New lagrangian approach for wet plume modelling

Jean-Marc Lacome, Frédéric Tognet, C. Olry, M. Nibart

HAL Id: ineris-00973695
https://ineris.hal.science/ineris-00973695

NEW LAGRANGIAN APPROACH FOR WET PLUME MODELLING

JM Lacome[1], F Tognet[1], C Olry[2], M Nibart[2]

[1]INERIS, Parc Technologique ALATA; 60550 Verneuil en Halatte, (France).
[2]Aria Technologies, 8 rue de la Ferme 92100 Boulogne-Billancourt, (France)

Abstract:
A new version of the lagrangian dispersion modelling system Micro-SWIFT-SPRAY (MSS developed by ARIA Technologies and ARIANET) has been developed in order to allow simulation of wet plume, microorganisms, insecticide or pesticide dispersion. For all these applications, it is necessary to take into account both gas and liquid phase evolution including mass and heat transfer. In the particular case of microorganisms distinct behaviors potentially occur when transported by the liquid and/or the gas phase. Following the MSS lagrangian approach, it is easy to define a mass quantity of vapor and a large number of droplets of the same diameter by a virtual particle. Hence a spectrum of different size of droplets can be model using several virtual particles. The development of the new module consists of modelling the physical phenomenon of evaporation and condensation inside a wet plume taking into account temperature and humidity of ambient atmosphere. Microphysics of droplet is solved using the classical laws of evaporation/condensation processes in the surrounding atmosphere. The calculated evaporation rate allows to estimate the diameter evolution and the temperature inside the droplet. The difficulty consists in characterizing the surrounding atmosphere. The interaction between droplets and ambient humidity has been performed on an eulerian frame. Two methods of two way coupling have been tested on academic cases (0D). The proposed paper will present the two approaches and the obtained results.

Key words: Microphysics, lagrangian, dispersion, modelling, spray, microorganisms, legionella, wet plume,

INTRODUCTION

Microphysical processes acting in a wet plume can be taken into account in 3D dispersion models like CFD. However, simulations can be complex to carry out and costly in computation time, particularly when a release have to be simulated over a few days to several weeks. Several Gaussian models offer simplified microphysics modules, however these models include simplified description of physics which is not relevant for complex flows which occur in urban areas. Even so applications may be multiple: transport of bioaerosols, plumes visibility and influence of wet plumes on plume dispersion. The development of a microphysics module in the Lagrangian model Micro Swift Spray allows to overcome the lack of tools available for these issues.

The basic of the new model is that virtual particles created by the lagrangian model include droplet spectrum of liquid water, vapor and microorganisms. Initially, the microorganisms are contained in water droplets. Evaporation rate is calculated for each droplet using the number of sherwood and correlation of Ranz and Marshall (1952 a,b). The evolution of droplet temperature is driven by the generic Lagrangian equation (Miller et al., 1998). Water vapor diffusion into the air is solved on a eulerian grid, this allows computation of diffusivity using the formulas of List (1963) and Bolz and Tuve (1976). Finally, the evolution of the density and temperature within the plume is determined by using the equations of Glendening (1984). When Water droplets are completely evaporated, microorganisms are released and start to disperse as free airborne. A simple biological model based on an exponential survival of microorganisms is applied at this specific moment when microorganisms are directly exposed to radiation, air temperature and humidity.

In the specific case of Legionella, accidental spread in the atmosphere due to contaminated cooling towers (CT), may disperse over a large distance (Nguyen, 2006). In this work a specific biological module has been developed and coupled with the MSS microphysic module. A first evaluation is done with the simulation of dispersion field campaign of biological aerosols performed by CSTB, DGA and INERIS.

MICROPHYSIC OF DROPLET

A multiplicity of thermo dynamical processes can occur within a plume released by a cooling tower. At the tower exit the plume is composed by a turbulent mixture of liquid droplets and vapour gas, which temperature is generally greater than ambient temperature. This bi-phase mixture is generally emitted with a vertical velocity that ranges from $\sim$ ms^{-1} to a dozen ms^{-1} for large towers and as the plume rise it will be transported by wind. The liquid fraction value at the tower exit could be approximately considered around $\sim$ 10% or less. This fraction is composed by a spectrum of droplets which evolves due to phenomena of nucleation, coagulation, evaporation,

condensation, all of them being influenced by the turbulence of the flow. The droplets can coagulate between them mainly within area of the plume with high number densities. Such a phenomenon contributes to decrease the number of droplets and to reach a diameter of equilibrium.

Heat transfers between droplets and vapour contribute to the evaporation of the droplets by heat mass transfer depending of the saturation level. Far away the droplets are assumed to reach an equilibrium temperature with the ambient air. The kinetics of evaporation and condensation strongly depends on the humidity saturation of the surrounding atmosphere. This latter evolves following interactions between the wet plume and the ambient flow which humidity level is a variable of primary importance. At the emission exit the droplets which are large enough can be affected by gravity, particularly those located in the surrounding of the release. In case of presence of drops with large radius (> 40 μm) (Bouzereau et al., 2008) precipitation phenomena could occur but it's unlikely the case in the investigated applications (CT). In the far field dispersion, the median diameter is smaller but sedimentation can also affect the vertical velocity of the droplet.

Due to the great number of phenomena described above it was decided to launch the development of the new model by focusing on modelling evaporation and condensation. These phenomena play major roles in the temperature and diameter equilibrium of the droplets and its lifetime in the atmospheric far field dispersion.

NEW LAGRANGIAN APPROACH FOR WET PLUME

In the LPD model Micro-SPRAY, the dispersion of a wet plume is simulated following the motion of a large number of fictitious particles, each one representing a part of the mass of vapour and liquid water emitted from sources of general shapes. Starting from a given spectrum of droplets, each virtual particle carries a large number of droplets sharing the same geometric and thermodynamic properties. Particle's transport is obtained applying an equation of motion where the particle velocity is split into a mean component driven by the local wind reconstructed by Micro-SWIFT and a stochastic component obtained by solving a 3-D form of the Langevin equation of the random velocity (Thomson, 1987).

As far as the wet plume has a vertical or oblique initial momentum and an initial buoyancy, five governing conservation equations of mass, energy, vertical momentum and the horizontal momentum are integrated for each particle at each time step, based on Glendening et al. (1984), Hurley (2005) and Hurley and Manins (1995). These equations are described as follow:

$$u_s = \sqrt{u_p{}^2 + v_p{}^2 + w_p{}^2} \tag{1}$$

with u_p, v_p, w_p velocities of particles at emission point.

$$B = g(\rho_a - \rho_p)/\rho_a \tag{2}$$

$$E = 2bu_e \tag{3}$$

$$u_e = \left[\alpha_1 \left| u_s - U_a \cos(\psi_p - \psi_a)\cos(\phi_p - \phi_a) \right| + \alpha_2 \left| U_a \left[1 - \cos^2(\psi_p - \psi_a)\cos^2(\phi_p - \phi_a) \right]^{1/2} \right| \right] \tag{4}$$

with a, p refer to air and plume, respectively, b is the plume radius (m), B is the buoyancy (ms^{-2}), E represents the entrainment rate (m^{2}s^{-1}), u$_e$ is the entrainment velocity (ms^{-1}) and Ψ and Φ are the vertical and horizontal angles. The following conservation equations are solved:

mass
$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2 \right] = E u_s \tag{5}$$

energy
$$\frac{d}{dt}\left[u_s b^2 B \right] = -\frac{\rho_p}{\rho_a} N^2 u_s w_p b^2 \tag{6}$$

vertical momentum
$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s w_p b^2 \right] = B b^2 u_s \tag{7}$$

x horizontal momentum
$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2 u_p \right] = E u_s u_a \tag{8}$$

y horizontal momentum

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}u_s\,b^2\,v_p\right] = E\,u_s\,v_a \tag{9}$$

where u_a and v_a are the horizontal components of the wind velocity, N^2 is the Brunt-Vaisala frequency. On one hand, by integrating this set of conservation equations, the temperature of the plume at the location of each virtual particle is known and used to drive the evaporation process of droplets. On the other hand, the concentration of water vapour is computed on an eulerian grid at each time step, using the background 3D field of specific humidity provided by Micro-SWIFT (Moussafir et al., 2004) and the vapour carried by fictitious particles. In each grid cell, concentration of vapor is compared to the saturation concentration and, as a result, evaporation or condensation can occur.

In grid cell where condensation or evaporation takes place, transfer of mass between vapor phase and liquid phase occurs internally to each virtual particle present in this grid cell. Where condensation happens, this transfer is done until the concentration of vapor is locally equal to the saturation concentration. Where evaporation happens, two different approaches can be followed:
 1) Microphysic of droplets disabled: Transfer from liquid phase to vapor phase is done until the concentration of vapor is equal to the saturation concentration.
 2) Microphysic of droplets enabled: evaporation rate at each time step is calculated for each type of droplets using the number of sherwood and correlation of Ranz and Marshall (1952 and 1953) together with the molecular diffusivity. This diffusivity can be computed by using the formulas of List (1963) or Bolz and Tuve (1976). Given this evaporation rate, mass and diameters of droplets are updated. Finally, the evolution of droplets temperature is also updated by using the following equation (Miller et al., 1998):

$$\frac{dT_{droplet}}{dt} = \frac{Nu}{3\text{Pr}}(\frac{\theta_1}{\tau_d})(T_{air}-T_{droplet})+\frac{L_v}{C_L}\frac{(d\,m_{droplet}/dt)}{m_{droplet}} \tag{10}$$

where $dm_{droplet}/dt$ is negative for evaporation, T_{air} and $T_{droplet}$ are respectively the local carrier plume temperature and the droplet temperature, L_v is the latent heat of evaporation, the ratio of the gas heat capacity to that of the liquid phase is $\theta_1 = C_{p,air}/C_L$, Pr is the gas phase Prandtl number; τ_d the particle time constant for Stokes flow and Nu the Nusselt number.

VALIDATION TEST (0D)

In order to validate the evaporation process when microphysic of droplets is enabled in MSS, the evaporation rates of several sizes of droplets subjected to different humidity, temperature and wind velocity conditions were computed. Results have been compared to measurements of evaporation rates and model predictions both described in Kincaid et al (1989). His model is based on modified Ranz and Marshall equations proposed by Goering et al. (1972). Figure 1 shows that the results obtained when using List diffusivity formula are in good agreement with both Kincaid's model and measurements.
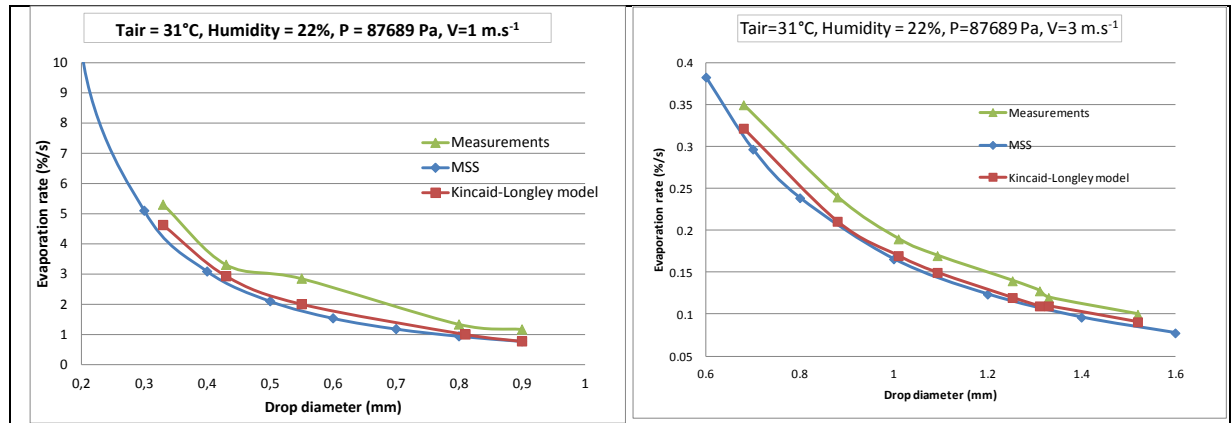

Figure 1: Evaporation rate of droplets in different conditions

Starting from initial droplet temperatures situated above and below the wet bulb temperature, the evolution in time of the temperature of the droplet was tracked until $|dT_{droplet}/dt| < \varepsilon$ (where ε is a small threshold value). Drops of temperature predicted by MSS and by the model used in Kincaid et al. (1989) are shown on Figure 2. Results from MSS calculation show that the temperature evolution is very similar to the Kincaid model prediction. However we notice that in MSS the droplet temperature drops below the wet bulb temperature. Shirai et al. (Shirai et al., 1971a,b) emphasized that measured droplet temperatures slightly lower than wet bulb temperatures were experimentally observed. An explanation provided in Kincaid et al. (1989) could be that a water droplet may evaporate more efficiently than a wick-covered thermometer.
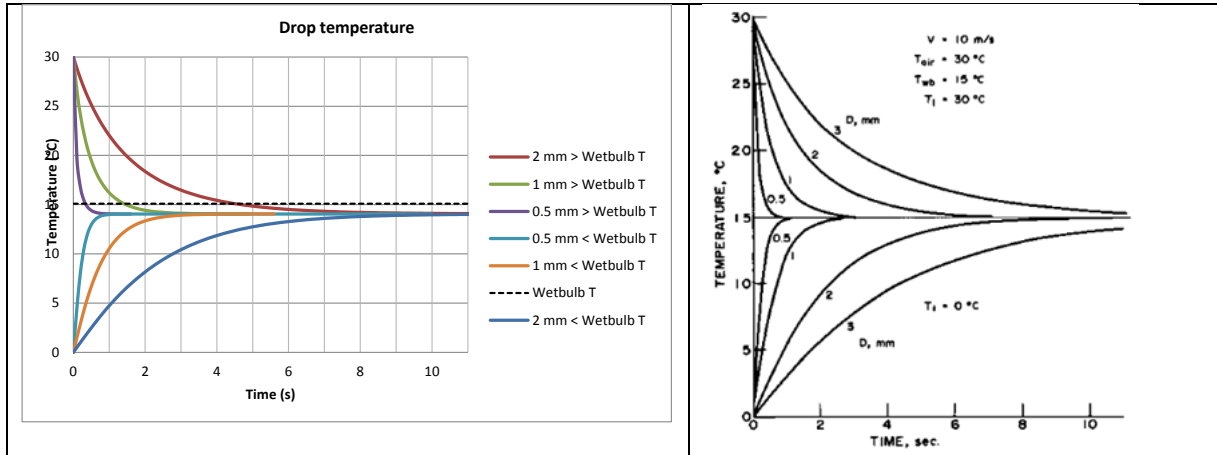

Figure 2: Evolution of temperature of droplets of different sizes, with initial temperature below or above the wet bulb temperature; left figure: prediction by MSS, right figure: Kincaid et al. (1989)

APPLICATIONS FOR A BIOLOGICAL MODEL

The model described above has been extended to model microorganism's transport. The underlying principle is that the virtual particles created by the lagrangian model include a droplet spectrum of liquid water, vapour and microorganisms. Initially, the microorganisms are assumed to be contained in water droplets. When water droplets are totally evaporated, microorganisms are released and transported as free airborne tracers. With respect to microorganisms, a consideration of sustainability must also be included in the code. An experimental laboratory approach specific to *Legionella pneumophila* has been carried out by CSTB and provided an useful knowledge (Ha T.L, 2005) on the bacteria sustainability using radiation, air temperature and humidity parameters. Following this experimental approach a model of sustainability has been set and coupled with the transport model. This biological model based on an exponential survival of microorganisms is applied during the free airborne transport only.

The main characteristics of this biological model are as follow:
- model is disabled for bacteria located in a virtual particle including water liquid,
- model is enabled for bacteria located in a virtual particle as soon as this particle is totally dry.
- When sustainability model is enabled, sustainability criteria are as follow:
  - Minimal and maximal temperature of sustainability (T_{min} and T_{max})
  - Net minimal and maximal radiation (Ray_{min} and Ray_{max})
  - Minimal and maximal relative humidity (HR_{min} and HR_{max})

For each -time step, the local temperature T, the local radiation Ray and relative humidity RH (taking into account the relative humidity provided by Meteorological input as well as the contribution of the water vapor contained in the wet plume) are checked with the following conditions :

$$T_{min} \leq T \leq T_{max} , \ Ray_{min} \leq Ray \leq Ray_{max} , \ HR_{min} \leq HR \leq HR_{max} \qquad (11)$$

At any time step Δt , if one or more of these conditions of sustainability is not satisfy, a number of spores lost by the virtual particle concerned is estimated. Naming α_i the decay parameter of the law of sustainability, the number of spores remaining after application of the survival model is as follows:

$$N_{spores}(t + \Delta t) = N_{spores}(t).e^{-\alpha_i \Delta t} \tag{12}$$

A study supported by the AFSSET (Agence Française de Sécurité Sanitaire de l'Environnment et du Travail) consisted of estimating the ability of the model Micro Swift Spray to predict the potential spread of microorganisms by an anthropogenic source resembling a cooling tower, by comparing data from the simulation with experimental measurements. Results were presented in the HARMO 14 session (Tognet, 2012) and parts of the conclusion are presented here. The simulation of the health risk caused by *L. pneumophila* aerosolization from a CT is possible but would require a finer characterization of the environment, the air flow conditions and source term, as well as additional knowledge on the ecology of *Legionella* before and after aerosolization (isolated bacteria in biofilm or with other interaction), the latter may be critical to the sustainability model. The choice of the model type (i.e. Gaussian, Lagrangian or Eulerian, with specific sustainability model or not) will depend on the expected accuracy and duration of the simulations requested by the authorities for the decision making process. It was experimentally demonstrated that, the dispersion of relative efficiencies of biocollectors is three times higher for these tests compared to controlled environment. While this does not preclude the ability of biocollectors to detect low concentrations of aerosolized microorganisms, the development of metrology is an important goal for improvement.

DISCUSSION AND CONCLUSION

The purpose of the present work is to develop a dispersion model for better understand outbreak consequences from a suspicious source of wet plume release over a few days to several weeks. If we consider that the modelling system Micro-SWIFT-SPRAY ensures a reliable description of the meteorological process in a reasonable computational effort, a model of evaporation/condensation for droplet has been implemented within the lagrangian dispersion model SPRAY. The droplet temperature is driven by the generic equation described in Miller et al., 1998. In order to validate (0D), evaporation rates of droplets, subjected to different conditions, were computed and comparisons with both Kincaid's model and measurements (Kincaid et al., 1989) give good agreements. A procedure of test case in 3D is presently carried out. By comparisons with both other lagrangian approach implemented in SPRAY (Mortarini et al., 2012) and CFD Code_Saturne (Bouzereau et al., 2008). These comparisons should provide hindsight on both lagrangian approach and eulerian approach.

REFERENCES

Bolz, R.E.,TUVE, G.L., 1976. CRC *Handbook of tables for applied Engineering Science*, 2nd Edition, Boca Raton (USA) : CRC Press, Inc, 1976. 1166 p. ISBN 0-8493-0252-8.

Bouzereau E., Musson Genon L. Carissimo B., 2008. Application of a semi-spectral cloud water parameterization to cooling tower plumes simulations. Atmospheric Research 90 (2008) 78–90.

Ha T.L., 2005, Etude de l'aérosol de *Legionella pneumophila*. Phd thesis report, Paris XII University.

Hurley, P.J., Manins, P.C., 1995. Plume Rise and Enhanced Dispersion in LADM. ECRU Technical Note No.4. *CSIRO Division of Atmospheric Research*, Australia.

Hurley P.J., 2005. The Air Pollution Model (TAPM) Version 3. Part1: Technical Description. *CSIRO Atmospheric Research Technical Paper* No. 71.

Goering, C. E., L. E. Bode and M. R. Gebhardt. 1972. Mathematical modelling of spray droplet deceleration and evaporation. *Transactions of the ASAE* 15(2):220-225.

Glendening J.W., J.A. Businger, and R.J. Farber, 1984., "Improving plume rise prediction accuracy for stable atmospheres with complex vertical structure". *J. Air Pollut. Control Ass.*, 34:1128–1133.

D. C. Kincaid, T. S. Langley. A Water Droplet Evaporation and Temperature Model. 1989; *Soil and Water Div. of ASAE*.

List, Robert J. 1963. Smithsonian Meteorological Tables. 6th rev. ed., The Smithsonian Institution, Pub. 4014.

Miller, R.S., Harstad, K., Bellan J., 1998. Evaluation of equilibrium and non-equilibrium evaporation models for many-droplets gas liquid flow simulation, Jet propulsion Laboratory, California Institute Technology, Passadena, *International Journal of Multiphase Flow* 24, 1998.

Mortarini L., Carlino G., Tinarelli G., Mauri L., Trini Castelli S., Anfossi D., 2012. Development of the microscale lagrangian particle dispersion model MicroSpray for the simulation of two-phase releases, *Harmo 14*, Kos, Greece.

Moussafir, J., Oldrini, O., Tinarelli, G., Sontowski, J., Dougherty, C., 2004. A new operational approach to deal with dispersion around obstacles: the MSS (Micro-Swift-Spray) software suite. *In: Proc. 9th Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, vol. 2, pp. 114-118.

Nguyen T. M. N, Ilef D., Jarraud S., Rouil L., Campese C., Che D., Haeghebaert S., Ganiavre F., Marcel F., Etienne J., Desenclos J.C., 2006. A community-wide outbreak of legionnaires disease linked to industrial cooling towers--how far can contaminated aerosols spread ? *The Journal of Infectious Diseases*, 193, 1, 102-111.

Ranz W. E. and Marshall W. R. 1952a. *Chem. Eng. Prog*. 48 141.

Ranz W. E. and Marshall W. R. 1952b. *Chem. Eng. Prog*. 48 173.

Shirai, K., S. Matsui and A. Shinjo. 1971. On the temperature change of sprayed water drops. I: Theoretical Study. *Transactions of the Japanese Society of Irrigatio. Drainage and Reclammation Engineering* 35:24-29.

Shirai, K., S. Matsui and A. Shinjo. 1971. On the temperature change of sprayed water drops. II: Experimental Study. Sprinkler Irrigation. *Transactions of the Japanese Society of Irrigation. Drainage and Reclamation Engineering* 35:30-35.

Thomson D.J. 1987. Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech.*, 180, 529-556.

Tognet F., Turmeau C., Ha Ti L., Tarnaud E., Rouïl L., Bessagnet B., Robine E., Morel Y., 2012, Numerical modelling of microorganisms dispersion in urban area: Application to legionella, *Harmo 14*, Kos, Greece.