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Computational Modeling of the Emission and Distribution of Gaseous Toxic Matters in the Atmosphere

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Physical, mathematical models and numerical calculation algorithm of toxic gas dispersion in an atmosphere were developed. They take into account air motion, gravity, complex relief, gases thermodynamics properties and presence of toxic matters variable source. The complete system of equations, describing the time-dependent three-dimensional two-component gas mixture flow, is written down in Cartesian co-ordinates. These equations are the conservation laws of gas mixture mass, impulse and energy and of gas admixture mass. The system of equations is complemented by equations determining heat-transfer properties of the gas mixture components. Set of the flow parameters in domain is calculated by means of the integral-interpolation Godunov's method. Developed computer system allows carry out effectively the engineering three-dimensional analysis of gas-dynamic mixing processes, to predict further distribution of gas mixture in open air or apartment with ventilation, and also to forecast the concentration of toxic gas across space.

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