Numerical simulation of water spray evaporation in a turbulent air flow

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Abstract. Water spray evaporation in a hot air flow is a common process for many industrial applications. Spray nozzles should be well adjusted and distributed specifically to achieve efficient evaporation. The present study addressed simulation of the process within the Eulerian-Lagrangian workframe with k-ε turbulence model. Simulation was carried out via OpenFOAM and postprocessed with ParaView. SprayFOAM solver was used to obtain a solution for 2D and 3D representations of the wind tunnel. Custom JANAF-based approximations were introduced for thermophysical properties of working mediums (air and water vapor). Obtained results were accurate enough to validate the presented model against adopted experimental data. Drift eliminator was modelled with virtual interfaces (baffles), which were tested in two scenarios: accumulating and removing droplets from the computational domain.

1. Introduction

Cooling towers are considered highly efficient in terms of waste heat rejection. Commonly they are engineered with semi-empirical correlations that usually provide sufficient accuracy. However, design optimization is usually out of reach.

Cooling towers operate in such a way that water injection in hot air flow is preferable in terms of design simplicity; however, well adjusted nozzles are required. Evaporation of water sprays in gas flow is well studied. A number of semi-empirical expressions for integral solutions are available [2–4,9,11]. Recent advances in the Eulerian-Lagrangian approach to simulation of two- and four-way coupled evaporating sprays induced numerous studies on the subject. One can see a steady growth of subject-related publications over the last five years (based on ScienceDirect search results). The following aspects of water spray evaporation were considered in these studies: evaporation rate (temperature driving force) [5, 7], droplet size distribution [8, 14], droplets dispersion (as a result of nozzle design and injection pressure) [8, 10, 14], injection direction [13, 14], spray relative velocity [14] and gas relative humidity [13, 14].

However, most of the models do not incorporate Lagrangian workframe, thus leaving two-way coupling unresolved. Another common shortcoming is the use of 2D computational domain, which can not fully predict turbulent flow that is intrinsically three-dimensional.

Simulation in reference work [13] does not account for drift eliminator and utilizes 2D computational domain without exit region. Considering the mentioned circumstances the present simulation was carried out to advance into the mechanics of the experiment [12].
2. Numerical Simulation

2.1. Governing Equations

2.1.1. Continuous phase

The simulation was made within the Eulerian-Lagrangian workframe, where the continuous phase was described with Reynolds Averaged Navier-Stokes (RANS) equations. Equations were closed with the $k$-$\epsilon$ turbulence model. The conservation equation reflected incompressibility of gaseous phase with droplets evaporation source term $S_{\text{evap}}$:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = S_{\text{evap}},
\]

\[
S_{\text{evap}} = \frac{\Delta m_d}{m_{d,0}} G_{in}^m.
\]

Here $\rho$ and $U$ are density and velocity of continuous phase, $m_{d,0}$ is an initial droplet mass, and $G_{in}^m$ is initial flow rate of liquid phase.

Momentum equation for continuous phase incorporates droplet momentum source term (fluid drag force) $S_{\text{mom}}$ among usual terms of pressure drop $\nabla p$, stress $\nabla \tau$ and gravitational force $\rho g$:

\[
\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) = -\nabla p + \nabla \tau + \rho g + S_{\text{mom}},
\]

\[
\nabla \tau = \nabla \cdot \mu_{\text{eff}} \nabla U + \nabla \cdot \mu_{\text{eff}} \left[ (\nabla U)^T - \frac{2}{3} \text{tr}(\nabla U)^T I_n \right],
\]

\[
S_{\text{mom}} = \sum \left[ \frac{18 \mu R e}{24 \rho_d d^2} (U_d - U) \right] G_{in}^m \Delta t.
\]

Here $\mu_{\text{eff}}$ is effective dynamic viscosity, $(\nabla U)^T$ is transposed velocity matrix, $tr$ denotes trace operator, $I_n$ is identity matrix ($n = 3$ for 3D case), $\mu$ and $Re$ are dynamic viscosity and Reynolds number of gaseous phase, $\rho_d$ and $U_d$ are density and absolute velocity of droplet with diameter $d$.

Specie equation describes dynamics of water vapor mass fraction $Y$ in overall flow due to water spray evaporation $S_{\text{evap}}$:

\[
\frac{\partial \rho Y}{\partial t} = \nabla \cdot (\rho U Y) - \nabla \cdot \mu_{\text{eff}} \nabla Y = S_{\text{evap}}.
\]

Energy equation describes temporal and spatial variation of full energy $E$ within a cell:

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot [U(\rho E + p)] = \nabla \cdot [\kappa_{\text{eff}} \nabla T - H J + \tau_{\text{eff}} \cdot U] + S_{\text{heat}},
\]

\[
E = mc_p T + \frac{U^2}{2},
\]

\[
S_{\text{heat}} = \frac{G_{in}^m}{m_{d,0}} \left[ m_{d, \text{in}} \int_{T_{\text{in}}}^{T_{\text{tref}}} c_p d T - m_{d, \text{out}} \int_{T_{\text{tref}}}^{T_{\text{tref}}} c_p d T - r (m_{d, \text{in}} - m_{d, \text{out}}) \right].
\]

Here $\kappa_{\text{eff}}$ is effective conductivity, $H$ is sensible enthalpy, $J = -D \nabla C$ is diffusion flux for concentration $C$ and diffusivity $D$ of evaporated water in air flow, $c_p$ is droplet isobaric specific heat, $r$ is evaporation heat of liquid phase, $\text{in}$ and $\text{out}$ indices denote droplet parameters on entrance and on exit of mesh cell respectively, $T_{\text{tref}} = (T_{\text{in}} + T_{\text{out}})/2$ is reference droplet temperature.

Full energy variation along with pressure force contribution are in the left hand side of (7). Right hand side of (7) considers heat transfer due to conduction, species diffusion, and viscous dissipation along with heat transfer between continuous and discrete phases $S_{\text{heat}}$. 

2
2.1.2. Discrete phase

Droplet dynamics was described by the Second Newton Law with the sum of external forces:

\[ m_d \frac{dU_d}{dt} = F_g + F_p + F_D, \]  
\[ F_g = \frac{1}{6} \pi d^3 \rho_d g, \]  
\[ F_p = \pi \rho f d^3 \frac{DU}{Dt}, \]  
\[ F_D = C_D \frac{\rho d^2}{8} (U - U_d)^2, \]  
\[ C_D = \frac{24}{Re_d} \left( 1 + \frac{1}{6} \frac{Re_d^{2/3}}{Pr^{1/3}} \right). \] 

Here \( F_g \) is gravitational force, which was set to act uniformly in the z-axis direction \( g(z) = -9.81 m/s^2 \), \( F_p \) is pressure gradient force, \( \frac{DU}{Dt} \) is material derivative of continuous flow velocity, \( F_D \) is drag force for spherical droplets with \( Re_d < 1000 \), \( C_D \) is drag coefficient.

Droplets dispersion was modelled with a gradient approach, which essentially pushed them in the direction of low values of turbulent kinetic energy (\( -\text{grad}(k) \)). However, for 2D computational domains with transverse symmetry there is a problem (the \( -\text{grad}(k) \) always points away from the axis of symmetry), so a workaround was implemented that pushes particles towards \( \pm \text{grad}(k) \). Dispersion sigma \( \sigma = \sqrt{\frac{2}{3}k} \) was used uniformly.

Ranz-Marshall heat transfer model was used for discrete phase with the following dimensionless coefficients of heat and mass transfer:

\[ Nu = 2 + 0.6 Re_d^{1/2} Pr^{1/3}, \]  
\[ Sh = 2 + 0.6 Re_d^{1/2} Sc^{1/3}. \] 

Here \( Re_d \) is a droplet Reynolds number, \( Pr \) and \( Sc \) are Prandtl and Schmidt numbers for gaseous phase.

Considering droplet heating and evaporation phases overall heat balance can be written as follows:

\[ m_d c_p \frac{dT_d}{dt} = h_d \pi d^2 (T_\infty - T_d) - \frac{dm_d}{dt} r. \]  

Here \( h_d = \frac{Nu \cdot k}{d} \) is the heat transfer coefficient of a droplet, \( T \) is gaseous phase temperature far away from the droplet.

Total evaporation rate was calculated as a sum of evaporation from droplet superheating (flash evaporation) and gaseous phase superheating:

\[ \Delta m_d = G_f + G. \]  

Evaporation due to droplet superheating \( (T_d > T_b) \) was rated as follows [1]:

\[ G_f = \frac{\alpha (T_d - T_b) A_d}{L(T_b)}. \]  

Here \( T_b \) is discrete phase boiling temperature, \( A_d \) is droplet surface area, \( L(T_b) \) is latent heat of liquid at boiling temperature, \( \alpha \) is empirical heat transfer coefficient that is being calculated in respect to superheating value \( \Delta T \).
\[
\begin{align*}
\alpha &= 760 \Delta T^{0.26}, \quad \text{for } \Delta T < 5 \, ^\circ C \\
\alpha &= 27 \Delta T^{2.33}, \quad \text{for } 5 \leq \Delta T < 25 \, ^\circ C \\
\alpha &= 13800 \Delta T^{0.39}, \quad \text{for } \Delta T \geq 25 \, ^\circ C
\end{align*}
\]

Evaporation due to gas superheating \((T_g > T_b)\) was rated as follows [15]:
\[
G = \frac{\pi d \kappa N_u}{c_p (1 + G_f/G) \ln \left(1 + \frac{h_{\infty} - h_b}{L(T_b)} (1 + G_f/G)\right)}.
\]

Here \(\kappa\) and \(c_p\) are thermal conductivity and specific heat of continuous phase.

2.2. Computational Domain and Mesh

A cuboid 585x585x3000 mm was used as a computational domain — wind tunnel. Water injection nozzle and drift eliminator were simulated with virtual interfaces, thus such a simple form was sufficient.

The computational domain was discretized with a set of uniform meshes. Cell sizes were in a range \(\Delta x = 5 - 20\) mm with corresponding capacity range \(N = 0.13 - 8.2\) million cells. Preliminary study showed no noticeable effect from local mesh refinement near the nozzle. Considering \(k-\epsilon\) modeling of turbulence no prismatic layers were applied to the walls to maintain \(y^+ > 30\).

2.3. Initial and Boundary Conditions

All initial and boundary conditions were set according to adopted experimental data [12] as strictly as possible. Initial conditions in the computational domain were set according to inlet conditions.

The moist air was used as a working medium of carrier flow. Humidity ratio was set to 5.04 g/kg considering dry and wet bulb temperatures 40.7 \(^\circ C\) and 19 \(^\circ C\). Thus water vapor and air mass fractions at the inlet were set 0.00504 and 0.99496 correspondingly at 313.85 K (40.7 \(^\circ C\)). Uniform velocity profile at the inlet (1 m/s) corresponds to experimental conditions, as fine wire mesh was used to stabilize the airflow.

Turbulent kinetic energy at the inlet was estimated with turbulent intensity \(I = 10\%\) as \(k = 1.5(\langle U' \rangle)^2 = 0.015 \text{ m}^2/\text{s}^2\). Turbulent dissipation rate at the inlet was estimated with hydraulic diameter \(d_h\) as \(\epsilon = \frac{C_0^{0.75} k^{1.5}}{0.07 d_h} = 0.09^{0.75} 0.015^{1.5} = 0.00736 \text{ m}^2/\text{s}^3\). Turbulent viscosity \(\nu_t\) and consequently thermal diffusivity \(\alpha_t = \frac{\rho \nu_t}{\rho c_p}\) at the inlet were set to zero. Adiabatic walls with no-slip condition and zero roughness were considered. All turbulent parameters mentioned above were set with appropriate wall functions.

Transverse virtual wall was set as a drift eliminator. It was introduced by a pair of wall interfaces (baffles) at \(y = 2.2\) m (0.2 m downstream of nozzle injector). These interfaces were treated with cyclic boundary conditions so they won’t affect continuous phase flow. However, Lagrangian particles (droplets) were instructed to escape the domain through this virtual wall. Thus measuring probes located downstream (at \(y = 2.3\) m) were unaffected by non-evaporated droplets. All outlet conditions were of mixed nature implying zero gradient \(\frac{\partial \psi}{\partial n} = 0\) for outflow and fixed value (equal to inlet value) for inflow.

2.4. Spray Cloud Characteristics

Discrete phase (water) was introduced into the computational domain via the virtual interface of the injector nozzle. The nozzle was located on the lateral axis at \(y = 2\) m, facing backwards. Hollow cone nozzle with 4 mm orifice and discharge coefficient \(C_d = 0.9\) sprayed 0.2071 kg/s of water at 308.25 K (35.1 \(^\circ C\)) in counterflow direction. Inner and outer angles of spray were
13.5° and 28.4° respectively. Droplet size distribution was reported in binned form [12] and was implemented likewise. Reported data can be summarized in arithmetic mean diameter $d_{10} = 197$ µm and Sauter mean diameter $d_{32} = 298$ µm.

Flow rate of injected water was ramped up to nominal value during the first second of simulation to relax solution. Primary breakup (atomization) of the spray was not modelled since initial droplet size distribution was set. Secondary breakup of droplets was modelled with 5000-15000 parcels per second by Enhanced Taylor Analogy (ETAB).

2.5. Thermophysical Properties

2.5.1. Continuous phase The continuous phase was treated as a multicomponent mixture of dry air and water vapor. Thus all thermophysical properties were calculated separately for each component and then combined according to their mass fractions. Expected temperature of the target process — which is heat recovery of flue gas — was considered to be in a range of 273-1100 K (0..827 °C). Thus default correlations were replaced in favor of accuracy. NIST-JANAF formulation was used to calculate molar heat capacity, enthalpy and entropy as follows:

\[
    c_p(T) = R \left( a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 \right),
\]

\[
    h(T) = R \left( a_0 T + a_1 T^2 + a_2 T^3 + a_3 T^4 + a_4 T^5 + a_5 \right),
\]

\[
    S(T) = R \left( a_0 \ln(T) + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 \right),
\]

Here $R = 8.3145 \text{ J/(mol·K)}$ is the universal gas constant, $\ln(T)$ is a natural logarithm of temperature.

Density for each specie was calculated as for a perfect gas:

\[
    \rho = \frac{P}{RT}.
\]

Air

Specific heat capacity of air at a temperature between 273 and 1100 K (0..827 °C) has a plateau, which makes analytical approximation an arduous task. However, OpenFOAM allows two-range definition of thermodynamic properties. This approach was utilized to precisely define molar heat capacity, enthalpy, and entropy of air with (22)–(24) and coefficients from Table 1.

| $T$, K | $a_0$     | $a_1$      | $a_2$      | $a_3$      | $a_4$      | $a_5$     | $a_6$     |
|--------|-----------|------------|------------|------------|------------|-----------|-----------|
| 300-1100 | 3.72891   | -1.82E-03  | 4.45E-06   | -3.11E-09  | 7.28E-13   | 414.37    | -7.36     |
| 273-300  | 3.503921775 | 0          | 0          | 0          | 0          | 433.9     | -6.45     |

Molecular viscosity of air was calculated with Sutherland approximation with coefficients, adopted for the temperature range mentioned above:

\[
    \mu_{\text{air}} = \frac{1.46e^{-6} \sqrt{T}}{1 + 110.62/T}.
\]
Water vapor

Water in a continuous phase is expected to be a vapor at atmospheric pressure. When $T < 373$ K water vapor was considered to be saturated. Molar heat capacity, enthalpy, and entropy of water vapor were defined with (22)–(24) and coefficients from Table 2.

Table 2. JANAF Thermodynamic coefficients for water vapor.

| $T$, K | $a_0$  | $a_1$  | $a_2$  | $a_3$  | $a_4$  | $a_5$  | $a_6$  |
|--------|--------|--------|--------|--------|--------|--------|--------|
| 373-1100 | 11.1605 | -3.95E-02 | 8.06E-05 | -6.91E-08 | 2.18E-11 | 3290.56 | -39.94 |
| 273-373  | 1.59259 | 1.19E-02 | 3.67E-05 | -2.91E-07 | 4.39E-10 | 4546.26 | 5.71   |

Molecular viscosity of water vapor was calculated with Sutherland approximation with coefficients, adopted for the temperature range mentioned above:

$$\mu_{\text{air}} = \frac{2.45e^{-6}\sqrt{T}}{1 + 1062.72/T}.$$  (27)

2.6. Mesh Dependency Analysis

Mesh dependency was checked on 4 meshes with average cell sizes 5, 10, 20, and 40 mm. Continuous phase temperature and humidity ratio (HR) were used as control parameters. Measurements were taken at every 10-th timestep in locations corresponding to adopted experimental data [12]: $x, y, z = -0.195, 2.3, 0.195, -0.195, 2.3, 0, -0.195, 2.3, -0.195, 0, 2.3, 0.195, 0, 2.3, 0, 0, 2.3, -0.195, 0.195, 2.3, 0.195, 0.195, 2.3, 0, 0.195, 2.3, -0.195$. Temperature discrepancy was negligible, thus humidity ratio was considered. Discrepancy between 5 and 10 mm meshes was less than 0.6%, thus the latter was used in the main simulations. Average values of 3 measurement points for each mesh are presented on figure 1.

Figure 1. Mesh dependency
2.7. Numerical Model Validation
Control parameters and measurements locations from mesh dependency analysis (temperature and humidity ratio of continuous phase) were used for model validation. Validation was conducted by comparison of simulation results with adopted experimental data [12].

Humidity ratios were calculated from dry and wet bulb temperatures available in experimental datasheets. Since reported temperature uncertainty was 0.3 K, humidity ratio uncertainty was considered 0.6 K.

Simulation results in three measurement points were sufficiently accurate, although not always within instrumental uncertainty range (see figures 2 and 3). Overall discrepancy between experimental measurements and simulation results was within 0.2% for temperature and within 7% for humidity ratio. Thus simulation results were considered to be accurate enough to validate the model.

![Figure 2. Validation by temperature.](image)

![Figure 3. Validation by humidity ratio.](image)
3. Results and Discussion

As droplets simulated with Lagrangian particles, their interaction with computational domain boundaries is crucial for the process. There are three main types of interaction: rebound, stick, and escape. That means the particles can be set to rebound back into the domain when hitting boundaries, stick to them or escape the domain through them.

Clearly, droplets should rebound from inlet boundary to prevent unintentional mass loss. Droplets also should escape the domain through the outlet. However, physical walls of the tunnel and virtual walls of drift eliminator are the subject to discuss. The base case was to treat tunnel walls and drift eliminator as escape interfaces for droplets. Physically droplets should stick to walls and form thin film to drain later downwards. However, it was assumed that liquid film contribution to heat balance of the flow is negligible. Thus film formation was discarded to simplify the model, as accumulating Lagrangian particles is a major slowdown factor for simulation.

To illustrate the effect of droplet–wall interaction scenario on temperature and humidity ratio distributions a 2D computation domain was considered. The 2D domain was a longitudinal central section of the original 3D domain. Cutting 2.5 magnitudes of mesh cells count, allowed us to simulate droplets sticking to the eliminator walls.

The results show noticeable temperature drop (about 3 K) and humidity ratio rise (3–4 g/kg of dry air) (see figures 4 and 5). Temperature drop was expected due to the eliminator acting as a wet porous medium where excessive evaporation occurs. The eliminator is acting as a wet porous medium where excessive evaporation occurs, which causes humidity ratio rise and temperature drop.

It should be mentioned that sticking droplets to the drift eliminator causes numerical instability, which in the present study was negotiated by solvers’ relaxation and limiting total parcels (groups of Lagrangian particles) count in the domain.
4. Conclusion
Numerical simulation of water spray evaporation in a counterflow of hot air was carried out with the OpenFOAM platform. Developed computational model incorporated custom definitions for thermophysical properties of the working mediums and utilized virtual interfaces (baffles) to represent a drift eliminator. The results of the present work can be summarized as follows:

(i) Overall temperature distribution is not affected by mesh resolution up to 40 mm cell size while using k-\( \varepsilon \) model. However, the model tends to overestimate humidity rate on meshes with cells larger than 20 mm.

(ii) Accumulation of droplets in the eliminator results in noticeable temperature drop (about 3 K) and humidity ratio rise (3-4 g/kg of dry air).

References
[1] Adachi M, McDonell V G, Tanaka D, Senda J and Fujimoto H 1997 SAE Tech. Paper Ser. 970871
[2] Belbari R, Ghiaus C and Allard F 2006 Solar Energy 80 1540
[3] Dickinson D R and Marshall W R 1968 AIChE J. 14 541
[4] Fisenko S P, Brin A A and Petruchik A I 2004 Int. J. Heat and Mass Transfer 47 165
[5] Lacour S O L, Flick D, Trinquet F, Leducq D and Vende P E 2020 Appl. Thermal Eng. 180 115652
[6] Montazeri H, Blocken B and Hensen J L M 2015 Building and Environment 83 129
[7] Okada S, Ohsaki S, Nakamura H and Watano S 2020 Chem. Eng. Sci. 115938
[8] Raoult F, Lacour S, Carissimo B, Trinquet F and Fournaison L 2018 Appl. Thermal Eng. 149 960
[9] Rivas A and Villermaux E 2016 Phys. Rev. Fluids 1 014201
[10] Safiullah, K N and Youichi O 2021 Int. Comm. Heat and Mass Transfer 123 105184
[11] Som S K and Dash S K 1993 J. Phys. D: Appl. Phys. 26 574
[12] Sureshkumar R, Kale S R and Dhar P L 2008 Appl. Thermal Eng. 28 349
[13] Sureshkumar R, Kale S R and Dhar P L 2008 Appl. Thermal Eng. 28 361
[14] Tissot J 2011 Improving the energy and environmental performance of refrigeration systems by misting air condensers (Doc. diss. in French, U. of Lorraine).
[15] Zuo B, Gomes A M and Rutland C J 2000 Int. J. Engine Research 1 321