NUMERICAL ESTIMATION OF THE FORMATION PROCESS OF ANTHROPOGENIC PRECIPITATION IN THE ATMOSPHERE

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Abstract. The processes of condensation of sulfur trioxide SO_3 and water vapor H_2O. Sulfuric anhydride is formed in flues of thermal power plants (TPP) by partial oxidation of SO_2 (up to 5 % of the total SO_2) from the combustion of high-sulfur fuels, and belongs to a class of mild-hazard products. Sulfuric anhydride in the interaction with water vapor, which refers to greenhouse gases, under certain conditions, it forms sulfuric acid.

1 Introduction

One of the factors of the negative impact of thermal power plants (TPP) on the environment is the possible formation of acidic precipitation in areas immediately adjacent to the TPP [1, 9]. Various pollutants released to the environment from the combustion of fuels [1].

In real practice the atmosphere always contains water vapor of natural origin [2]. In addition, a significant increase of the water vapor concentration in the air is possible in areas adjacent to the power plants by emissions of H_2O due to the work of the heat engineering equipment of the station [1, 3]. The analysis of processes of sulfuric acid drops formation in the air upon jointly proceeding processes of condensation of SO_3 and H_2O vapors on the condensation nuclei surface is of interest.

According to [1] it was assumed that the formation of sulfuric acid drops is the result of condensation of SO_3 and water vapor at the surface of the "condensation nuclei" – microscopic drops of water. The speed of the thermodynamic process significantly depends on the temperature [4]. Accordingly the reliability of the simulation results of condensation process is determined by the accuracy of the condensation surface temperature determination.

2 Study technique

The mechanism of the sulfuric acid formation [1] is based on cooperation, where sulfurous anhydride SO_3 is absorbed by water vapor.

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$$SO_3 + H_2O \rightarrow H_2SO_4 + Q \qquad (1)$$
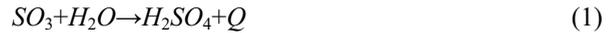
The process of transfer of energy, momentum and mass in these circumstances is described by the system of non-stationary partial differential equations [5]. It is considered that the temperature and concentration on the left border of the solution domain (chimney of TPP) do not depend on time. Unsteady two-dimensional equations of mixed convection in the approximation of the Boussinesq approximation [6] are used to model the changes in the main sought for functions.

Calculation of the condensation rate was conducted using the formula [4]:

$$W_i^K = \beta \cdot \frac{P_A - P_{0i} \cdot \exp\left(-\dfrac{E_i}{R \cdot T}\right)}{\sqrt{\dfrac{2 \cdot \pi \cdot R \cdot T}{M}}}, \qquad (2)$$

where P_A – the atmospheric pressure, Pa; P_{0i} – the preexponent, Pa; E_i – the activation energy of process of condensation, J/kg; R – universal gas constant, J/(mol·K); M – molar mass, kg/mol; β – the coefficient of condensation.

To solve the formulated boundary problem it was used the algorithm [7], developed for the decision of tasks of conjugate heat transfer in areas with a local energy source. Assessment of reliability of the obtained results was performed by verification of difference scheme conservative similar to [8].

The value of the coefficient of condensation of water vapor was varied in the range from 0.05 to 0.4. Below are the results of numerical simulation of growth of sulfuric acid drops in the condensation process of sulfur dioxide and water vapor, calculated at a wind speed of 5 m/s in summer.

Figure 1 shows the changes of the sulfuric acid drop sizes, depending on the time at various initial sizes of condensation nuclei.
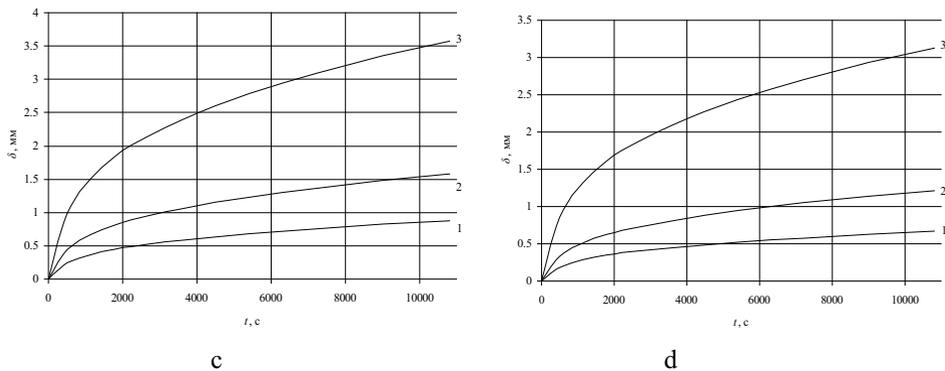

a

b
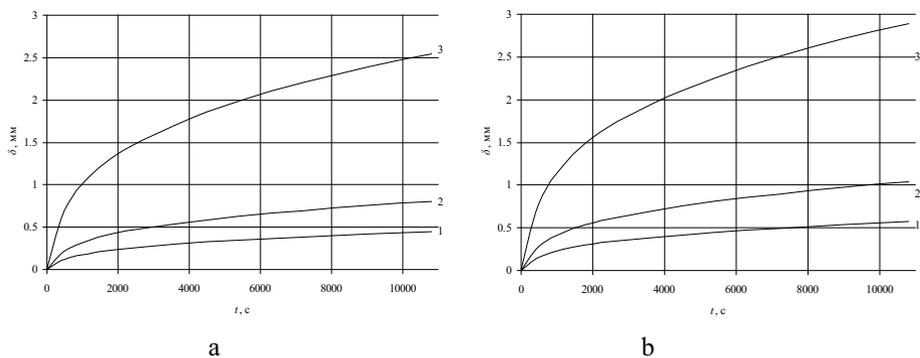
Fig. 1. Changes of the sulfuric acid drops size ($1 - \delta_0 = 0.8 \cdot 10^{-6}$ m; $2 - \delta_0 = 1.0 \cdot 10^{-6}$ m; $3 - \delta_0 = 5.0 \cdot 10^{-6}$ m; δ_0 – the initial size of the condensation nuclei): a) $\beta = 0.05$; b) $\beta = 0.1$; c) $\beta = 0.2$; d) $\beta = 0.4$.

The results (Fig. 1) of numerical investigations show that when the coefficient of condensation $\beta = 0.05$ it is possible to form the sedimentary acid precipitation already through 1800 s since the beginning of the process on the condensation nuclei surface $\delta_0 = 5.0 \cdot 10^{-6}$ m. Further course of the simultaneous condensation process of sulfur dioxide and water vapor promotes the formation of sulfuric acid drops with sizes to $2.5 \cdot 10^{-3}$ m during the analyzed time interval.

It was established that formation of acid precipitation occurs on the condensation nuclei surface at $\delta_0 = 1.0 \cdot 10^{-6}$ m during 9000 and 7200 s, respectively, in the range of changes of the condensation coefficient from 0.1 to 0.2. For the considered period of time, the formation of sulfuric acid drops in the airspace adjacent to the power plants, with size from $1.0 \cdot 10^{-3}$ m to $1.2 \cdot 10^{-3}$ m is possible. Numerical evaluation of the particle border growth on the condensation nuclei surface at $\delta_0 = 5.0 \cdot 10^{-6}$ m illustrates the possibility of the sulfuric acid sedimentary drops formation during the 1800 s and 600 s since the beginning of the simultaneous introduction process of sulfur dioxide and water vapor at the surface of the "embryo".

3 Conclusion

The formation of sulfuric acid drops in the atmosphere of the Earth occurs more intensive on the condensation nuclei surface with initial size from $1.0 \cdot 10^{-6}$ m to $5.0 \cdot 10^{-6}$ m when the coefficient of condensation $\beta = 0.05$ as the researches have shown.

References

1. Ju. A. Izrajel', I. M. Nazarov, A. Ja. Pressman, *Acid rains* (Gidrometeoizdat, Leningrad, 1989) [in Russian]
2. D. V. Gvozdyakov, Web of Conference **82**, 01026 (2015)
3. A. K. Vnykov, *Protection of atmosphere from emissions of energy facilities* (Energoatomizdat, Moskva, 1992) [in Russian]

4. A. D. Labuncov, *Physical fundamentals of Energy* (MEI Publ., Moskva, 2000) [in Russian]
5. P. Rouch, *Computational fluid dynamics* (Moskva, World, 1980) [in Russian]
6. Paskonov, V.I. Polezhaev, L.A. Chudov, *Numerical simulation of processes of heat and mass transfer* (Nauka, Moskva, 1984) [in Russian]
7. G. V. Kuznetsov, J. Eng. Phys. **79,** 56 (2006)
8. G. V. Kuznetsov, J. Eng. Thermophys. **18**, 162 (2009)
9. K. V. Slyusarskiy, M. K. Bejsekov, J. V. Marysheva, Y. Ja Rakov, MATEC Web of Conferences, **37**, 01053