Numerical Study on Droplet Evaporation Simulation Scheme and Evaporation Characteristics of Salt-containing Desulfurization Wastewater

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Keywords: Desulfurization Wastewater, Salt-Containing Droplets, Evaporation Characteristics, Numerical Simulation.

Abstract: In order to accurately simulate the evaporation characteristics of salt-containing desulfurization wastewater in high temperature flue gas, five simulation schemes for droplet evaporation of desulfurization wastewater were discussed based on DPM model of FLUENT platform and combined with the actual composition of desulfurization wastewater. A simulation scheme for realizing the influence of soluble salts and suspended solids on the evaporation of wastewater droplets was determined. The differences of evaporation characteristic parameters such as evaporation time, evaporation distance, particle size change and mass change of wastewater droplets obtained under different schemes were explored, and the evaporation characteristics of wastewater with different salt content were studied. The results show that the evaporation characteristics of different schemes are different. It is recommended to use the evaporation simulation scheme considering the actual composition of desulfurized wastewater in the simulation; The greater the salt content, the shorter the time and distance required for evaporation of waste water droplets. Under the research conditions in this paper, when the salt content of wastewater is doubled, the particle size of remaining particles increases by 10.3%, the relative mass of remaining particles increases by a percentage of 2.3, the total evaporation time and the total evaporation distance decrease by 6% on average.

1 INTRODUCTION

Since 2015, the government has issued a series of pollution control policies, which put forward the requirement of near zero discharge for desulfurization wastewater from thermal power units. At the same time, the increase in desulfurization wastewater from large thermal power units increases the task of treatment. Therefore, concentration and reduction become necessary before the terminal treatment of desulfurization wastewater. Atomization evaporation is one of the terminal treatment technologies of desulfurization wastewater treatment process and has a certain application in engineering. However, with the concentration and reduction of desulfurization wastewater, the composition of wastewater changes. Correspondingly, wastewater droplet evaporation characteristics will also change. How to accurately master the evaporation characteristics of wastewater droplets is of great engineering significance for better application of atomization evaporation technology and improvement of desulfurization wastewater treatment effect.

In previous studies, the treatment of wastewater droplets was different. Ref. (Zhang 2011, Kang 2013, Min 2019) considered that water accounted for the majority of desulfurization wastewater, and treated desulfurization wastewater as pure water which can evaporate completely. Ref. (Chen 2016, Ran 2016, Wang 2019) still thought that desulfurization wastewater could be evaporated totally, the difference was that they considered the physical property difference between waste water and pure-water. In fact, desulfurization wastewater contains Ca, Ma, Cl and SO_3 as well as suspended solids (Wu 2006). Especially after concentration and reduction, the proportion of soluble salts in desulfurization wastewater becomes larger. Therefore, above research work has shortcomings.

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Yu, G. and Zhang, L.
Numerical Study on Droplet Evaporation Simulation Scheme and Evaporation Characteristics of Salt-containing Desulfurization Wastewater.
DOI: 10.5220/0011175800003443
In *Proceedings of the 4th International Conference on Biomedical Engineering and Bioinformatics (ICBEB 2022)*, pages 18-25
ISBN: 978-989-758-595-1

In recent two years, researchers started paying attention to the influence of soluble salts in desulfurization wastewater on droplet evaporation. Ref. (Xiong 2020) researched the influence of soluble salts on droplet evaporation characteristics by using a shell formation model. Ref. (Yang 2020) regarded desulfurization wastewater as homogeneous salt solution and took into account the influence of salt crystallization on droplet evaporation characteristics during the numerical study. However, the research on atomization evaporation of saline desulfurization wastewater is not enough. How to consider the actual composition of desulfurization wastewater and how to use the droplet model provided by the numerical simulation platform to simulate the evaporation process of desulfurization wastewater more accurately? What are the differences in evaporation characteristics between different numerical simulation schemes for wastewater droplet evaporation? These are all worthy of in-depth study.

Based on the above analysis, combined with the actual composition of desulfurization wastewater, this paper discussed several research schemes on how to simulate the droplet evaporation of desulfurization wastewater on FLUENT platform. and obtained the evaporation characteristics in several aspects under different schemes. A simulation research scheme which could realize the influence of soluble salts and suspended solids on the droplet evaporation of wastewater was determined. At last, the evaporation characteristics of desulfurization wastewater with different salt content were studied

2 MATHEMATICAL MODEL OF DESULFURIZATION WASTEWATER EVAPORATION

It is generally considered that the evaporation process of desulfurization wastewater in flue gas is a dilute two-phase flow.

2.1 Control Equation of Continuous Phase

Continuous phase flue gas is considered as a mixture of dry flue gas and water vapor. The flow and heat exchange processes are described in a general form as follows (Feng 2019):

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\mathbf{U}_f\phi) = div(\Gamma_\phi grad\phi) + S_\phi \qquad (1)$$

in equation: ϕ is a general variable for different equations; ρ is density of flue gas; $\mathbf{U}_f$ is the velocity vector of flue gas; Γ_ϕ is a general diffusion coefficient; S_ϕ is a general source term, which represents the droplet evaporation, the interaction force between flue gas and droplets, the heat required for evaporation.

2.2 Trajectory Equation of Discrete Phase

The trajectory equation of atomized droplets can be obtained by integrating the particle forces in Laplace coordinates (Jen 2005):

$$\frac{\mathrm{d}\mathbf{U}_P}{\mathrm{dt}} = F_D(\mathbf{U}_f - \mathbf{U}_p) + \frac{\mathbf{g}(\rho_p - \rho_f)}{\rho_p} \qquad (2)$$

in equation: $\mathbf{U}_p$ is the velocity of particle; $F_D(\mathbf{U}_f - \mathbf{U}_p)$ is the drag force acting on unit mass particle.

2.3 Heat and Mass Transfer Equation between Two Phases

During the process of evaporation, there is heat and mass transfer phenomena between flue gas and droplets. The droplets may have three different phenomena: heating, evaporation and boiling. When the droplet temperature is lower than the "critical" evaporation temperature, only heat transfer exists between the droplet and the flue gas. When the droplet temperature is higher than the "critical" evaporation temperature and lower than the boiling point temperature, the heat absorbed by the droplet is used for both temperature rise and evaporation (i.e. unsteady evaporation) and then enters the steady evaporation stage, the heat is fully used for droplet evaporation. When the temperature reaches the boiling point, the droplets absorb heat and boil.

Generally, atomization evaporation of desulfurization wastewater is the above evaporation phenomena. Without considering the influence of radiation, the droplet temperature equation and the evaporation rate formula determined by the convection mass are as follows (Miura 1977):

$$M_p c_p \frac{dT_p}{dt} = hA_p(T_f - T_p) + \frac{dM_p}{dt}\gamma \qquad (3)$$

$$\frac{dM_p}{dt} = k_c A_p \rho_p ln(1 + B_m) \qquad (4)$$

in equation: M_p is droplet mass; c_p is the specific heat capacity of the droplet; A_p is the surface area of the droplets; T_f、T_P is separately the temperature of flue gas and the droplets. h is the convection heat coefficient of the droplet surface; γ is the latent heat of vaporization; k_c is the mass transfer coefficient;B_m

is the Spalding mass transfer number.

If the droplet contains solids, the remaining particle will enter the heating process after all the evaporable components evaporate. The temperature equation is as follows (Miura 1977):

$$M_p c_p \frac{dT_p}{dt} = hA_p\left(T_f - T_p\right) \qquad (5)$$

3 DISCUSSION ON SIMULATION SCHEME OF DROPLET EVAPORATION

The treatment scheme of wastewater droplet evaporation simulation is related to the components of desulfurization wastewater and the discrete phase model provided by the numerical simulation platform.

3.1 Component Analysis of Desulfurization Wastewater

Desulfurization wastewater is the most difficult terminal wastewater in thermal power plant, in which there are many kinds of pollutants such as suspended solids, salt content, heavy metal, fluoride and so on. Measurement results showed that desulfurization wastewater after pretreatment still contains Cl^-, SO_4^{2-}, Na^+, K^+, Mg^{2+}, Ca^{2+} and suspended solids. Therefore, desulfurization wastewater is generally considered to consist of pure water, soluble salts and suspended solids (Liang, 2019). Because the crystallization of salts and existence of suspended solids would affect the droplet evaporation characteristics, the simulation scheme of wastewater droplet considering the existence of these substances is a more reasonable scheme.

3.2 Discussions on Discrete Phase Model of FLUENT Simulation Platform

FLUENT platform could simulate many physical phenomena such as flow, heat transfer, mass transfer, combustion, radiation and so on. The platform provides several particle models for discrete phase simulation. Both droplet model and multicomponent model are suitable for simulating droplet evaporation. Droplet model is mainly used to simulate the evaporation of homogeneous droplets which the physical parameters doesn't change during the simulation. Therefore, droplet model can't simulate the crystallization of soluble salts and the presence of suspensions. The multicomponent model can define several components of the droplet, and can define the physical properties and evaporation of each component separately. With the evaporation or crystallization of the droplet components, the composition and physical properties of the droplet change during the simulation. Therefore, the multicomponent model could simulate the mixture with salt crystallization and suspension, and realize different simulation schemes of wastewater droplets by defining the composition and content.

3.3 Discussion on Droplet Evaporation Scheme of Desulfurization Wastewater

Based on the above analysis, combining with the DPM model provided by FLUENT simulation platform, considering the actual composition of desulfurization wastewater and the treatment scheme of desulfurization wastewater droplets in previous literatures, the following five schemes which may simulate the evaporation of wastewater droplets are determined:

(1) Scheme 1: Disregard soluble salts and suspended solids, treat wastewater as pure water, select droplet model.

(2) Scheme 2: Disregard suspended solids, treat wastewater as a mixture of pure water and soluble salt, select droplet model.

(3) Scheme 3: Treat wastewater as a mixture of pure water, soluble salt and suspended solids, select droplet model.

(4) Scheme 4: Disregard suspended solids, treat wastewater as a mixture of pure water and soluble salt, select multicomponent model, define the physical properties and proportion of pure water and soluble salt respectively.

(5) Scheme 5: Treat wastewater as a mixture of pure water, soluble salt and suspended solids, select multicomponent model, define the physical properties and proportion of pure water, soluble salt and suspension respectively.

4 RESEARCH OBJECT AND CALCULATION CONDITION SETTING

4.1 Research Object

Taking the evaporation of desulfurization wastewater in flue as an example, above five schemes of desulfurized wastewater are compared. The flue between air preheater and dust collector of one unit is chose. Fig.1 gives the size of the flue and the plan of the nozzle. Tab.1 gives the relevant parameters of the flue gas and atomized wastewater.

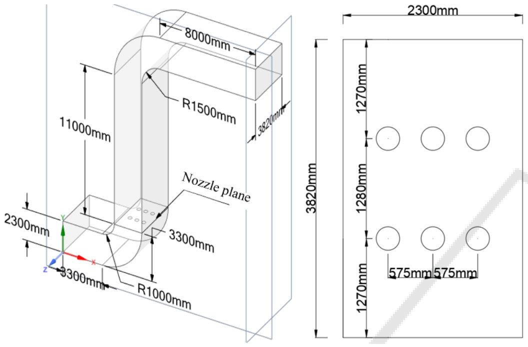


Figure 1: Flue structure and nozzle layout.

Table 1: Related parameters of flue gas and wastewater.

Parameter	Unit	Value
Flue gas flow rate	m/s	10
Flue gas temperature	K	433
Mass fraction ratio of water vapor in flue gas	%	0.08
Waste water temperature	K	323
Waste water quantity	t/h	4.2
Number of nozzles		6
Droplet injection rate	m/s	5
Droplet size	μm	60

4.2 Composition of Desulfurization Wastewater

The main content of desulfurization wastewater is shown in Tab.2. Refer to Ref. (Liang, 2019), it is assumed that the soluble salts containing in the wastewater are $CaCl_2$, $MgCl_2$, NaCl, $MgSO_4$ and KCl. The contents of the soluble salts are calculated.

It is assumed that the suspension in wastewater is mainly calcium sulfate. The content is 70mg/L according to the national standard. Tab.3 shows the composition and physical properties of desulfurization wastewater.

Table 2: Main ion content in wastewater.

Ions	Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	Cl^{-}	SO_4^{2-}
Content(mg/L)	500	3954	683.5	175.2	6594.5	9600.3

Table 3: Composition and physical parameters of wastewater.

Component	Water	Soluble salts					Suspended solids
		$CaCl_2$	$MgCl_2$	NaCl	$MgSO_4$	KCl	$CaSO_4$
Content (g/L)	978.32	1.388	6.151	1.738	12.00	0.335	0.07
Density (kg/m^3)	1000	2152	2325	2165	2660	1984	2960
C_P (J/kg·k)	4180	657.5	752.6	870.4	805.5	657.5	733.8

4.3 Calculation Condition Setting

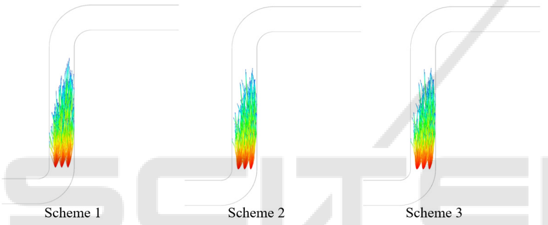
Three sets of grids with total numbers of 1.17, 2.03 and 2.4 million are generated. After verification of grid independence, the number of grids used for calculation is 2.03 million.

In the simulation, it is considered that the continuous phase is composed of dry flue gas and water vapor. The component transport model is used to consider the evaporative mass transfer of droplets. The inlet of flue is set as the velocity inlet boundary, the outlet is set as the pressure outlet boundary and the wall is insulated without slip. Discrete phase droplets are injected from nozzles with uniform particle size(60μm). The droplet trajectory is calculated by discrete random walk model. The wall collision model adopts capture type and the flue outlet is escape type. The discrete phase and the continuous phase are coupled and the steady-state tracking method is used with the maximum iteration step of 50000. SIMPLE algorithm is used for pressure-velocity calculation and second-order upwind mode is used for equation discretization. The physical parameters of waste water droplets in different schemes are set according to Tab.3.

5 DISCUSSION OF SIMULATION RESULTS OF DIFFERENT DROPLET EVAPORATION SCHEMES

5.1 Particle Motion Analysis

According to the above numerical methods, the simulation of five schemes for droplet evaporation of wastewater was completed. The continuous phase flow fields obtained have little difference, but the particle motion is different. Fig.2 shows the particle motion of five schemes. It can be seen qualitatively that the wastewater droplets of Scheme1, 2 or 3 evaporate completely in a vertical flue, only the evaporation processes are slightly different. However, for Scheme 4 or 5, there are residual particle after wastewater evaporation due to the salt or suspended solids. The residual particles are discharged with the flue gas.



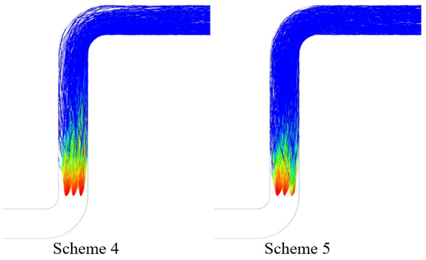


Figure 2: Droplet trajectory of each scheme.

5.2 Comparison of Evaporation Characteristics

Table 4 shows the evaporation time and distance of the wastewater droplets under each scheme. It can be seen that the time and distance required for droplet evaporation in Scheme 1, 2 or 3 are not significantly different, and the minor differences are mainly caused by the slight changes of physical parameters of wastewater, such as density and specific heat capacity. However, compared with the first three schemes, the evaporation time and distance are longer in Scheme 4 or 5 due to considering the presence of crystalline salts and suspended solids, because these have adverse effects on droplet evaporation. The research object in this paper has a vertical flue of 12.5m. The simulation results in Tab.4 shows that the droplets have evaporated completely before leaving the bend and do not impact on downstream equipment.

Table 4: Evaporation time and distance of each scheme.

Scheme	1	2	3	4	5
Average evaporation time (s)	0.603	0.586	0.586	0.621	0.624
Complete evaporation time (s)	0.975	0.978	0.978	1.311	1.307
Average evaporation distance (m)	5.900	5.680	5.680	5.930	5.993
Complete evaporation distance (m)	9.197	9.201	9.201	12.08	12.03

Fig.3 shows the variation of droplet temperature with evaporation time. It can be seen that the evaporation first experienced the unsteady stage since the droplets of Scheme 1, 2 and 3 are all pure solutions. Then the evaporation rapidly enters a steady stage with a temperature of about 331.8K until the droplets completely evaporate. For Schemes 4 and 5, the unsteady evaporation stage is relatively slow, because of the salt or suspended solids in Schemes 4 and 5, which may need additional heat to rise temperature. Then the evaporation also enters a steady stage with almost the same evaporation temperature as the first three schemes. After the steady evaporation lasts for a short time, all the water evaporates, the remaining crystalline salts or solids begin to absorb heat and rise temperature. In addition, duo to discard the suspended solids in Scheme 4, the temperature of wastewater droplet is slightly different from that in Scheme 5.

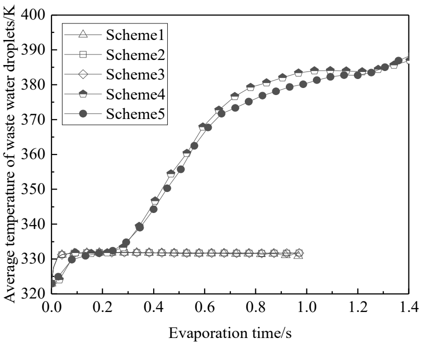


Figure 3: Variation of average temperature of droplet with time of each scheme.

Fig.4 compares the change of droplet mean diameter with evaporation time. It shows that the average droplet size of the five schemes decreases rapidly with evaporation time in the early stage of droplet evaporation, and the change rate is basically the same. However, during the later stage of evaporation, the change of average droplet size is different. The results of Scheme 1, 2 and 3 show that the droplets evaporate completely and rapidly, while the average particle size of Scheme 4 and 5 tend to a fixed value due to the retention of crystalline salts and suspended solid.

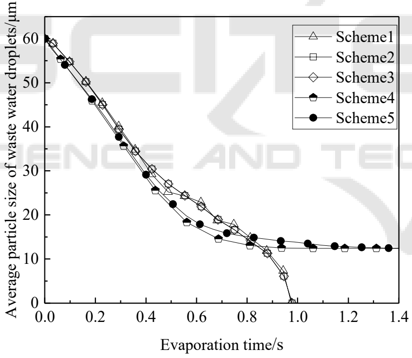


Figure 4: Variation of average size of droplet with time of each scheme.

Fig.5 is a graph of the change of the relative mass of droplets with evaporation time. It can be seen from the figure that the change trend of droplet mass obtained by each scheme is basically the same. In the early stage of evaporation, the droplets are evaporated quickly by about 50% due to the large temperature difference between droplets and flue gas. For the remaining 50% mass, the heat transfer between droplets and flue gas is reduced due to the reduction of temperature difference between droplets and flue gas and the reduction of droplet surface area. Therefore, it takes a long time to completely evaporate.

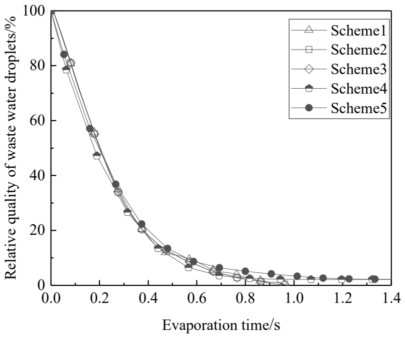


Figure 5: Variation of relative mass of droplet with evaporation time of each scheme.

By comparing the simulation results of the above five schemes, it is easy to find that the characteristics of droplets simulated by the first three schemes using droplet model have the same trend, and there are slight differences among them, mainly due to the different settings of physical properties of wastewater droplets. Similarly, the evaporation characteristics obtained by the multicomponent model have the same trend. The difference between Scheme 4 and Scheme 5 is mainly due to whether the presence of suspended solids is considered and is especially in the later stage of droplet evaporation. Due to better consideration of the actual composition of wastewater, Scheme 5 is recommended in this paper.

6 EVAPORATION CHARACTERISTICS OF WASTEWATER WITH DIFFERENT SALT CONTENT

On the basis of the above wastewater components, it is assumed that the wastewater is concentrated to different degrees. Using Scheme 5, the evaporation characteristics of droplets with different salt content are further studied.

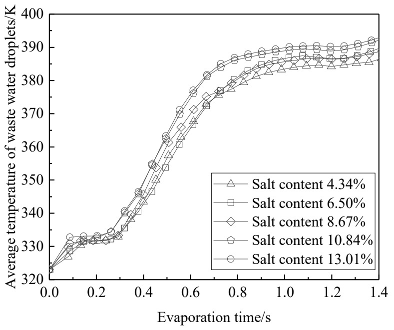


Figure 6: Variation of average temperature of droplet with different salt content with evaporation time.

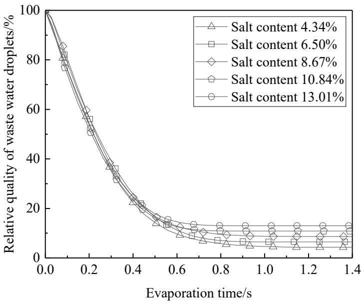


Figure 7: Variation of average particle size of droplet with different salt content with evaporation time.

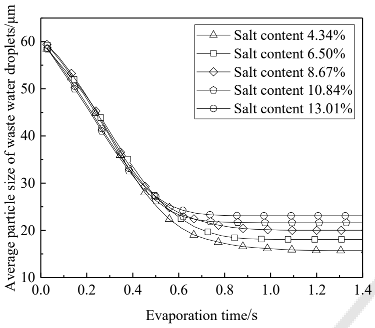


Figure 8: Variation of relative mass of droplet with different salt content with evaporation time.

Fig.6-8 show the variation of average temperature, average particle size and relative mass with evaporation time when droplets of desulfurization wastewater with different salt content evaporate. Fig.6 shows that the less the salt content, the later the wastewater droplets enter the steady evaporation, the longer the steady evaporation duration, the lower the steady evaporation temperature, and the lower the temperature of the final particles. It can be seen from Fig.7 and Fig.8 that with the increase of salt content, the earlier the particles enter the stage of constant particle size and mass, indicating that the complete evaporation time of droplets becomes shorter. At the same time, it can be seen that the larger the salt content, the larger the diameter and mass of the final remaining particle.

Finally, the evaporation time, distance and residual relative mass of wastewater with different salt content are extracted from the simulation results as shown in Tab.5. It can be seen that the relative mass of the remaining particles obtained by the numerical simulation is the same as the mass fraction of salt in wastewater before evaporation, which also shows the accuracy of the calculation to a certain extent. In addition, the table shows that the higher the salt content, the shorter the time and distance required for the evaporation of wastewater droplets, and the greater the influence on the evaporation characteristics. Therefore, for the atomization evaporation simulation of desulfurization wastewater after concentration, it is more necessary to adopt wastewater droplet simulation scheme considering the existence of crystalline salt precipitation and suspended solids.

Table 5: Evaporation time and distance of droplets of wastewater with different salt content.

Salt content (%)	4.336	6.505	8.673	10.841	13.009
Relative mass of remaining particles (%)	4.336	6.505	8.673	10.841	13.009
Residual particle size (μm)	15.74	18.10	20.01	21.66	23.12
Average evaporation time (s)	0.602	0.587	0.566	0.503	0.489
Maximum evaporation time (s)	1.252	1.134	1.093	1.034	0.971
Average evaporation distance (m)	5.820	5.717	5.400	4.907	4.744
Maximum evaporation distance(m)	11.71	10.23	10.48	9.25	9.25

7 CONCLUSION

The variation of evaporation characteristics of wastewater droplets needs further consideration under the background of concentration and reduction, which needs comprehensive analysis combined with wastewater composition and droplet treatment scheme. By comparing evaporation simulation schemes of wastewater droplet and exploring the influence of salt content on droplet evaporation characteristics, the following conclusions are obtained:

(1) The evaporation characteristics of wastewater droplets obtained by different simulation schemes are different. For the simulation scheme considering salt or suspended solids, the unsteady evaporation process is slow, and the temperature rise of residual particle

after evaporation of wastewater droplets can be simulated, and the evaporation time and evaporation distance are longer.

(2) Scheme 5 takes into account the actual composition of desulfurization wastewater. The simulation scheme is recommended when simulating atomization evaporation of wastewater.

(3) Under the research conditions in this paper, when the salt content of wastewater is doubled, the particle size of remaining particles is increased by 10.3%, the residual relative mass is increased by a percentage of 2.3, and the total evaporation time and distance are reduced by 6% on average.

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