CFD modelling of the condensation, evaporation, coagulation and crystallization processes in the cooling tower emissions

M I Ershov¹,²*, V G Tuponogov¹, N A Abaimov¹, M A Gorsky¹

¹ Department of Thermal Energy and Engineering, Ural Federal University named after the first President of Russia B. N. Yeltsin, 620002, 19 Mira Street, Ekaterinburg, Russia
² PLM Ural Group, 620131, 16-b Metallurgov Street, Ekaterinburg, Russia

*E-mail: ershov1807@gmail.com

Abstract. The aim of the paper is to develop the CFD model for the environmental impact assessment of the cooling tower. The methods applied for this problem are the single-phase turbulent multispecies flow modelling with the DPM Lagrangian particle tracking. The simulations have been carried out in the steady state SIMPLE solver using the ANSYS Fluent software. User Defined Functions have been defined to enhance the accuracy and versatility of the modelling approach in terms of turbulence, fog formation, evaporation, coagulation and crystallization modelling. The Chalk Point cooling tower experiment, laboratory tests with freezing droplets and analytical correlations are used to verify the customized parts of the new CFD model. The arbitrary small-town geometry is used to demonstrate the simulation capabilities of the fog and drift deposition as well as the temperature and relative humidity values near ground and buildings. The results indicate that the new CFD model is able to predict the cooling tower plume parameters, icing and salt contamination risks as well as drift deposition.

1. Introduction

The current economic and ecological imperatives mandate green transition and energy stewardship. Cooling towers can cool huge amounts of water for industrial enterprises. However, their use entails a number of environmental hazards, including [1]:

1) soil contamination with chemicals from the water treatment system;
2) soil waterlogging;
3) thermal pollution;
4) icing of surrounding structures.

In order to take into account all possible risks when designing a cooling tower, it is necessary to simulate the behavior of steam and entrainment droplets from the cooling tower, taking into account the influence of the flow turbulence.

It is an accepted practice to simulate the cooling tower performance using numerical methods [2]. Among all the numerical methods, there is the Computational Fluid Dynamics that can offer a fast, flexible and efficient means of modelling.

There is a rich body of literature on the cooling tower modelling. Most of the research works have focused on the cooling tower performance in warm and temperate climates with the ambient temperature above 10 °C [2-4]. However, the most interesting effects for cold climates such as fog formation, coagulation and icing have not been considered.
The proposed numerical model of the macroscale heat and mass transfer between emissions from a cooling tower and the environment consists of two independent parts.

In the first part, a single-phase steady-state problem of the formation and evaporation of mist droplets is solved, taking into account the latent heat of vaporization. The fog droplets are represented by the transport equation of the custom UDS scalar, which coincides with the water vapor transport equation.

In the second part, the trajectories and parameters of water droplets carried away from the cooling tower are calculated on the resulting field of the flow of moist air and fog. The implementation of the UDF functions allows these droplets to evaporate, grow due to collisions with fog droplets, and crystallize.

The capabilities of the model were demonstrated by the example of calculating the risk of icing of buildings near a cooling tower at negative outdoor temperatures in the approximation of an isothermal atmosphere.

The Ansys Fluent program was used for the calculations. ANSYS Fluent is a general purpose CFD software, which has the capability of simulating pervasive engineering problems, such as fluid flow, heat transfer, turbulence and chemical reaction.

During the numerical simulation, three-dimensional fields of thermodynamic parameters (temperature, velocity, species mass fractions, pressure), as well as the water deposition both in liquid and solid phases on the surfaces of buildings were obtained.

2. Physical models

The basis of the problem is the aerodynamics with proper modeling of turbulence (momentum exchange) and mixing processes (heat and mass exchange). When the ambient air and cooling tower plume mix, the zones supersaturated with water vapor form. In such areas, a mist is instantly formed from small drops of water. The mechanism of fog formation is heterogeneous condensation. Large droplets carried away from the cooling tower (drift droplets) grow in the fog by collisions with small fog droplets due to the coagulation mechanism. Large droplets cannot stay in the fog cloud for a long time, they settle and enter the zone of evaporation, where their mass decreases. The deposition of drops on the ground or the flow rate of falling drops per unit surface is determined by the ballistics of the drop. At subzero temperatures, it is important to know the phase state of the falling drop. If there is supercooled water in the drop upon contact with the structure, icing will occur. It is important to take into account the mechanisms of heterogeneous crystallization.

2.1. Turbulence

The turbulence is modeled using the neutral atmospheric boundary layer conditions. It is assumed that heat and mass exchange in the vertical direction is zero. The temperature is independent of height (isothermal atmosphere). Such conditions are normal for strong wind and cloudy weather. The turbulence inlet profile was taken from [5].

2.2. Evaporation

In its simplest form, the problem of evaporation of a single stationary spherical drop was solved by Maxwell in 1877. If the drop moves relative to the flow, then the mass transfer coefficient \( k \) (m/s) is introduced through the dimensionless Sherwood number \( Sh \) (1) according to the Ranz-Marshall equation [6]:

\[
Sh = k \cdot d \left( \frac{D}{D} \right) = 2.0 + 0.6 \cdot Re_d^{1/2} Sc^{1/3},
\]

where \( d \) – droplet diameter, m; \( D \) – diffusion coefficient of air, m\(^2\)/s; \( Re_d \) – droplet Reynolds number.

2.3. Condensation (Fog formation)

According to the findings [7], the moist air from the cooling tower, mixing with the ambient air, will form a mist of droplets with a diameter of 1 to 10 microns on heterogeneous condensation centers. In
such zones relative humidity values of about 105% may exist. The difference between the initial moisture content and the final one during the formation of fog droplets is called the specific water content of the cloud. This value is crucial for the simulation of drift droplets growth due to coagulation. At a relative humidity of 100-105%, the growth of drift droplets due to diffusion alone is negligible. During the formation of fog, the latent heat of vaporization and the removal of steam from the cloud are taken into account.

The condensation mass flux \( m = \frac{2 \cdot \sigma}{2 - \sigma} \left( \frac{M}{2 \pi R} \right)^{1/2} \left( \frac{P_i}{P_v} - \frac{P_v}{T^{1/2}} \right) \), (2)

where \( \sigma \) – condensation coefficient; \( M \) – molar mass of air, kg/mol; \( P_i \) – steam partial pressure at saturation near the droplet surface, Pa; \( R \) – universal gas constant, J·K\(^{-1}\)·mol\(^{-1}\); \( P_v \) – steam partial pressure far from the droplet, Pa; \( T \) – droplet temperature, K.

2.4. Coagulation

The cooling tower drift droplets grow in the fog as they collide and coagulate with the small aerosols. The drift droplet growth can be calculated using equation (3) according to findings [7]:

\[
\tau = \frac{4 \cdot \rho}{\xi \cdot \delta \cdot c_i} (\ln r_2 - \ln r_1),
\]

(3)

where \( \tau \) – growth time, s; \( \rho \) – droplet density, kg/m\(^3\); \( \xi \) – droplet capture coefficient; \( \delta \) – fog water content, kg/m\(^3\); \( c_i \) – coagulation constant, s\(^{-1}\); \( r_2 \) – final droplet radius, m; \( r_1 \) – initial droplet radius, m.

2.5. Crystallization (Solidification)

To improve the accuracy of building icing simulation, the method for estimating the phase state of a falling drop was introduced (if the water droplet is supercooled, the icing will take place, if water is already frozen there will be no icing).

The model used was proposed by [9]. The model considers a freezing drop consisting of ice and supercooled water, with water contained in the center of the drop and ice on its periphery. The crystallization of the drop occurs in the direction from the periphery to the center, since in any particle, the outer surface freezes first. At the point of contact of ice and water, the temperature is approximately 0°C. Crystallization occurs at a surface temperature below 0°C. First, a thin layer of ice is instantly formed at the periphery, and then the process of transient crystallization is started.

2.6. User Defined Functions (UDF)

The following UDF macros have been used to introduce the advanced physics:

1) DEFINE_DPM_LAW – defines the droplet heat and mass transfer with ambient air (heating, evaporation, coagulation).

2) DEFINE_ADJUST – calculates the precise relative humidity and other auxiliary parameters and stores them in the user defined memory locations.

3) DEFINE_DPM_SCALAR_UPDATE – tracks the droplet density during the crystallization as a user defined scalar.

4) DEFINE_DPM_PROPERTY – applies the calculated density to the droplet.

5) DEFINE_DPM_EROSION – provides effective drift deposition monitoring taking into account the droplet phase state (supercooled or frozen).

6) DEFINE_SOURCE (3 macros) – applies the sources of steam, aerosols and heat for the fog formation modelling.

7) DEFINE_PROFILE (3 macros) – applies the ambient inlet profiles of speed and turbulence for the neutral atmospheric boundary layer.

3. Verification
A natural draft cooling tower geometry was used to verify the aerodynamic models. The height of the tower was 124 m and the diameter was 54.8 m. The air temperature from the cooling tower was 42 °C (100% humidity). The air velocity at the outlet of the tower was 4.5 m/s. The mass flow rate of the drift droplets was 0.328 kg/s. The droplet diameter distribution was set according to the Rosin-Rammler formula (max 1 mm, min 1 µm). Weather conditions: temperature: 11 °C, relative humidity 75%, wind speed 8 m/s.

The height and length of the cooling tower plume was verified by means of the analytical formula of Briggs [3]. Verification of the droplet deposition on the ground was performed based on the results of the Lucas CFD simulation [3].

The mechanism of droplet crystallization was verified by modeling the laboratory test [10]. The free fall and crystallization of droplets with diameters of 0.5 mm, 1 mm, and 2 mm in a cylindrical chamber at temperatures of -20 and -30 °C and atmospheric pressure was simulated.

The simulation results differ from the experimental data by less than 5%. Thus, the verification showed satisfactory agreement between the simulation and experimental data.

4. Problem setting
The task is to simulate a turbulent multiphase multicomponent flow of a homogeneous mixture of air and steam, taking into account the trajectories of water droplets. The heat and mass transfer of water droplets with evaporation, coagulation and crystallization are to be modeled.

The domain is presented in the form of a settlement with a mechanical draft cooling tower, which includes 10 fans with the diameter of the output section of the diffuser 6.7 m. The fans are arranged in two rows of 5 pieces, and both rows take the same air flow from the street, which is necessary for the uniform operation of the aerodynamic path of each section of the cooling tower. The height of the cooling tower is 19 meters. The height of the buildings is from 4 to 23 meters.

Most of the domain is the enclosure in the form of a rectangular box with a height of 700 m, a width of 600 m and a length of 5000 m.

The atmospheric air inlet is represented by the Velocity Inlet boundary condition. The profiles of velocity, turbulent kinetic energy and dissipation rate were set for the conditions of the neutral boundary layer for areas with obstacles in the form of dispersed houses and farmlands (aerodynamic roughness length 0.5 m). It was assumed that at an altitude of 30 m above the ground, the air velocity is 9 m/s. Wind direction is from the cooling tower to the stadium. The ambient air temperature was set to be constant in height and equal to 271 K with a relative humidity of 95%. Atmospheric air outlet – Pressure Outlet with Prevent Reverse Flow function.

The surface of the earth and buildings was considered as a heat-conducting 1D wall with a thermal conductivity like that of clay (1.5 W m⁻¹ K⁻¹) and a thickness equal to the depth of the ground freezing (1 m). At the freezing depth, the temperature was 273 K.

The humid air left the cooling tower at a speed of 8 m/s and temperature of 305 K and a humidity of 100%. The turbulence at the fan outlet was set as Intensity =10%, Length Scale = 3 m.

The drift droplet flow rate was 0.1 kg/s. The diameter of the droplets was assumed to be 350 microns to demonstrate the operation of the model. The Symmetry condition was assigned to the top and sides of the settlement to the domain boundaries. Atmospheric pressure was 101325 Pa.

Pressure-based Steady State solver with SIMPLE Pressure-Velocity Coupling was used. Solution limits for the Maximum turbulent viscosity ratio were raised to 1e+09 in order to properly model turbulence in the atmospheric boundary layer.

Droplets were treated as spherical with the default Turbulent Dispersion enabled.

The simulation was carried out in the CFD software ANSYS Fluent 2021 R1.

5. Results and discussion
The results are presented in figures 1-4. The figure 1 shows the scene object containing all the ground and building surfaces and two contour plots for the deposition rates of snow (frozen droplets) and water (supercooled droplets). Due to the warm winter conditions, the amount of frozen droplets is negligible.
However, the amount of supercooled water hitting the surfaces is sufficient and exceeds the initial drift droplet flow rate by 1.5 because of the coagulation process.

**Figure 1.** Deposition rates of snow (white colouring) and water (bgr colouring) in kg·m⁻²·c⁻¹.

The figures 2-4 show the x=0 plane of the domain near the cooling tower and buildings with the contour plots of the relative humidity, fog aerosol mass fraction and flow temperature. According to the figure 2, although the fog formation sources are implemented, the zones with supersaturation still remain in the vicinity of cooling tower fans.

**Figure 2.** Relative humidity in the cooling tower plume.

**Figure 3.** Mass fraction of the fog aerosol (small droplets).
Figures 3 and 4 indicate that the turbulent mixing processes are strong enough to dissipate the fog droplets and cool the plume down fast.

6. Conclusion
Analysis of the data obtained using the verified CFD model has demonstrated the following.
1) The mathematical model presented, consisting of two coupled sets of conservation equations for the continuous and discrete phases with extra UDFs, was incorporated in the general-purpose CFD code Fluent to simulate drift evaporation, coagulation, crystallization and deposition.
2) For cooling tower applications, one can evaluate the environmental flow patterns (temperature, velocity, pressure, humidity, liquid water content) through the 3-D steady-state turbulent flow modeling.
3) The zones with supersaturation are in the vicinity of cooling tower fans. The turbulent mixing processes are strong enough to dissipate the fog droplets and cool the plume down fast.

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