(\frac{(z-h)^2}{2\sigma^2_y}+\frac{(z+h)^2}{2\sigma^2_z}\right)} \quad (3)$$

where: h-release the height ;Q -source strength.

2.2.Diffusion parameters

In the above diffusion process, it is actually very difficult to determine the diffusion parameters σ_x, σ_y, σ_z. Generally speaking, it requires meteorological observation under specific conditions and a lot of calculation work. In practice, only conventional observations are available. In order to easily and efficiently calculate the diffusion parameters based on the available data, researchers conducted in-depth research and came up with some effective methods, including Pasqual diffusion curve method, GB/T formula and Briggs[10] formula.

On the basis of the above methods, China formulated the national standard "Technical Methods for Formulating Local Air Pollutant Emission Standards" [11] according to the actual situation. After determining the atmospheric stability, the diffusion parameters were calculated by the following two formulas:

$$\sigma_{xy}=\gamma_1 x^{a_1} \quad (4)$$

$$\sigma_z=\gamma_2 x^{a_2} \quad (5)$$

where : h-release the height ;Q -source strength.

3. Variational assimilation model of Chemical leakage hazard diffusion

Based on variational assimilation theory and Gaussian plume model, the mathematical modeling of battlefield chemical hazards is carried out.The basic function of the variational assimilation scheme is to input the workflow of variational assimilation in combination with the prevailing meteorological conditions, observed data, etc., after a chemical hazard event occurs. When the error statistics are reduced to an acceptable range, the concentration analysis value of the hazard field will be output to reflect the hazard degree under the current state, providing a decision basis for subsequent rescue operations and post-evaluation.

3.1.Variational assimilation principle

The mathematical expression of variational method[12,13] is a functional extreme value problem with constraints. The domain of the functional is the space-time of the given mode integral, the composition of the function is the sum of the pairwise variances of the observed value, the forecast value and the analysis value, and the mode equation is the constraint condition.

3.1.1.Three-dimensional variational assimilation algorithm(3d-var)

Three-dimensional Variational Algorithm(3D-VAR) refers to an assimilation Algorithm [14] for obtaining the optimal solution of analysis field in three-dimensional space, and its principle is shown in Figure 1.

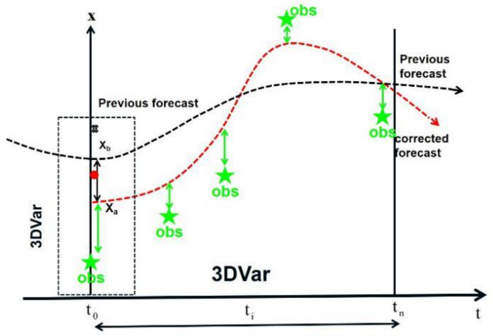

Figure 1 Three-dimensional variational schematic diagram

The objective function of this algorithm[14] is:

$$J(x)=\frac{1}{2}(x-x_b)^T B^{-1}(x-x_b)+\frac{1}{2}(H(x)-y_o)^T R^{-1}(H(x)-y_o) \quad (6)$$

Where: x-Analysis value; x_b -background value; H-observation operator; y: observation vector; B-Background error covariance matrix; R-Observation error covariance matrix.

By obtaining the minimum value of the objective function, the analysis value and the truth value are fitted repeatedly, and the minimum distance is used to show the minimum difference between the two, so as to obtain the optimal value.

The gradient of the objective function is used to compute the analysis field:

$$\nabla J(x)=B^{-1}(x-x_b)+H^T R^{-1}(H(x)-y_o) \quad (7)$$

The value that makes the above equation zero is the optimal value:

$$x_a=x_b+\left(B^{-1}+H^T R^{-1} H\right)^{-1} H^T R^{-1}\left(y-H(x_b)\right) \quad (8)$$

3.1.2.Algorithm process

In the 3d-var process, after pre-processing the data, input the set observation parameters and model parameters, model the error covariance matrix, calculate the weight matrix, then calculate the objective function and its gradient, and then iteratively solve the minimum value of the objective function through the optimization algorithm.

4. Establishment of chemical hazard diffusion variational assimilation model

Error is an inevitable topic in the whole assimilation process, which, from a mathematical point of view, can be understood as the process of minimizing error.Before the assimilation, the error is mainly reflected in the background error covariance matrix B, which is an important part of the whole assimilation process and determines the error of the analysis field together with the observation error covariance. Therefore, before the assimilation process begins, the error must be corrected to reduce the error of the analysis value as much as possible and improve the accuracy.

4.1.Background error covariance matrix-B

The accuracy of the analysis results[15] is directly determined by the fact that only 15% of the analysis field parameters generated by the assimilation system are from the observed data, while the remaining 85% are from the background field [17].In the physical sense, the background field is the state field of the region before assimilation, and it continuously integrates the observed data in the assimilation cycle into the latest analysis field.The definition is as follows:

$$B=(x^{true}-x_b)^T\left(x^{true}-x_b\right)=\varepsilon_b^T\varepsilon_b \quad (9)$$

Where, x^{true} - truth value, ε_b -background error. Since the truth value is unknown at many times, the B matrix is also expressed as:

$$\mathrm{B}=\overline{\left(\varepsilon_b-\overline{\varepsilon_b}\right)\left(\varepsilon_b-\overline{\varepsilon_b}\right)^{\mathrm{T}}} \tag{10}$$

It can be seen that The B matrix is a positive definite symmetric matrix, and the eigenvalues are all non-negative.The background error covariance matrix can be written as:

$$\mathrm{B}=\begin{bmatrix} \operatorname{var}(e_1) & \operatorname{cov}(e_1,e_2) & \operatorname{cov}(e_1,e_3) \\ \operatorname{cov}(e_2,e_1) & \operatorname{var}(e_2) & \operatorname{cov}(e_2,e_3) \\ \operatorname{cov}(e_3,e_1) & \operatorname{cov}(e_3,e_2) & \operatorname{var}(e_3) \end{bmatrix}$$

Each of these elements reflects the correlation of the background error at the two locations, and the correlation between the two variables. Diagonal elements or diagonal matrices represent the background error variance, while non-diagonal elements and matrices represent the covariance.

In order to reflect the background field more accurately, a mathematical model is established for correction. It is defined that the background field correlation coefficient $\mathrm{b}\left(\mathrm{x},\mathrm{x}_0\right)$ between x , x_0 two points is a function of the distance $\mathrm{dist}\left(\mathrm{x}\text{-}\mathrm{x}_0\right)$ between two points:

$$\mathrm{b}\left(\mathrm{x},\mathrm{x}_0\right)=\mathrm{dist}\left(\mathrm{x}\text{-}\mathrm{x}_0\right)e^{-\frac{\mathrm{dist}\left(\mathrm{x}\text{-}\mathrm{x}_0\right)^2}{2}} \tag{11}$$

4.2.Observation error covariance matrix -R

R is the observation error covariance matrix, which contains statistical information about the observation error. For many observation systems, observation errors at different locations are statistically independent of each other. Similarly, before determining the covariance matrix of the observation error, assuming that the observation error is unbiased.

Observation error generally includes observation operator error, instrument error and representative error.The error of observation operator is mainly caused by the insufficient or one-sided understanding of the relation between two different kinds of data. It mainly occurs in the case of indirect observation. The representativeness error generally comes from two aspects: first, the model is not perfect and cannot be measured completely accurately; Second, due to the limited model resolution, the observation system with a resolution of 3km certainly cannot reflect the regional state within a range of 10km.This kind of error can be reduced by means of high density observation and improved model resolution filtering. The instrument error is carried out when leaving the factory, generally with data parameters. The parameters can be adjusted appropriately considering the actual situation such as equipment aging and long service time. In addition, as far as the current research level is concerned, there are few good solutions at home and abroad. In general, the processing of R is quite simplified. In the case that the observations are independent of each other, it can be reduced to diagonal matrix processing to facilitate the calculation in the next step.

5. Typical Case Analysis

In order to verify the assimilation capability of the model and the influence of various parameters on the assimilation quality, numerical simulation experiments are used for analysis in this section.

Firstly, the diffusion model of hazardous substances is run to obtain the concentration of each grid point in the hazard region, which is taken as the background concentration field, and this time is denoted as the 0 moment of the assimilation window. Run the diffusion model forward, and for simplicity, take the predicted value of the resulting model as the "true value";

Secondly, the position of the observation point is set in the hazard area, and the predicted atmospheric stability concentration at the position of the observation point is output and recorded as the observation data. At the same time, another set of diffusion models was run with the parameters unchanged, and 10% random error was added to the initial prediction results. Then the observed

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values were used to assimilate the predicted values with errors, and the assimilation effect and convergence were tested.

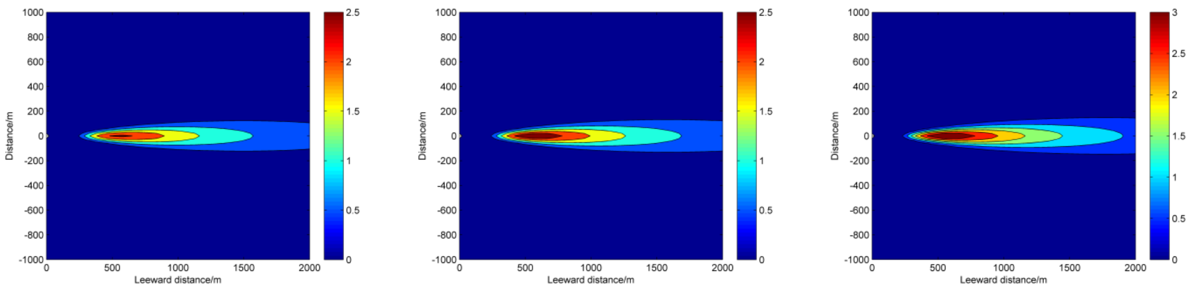
Condition setting: Suppose a single chemical substance leakage occurs in the chimney of a chemical plant in a plain area, and the source term information and meteorological information at that time have been obtained, and observation equipment with output function has been equipped in the plant to prevent accidents. Other conditions are shown in the table below:

Table 1 Test condition setting

Parameter	Value	Parameter	Value
Area	2×2km	Diffusion- Parameter	GB/T
Source strength	100kg	Height	12m
resolution ratio	50m	observation error	5%
Wind speed	2.5m/s	Number of observation points	25
Wind direction	Due west	Interval time	30s
atmospheric stability	C	Forecast time	2h

In order to make the experiment as simple as possible, the external conditions should be idealized without considering the influence of bad weather such as rainfall and lightning. In addition to assimilation effect analysis, convergence and process errors are also analyzed in this section.

Firstly, the diffusion diagram of background field, real field and model prediction field :



(a)background field (b)true value field(30 min) (c)forecast field(30 min)

Figure 2 Concentration field comparison diagram

It can be analyzed from the figure that the concentration diagram predicted at the beginning of diffusion and the background field of this experiment have more or less concentration distribution in the whole diffusion region. However, after 30 minutes of diffusion, the concentration of substances in other regions seems to be zero except the primary clouds of hazardous substances. At the same time, when the random error is added, it is obvious that there is a difference between the predicted value and the true value.Take the number of iterations as 1000, and the figure below is the assimilation effect diagram of the experiment, convergence and error change:

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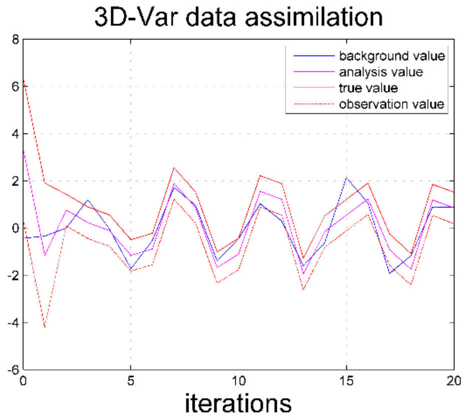
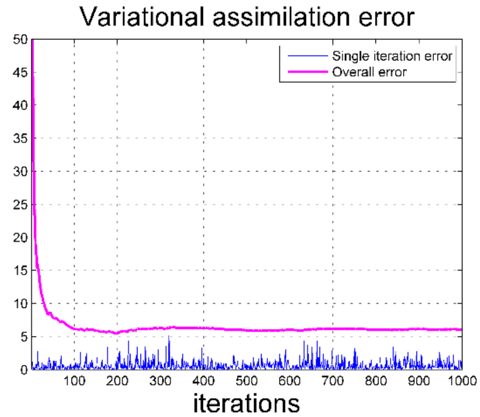
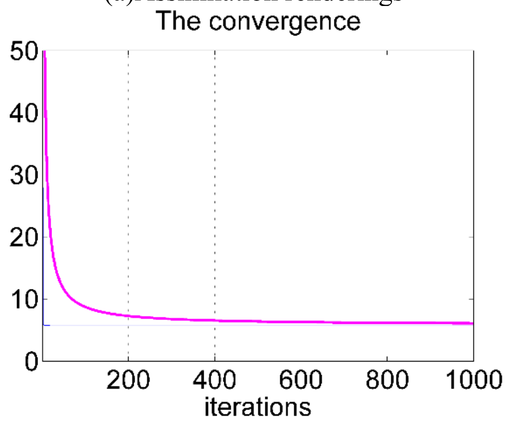


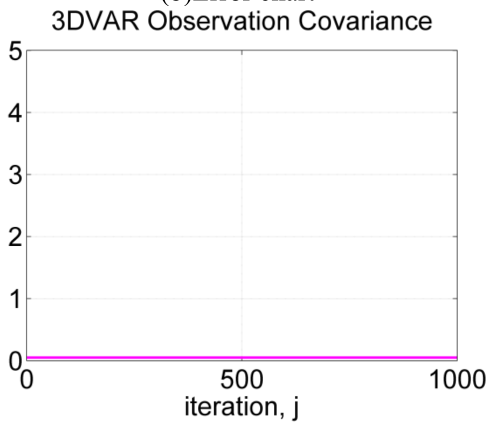
(a)Assimilation renderings



(b)Error chart



(c)Assimilation convergence

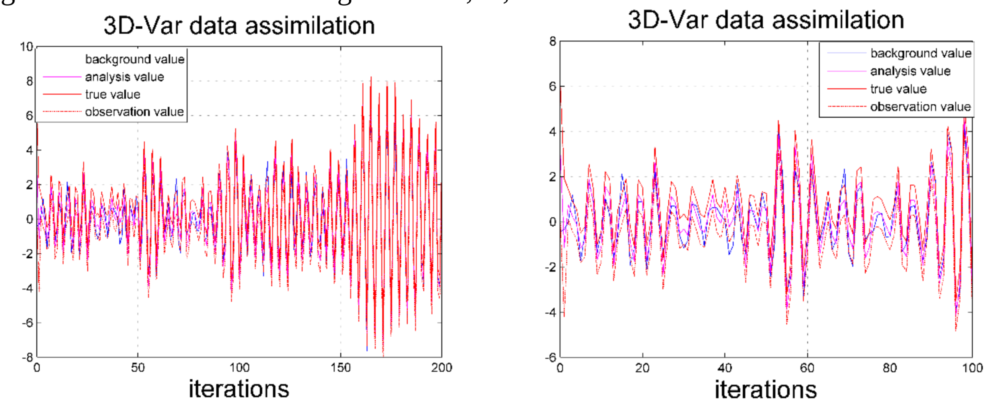


(d) Observation error chart

Figure 3 Experimental renderings

It can be seen from the figure that, through assimilation, the analysis value is closer to the truth value than the observed value, while the background value has obvious deviation from the other three curves in the initial state, and gradually fits into the other several curves after a certain number of iterations.Since the observation error covariance matrix R is a diagonal matrix, and the diagonal elements are mean square error and fixed value, the variance of the observation field remains unchanged no matter how many iterations and how long the assimilation time window is.Although the single error in the assimilation process varies from time to time, it tends to converge and become stable after about 200 falls.Similarly, as the number of iterations increases, the variance of the background field of assimilation gradually converges, and the number of iterations is also around 200.

The figure 4 is the assimilation diagram of 20,50,100 and 200 iterations:



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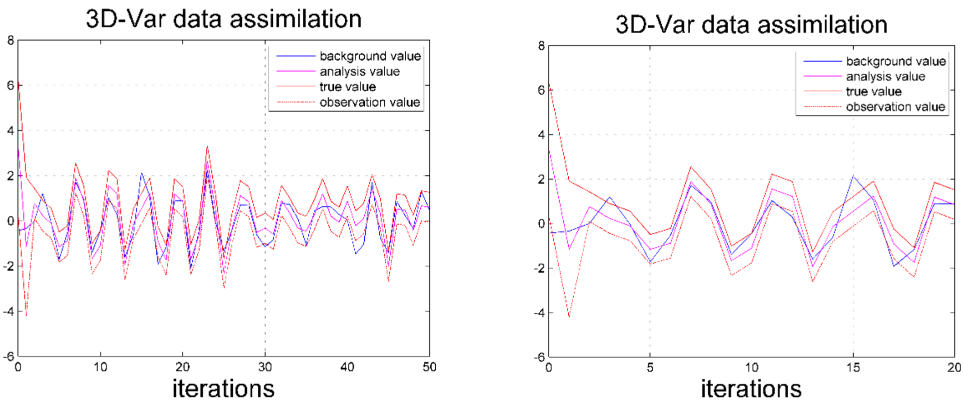

Figure 4 Assimilation effect under different iteration times

As can be seen from the comparative analysis in the figure above, after 200 iterations, the assimilation basically achieves the effect, and the degree of fitting among all curves increases and begins to converge. This is also consistent with the analysis in the figure above that the assimilation process begins to converge after 200 iterations. After the concentration information in the hazard region is assimilated, the concentration of hazardous substances gradually approaches the truth value and fluctuates around it. With the advance of time and the increase of observation data, the assimilation result becomes more and more stable, and the 10% random error added at the initial time is gradually eliminated, reaching the state of convergence.

6. Conclusion

In this paper, the application of four-dimensional variable fraction data assimilation in chemical hazard diffusion prediction is systematically studied and verified. Firstly, the instantaneous release model and continuous release model of Gaussian diffusion model are studied respectively, and the diffusion parameters suitable for chemical hazard prediction are proposed. Secondly, a variational assimilation algorithm suitable for chemical hazard prediction is constructed. The assimilation scheme, background error covariance matrix, observation error covariance matrix and optimization algorithm are modelled , and the optimization steps are defined. Finally, through MATLAB simulation, the assimilation quality and convergence of the algorithm are tested and compared. However , in order to prove the influence of parameters, idealized numerical experiments are applied in the sample analysis to simplify the experimental conditions. The following research needs to further refine the experimental conditions and make more detailed analysis.

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