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Numerical Method for Determining the Droplet Size Distributions of Spray Nozzles Using a Two-Zone Model

W. Plumecocq*, L. Audouin, J.P. Joret, H. Pretrel

Institut de Radioprotection et de Sûreté Nucléaire (IRSN), PSN-RES, SA2I, LEF, Cadarache, St
Paul-Lez-Durance Cedex, 13115, France

* Corresponding author -E-mail address: william.plumecocq@irsn.fr

ABSTRACT

The water spray systems is widely used for fire safety area and is a well-established technique for providing safety and protection of nuclear installations and also in industrial facilities. One major challenge is to be able to properly determine the technical features of the water spray system that are required for predictive simulations. For that, a Phase Doppler Interferometer (PDI) device, that is a complex and challenging laser technique, is often used to measure the droplet size distributions and the droplet velocities. However, some usual water spray models can require as input parameters only an overall droplet size distribution and an initial velocity and some statistical methods are needed to determine them from local accurate measurements. In this paper, it is addressed a new calibration approach for assessing the input parameters of this modeling by using large-scale and well-controlled fire tests. Then, by introducing some correlations to take into account different operating conditions of the pressure at the nozzle head, this technique is validated on other large-scale fire tests. After discussing thoroughly the results, this new method shows that it can be a valuable and efficient tool for determining the overall features of water spray systems linked with the modeling of water spray system used in this study.

Keywords: SYLVIA, Fire modeling, Spray modeling, Droplet size distribution

NOMENCLATURE

Acronyms

PDI	Phase Doppler Interferometer
PID	Proportional–Integral–Derivative

Symbols

A	Cross-section area of the branch [m ²]
B _M	Spalding number for the mass [-]
$\bar{c}$	Average molar concentration [mol m ⁻³]
C _D	Drag coefficient [-]
CMD	Count median diameter [m]
d	Diameter [m]
D _A	Nozzle orifice size [m]
$\bar{D}$	Average diffusion coefficient [m ² s ⁻¹]
f	Distribution function of droplets [m ⁻⁴]
g	Gravity acceleration [m s ⁻²]
h	Branch's characteristic function [Pa]
H	Specific enthalpy [J kg ⁻¹]
HRR	Heat release rate [W]
k	Orifice flow coefficient [l min ⁻¹ bar ^{-0.5}]
L	Length of a branch [m]
m	Mass [kg]
MMD	Mass median diameter [m]
M	Molar mass [kg mol]

Nu	Nusselt number [-]
n_0	Number concentration of droplets [m^{-3}]
P	Total pressure [Pa]
Pr	Prandtl Number [-]
Q	Volumetric flow-rate [$\text{m}^3 \text{s}^{-1}$]
Q_m	Mass flow-rate [kg s^{-1}]
R_{lin}	Aeraulic resistance (linear part) of a resistive element [$\text{kg s}^{-1} \text{m}^{-4}$]
R_{quad}	Aeraulic resistance (quadratic part) of a resistive element [m^{-4}]
RH	Relative humidity [%]
S_l	Source term l of the ODE system [-]
Sc	Schmidt number [-]
Sh	Sherwood number [-]
t	Time [s]
T	Temperature [K]
U	Internal energy per unit volume [J m^{-3}]
v	Velocity [m s^{-1}]
X	Molar fraction [-]
We	Weber number [-]
z	Height [m]

Greek letters

α	Nozzle coefficient [-]
γ	Specific coefficient depending on the conservation equation [-]
ε	Emissivity [-]
λ	Thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$]

$\emptyset$	Physical quantity of interest (mass, enthalpy, mass fraction...) [-]
ρ	Density [kg m^{-3}]
σ	Stephan-Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]
σ_g	Geometric standard deviation [-]
σ_w	Surface tension of droplet [N m^{-1}]
ρ_g	Geometric standard deviation [-]

Subscripts

dn	Downstream
g	Gas
i	Interface
l	Index of the source term in the ODE system
lin	Linear
low	Lower layer (2-zone modeling)
quad	Quadratique
s	Water vapour
up	Upstream or upper layer (2-zone modeling)
w	Water droplet
∞	Bulk

1 INTRODUCTION

Water spray systems used for fire safety area is a well-established technique for providing safety and protection of industrial and nuclear installations. The research in the domain of water spray systems remains important due to the complexity involved in predicting the interaction between the water sprays and the fire environment. Indeed, a continuous

research activity is underway to improve the capability of modeling and predicting tools ([1]-[6]), to measure accurately the characteristics of water spray systems ([7]-[10]) and to investigate the efficiency of such systems ([11]-[13]) depending on the technique of water spraying of interest and on the objectives sought (for instance, fire extinction by flame cooling and oxygen concentration reduction through an increase of water vapor content, reduction of the aggressive features of hot smoke by gas cooling and soot removal by spray droplets or protection of structural elements by direct or indirect cooling).

The main advantages of sprinkler or deluge water spray systems are the wide availability, the relative low cost, the low level of operating pressure (<5 bar except for water mist system) and a good efficiency in fire suppression if enough large amounts of water are supplied in relevant location and early time. An accurate experimental characterization of the spray nozzle in terms of droplets size distribution at injection and initial velocity of droplet is required as input data for predicting tools since droplet evaporation kinetics is highly dependent on droplet size and droplet fall time. Nevertheless, determining the water spray characteristics could be very challenging due to the design of spray nozzles (i.e. the geometric features of sprinkler head) mainly made for practical engineering goals involving often the complexity of water spray behavior (especially the breakup process of water jet inducing large variations of droplet size and velocity close to the nozzle, and various spray diameter). In order to determine the main technical features of a water spray system, a Phase Doppler Interferometer (PDI) device is generally used to measure the droplets size distributions and the droplets velocities allowing to perform accurate local measurements. Nevertheless, some usual water spray models ([1], [6]) can require as input parameters only an overall droplet size distribution and an initial velocity. Thus it is needed to process some statistical methods over these experimental data to determine

them. A second difficulty is linked to the high sensibility of droplets size distribution and droplets initial velocity due to the pressure effect at nozzle head. Indeed, an initial characterization of a water spray system is performed at a given pressure for the nozzle head before using in fire scenario. However, a slight change of water flow-rate (i.e. pressure head) can lead to significant variations of droplets size distribution and droplets initial velocity. Thus, an adjustment on both droplets size distribution and on droplets initial velocity must be performed in predictive simulations in case of change of spray water flow-rate compared to the one used during the initial characterization of the water spray system. The last difficulty lies on the experimental measurement of droplets initial velocity used as input data in spray modeling. Water droplets from sprinkler or deluge spray nozzles are produced by impingement of the water jet on the deflector of the nozzle. Droplet velocities measurements are consequently performed several tens of centimeters below the spray nozzle (see [8] for instance). At this elevation, the droplets are under-relaxed and so the velocity measurements do not correspond strictly to initial velocity of droplets.

As an alternative way for defining the features of spray nozzles, a numerical method for determining droplets size distributions and droplets initial velocity is then developed using both the SYLVIA two-zone model [25] and experimental data [11]. Indeed, this approach proposes to perform a calibration of spray modeling by means on full-scale fire tests in enclosure, for which the fire power and the ventilation system are perfectly controlled.

After a brief description of SYLVIA software (see also the appendix) and of the water spray modeling, this work addresses a new calibration approach for assessing the input parameters of this modeling by using large-scale scale fire tests in DIVA facility [11]. Then, this technique is validated on other fire tests having different pressure heads for the water spray nozzles. The results of this study are discussed thoroughly and show that this

new approach can be a valuable and efficient tool for determining the overall features of water spray systems based on the spray modeling used in this work.

2 BRIEF DESCRIPTION OF SYLVIA SOFTWARE

The SYLVIA software [25] is developed at the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) to simulate a full ventilation network, fire scenarios in a highly confined and ventilated facilities, and airborne contamination transfers inside nuclear installations. This software is based on a zone approach which consists in calculating mass and energy balances in each of two zones, separated by an interface, which constitute the enclosure (fire room or not): the lower zone simulating the fresh gas and the upper zone simulating the combustion products and the gas entrained by the plume. In a zone approach, a plume feeds the upper zone of the fire room, whose volume increases, which has the effect of lowering the interface if the gas flow in the exhaust duct or at the level of openings of the fire room is not sufficient to remove all gases supplied by the plume. An overview of the main technical features of SYLVIA software is available further in appendix 7.

3 SPRAY MODELING

3.1 Model description

3.1.1 Droplets size distribution

The spray model implemented in the SYLVIA software is based on mass and heat transfers between droplets and surrounding gas during their fall [1]. No direct interaction between spray droplets and the fire source is modeled. The rates of mass and heat transfers between surrounding gas and falling droplets during the evaporation process are strongly dependent on the droplet size. To characterise statistically the droplet size in a control volume, a

concept of distribution function $f(r)$ is introduced whose mathematical properties are similar with those of a density of probability. This function is such as the number of droplets per unit of volume for droplet diameters from d_w to $d_w + dd_w$ is:

$$(1) \quad dn = f(d_w) dd_w$$

In practice, the droplets size distribution produced by most of spray nozzles are often well represented by a log-normal distribution function as:

$$(2) \quad f(d_w) = \frac{n_0}{\sqrt{2\pi} d_w \ln \sigma_g} \exp \left[-\frac{\left(\ln \frac{d_w}{CMD} \right)^2}{2 (\ln \sigma_g)^2} \right]$$

The log-normal distribution function requires the knowledge of two parameters for determining it: the geometric standard deviation σ_g that describes the dispersion of the distribution function and the count median diameter (CMD) or the mass median diameter (MMD). The CMD diameter is defined such that the number of droplets having diameter less than the CMD one is equal to half the total number of droplets. It is the median of the number distribution. The MMD diameter is equivalent to the CMD diameter for the mass. For a log-normal distribution function, The MMD diameter is directly related to CMD one by the following equation:

$$(3) \quad MMD = CMD \exp \left[3 \cdot \ln(\sigma_g)^2 \right]$$

3.1.2 Dynamics of droplets

Droplets are assumed to fall down vertically from their injection area (no interaction is considered with room walls). Gas environment is assumed to be steady during a droplet fall (i.e. it is assumed that the characteristic time for a droplet fall is significantly less than the characteristic time for changing the mean gas conditions in the enclosure). The thermal resistance inside the droplet is assumed to be negligible (i.e. thermally thin assumption

for droplets). In a previous study [1], it has been shown that this assumption is well-established. Coalescence of droplets is also neglected according to low droplet fall heights in fire applications (several meters).

The evolution of mass, velocity and temperature of a droplet during its fall is obtained by solving a set of coupled equations for the mass, momentum and energy balance:

$$(4) \quad \frac{dm_w}{dz} = \pi d_w Sh_g \bar{D}_s \bar{c}_g M_w B_M / v_w$$

$$(5) \quad \frac{d}{dz}(m_w v_w) = m_w g / v_w - \frac{\pi d_w^2}{8} C_D \rho_g v_w$$

$$(6) \quad \frac{d}{dz}(m_w H_w) = (\pi d_w \lambda_g Nu_g (T_g - T_w)) / v_w + \epsilon \sigma \pi d_w^2 (T_g^4 - T_w^4) / v_w + \frac{dm_w}{dz} H_s$$

The Spalding number for mass transfer is given by:

$$(7) \quad B_M = \frac{X_{\infty} - X_{sw}}{1 - X_{sw}}$$

Knowing both the gas conditions and the injection conditions of droplets (velocity, diameter and temperature), the dynamics of droplets is defined by the expression of the three dimensionless numbers Sh_g , Nu_g and C_D . The Nusselt number Nu_g and Sherwood number Sh_g are deduced from steady evaporation in dry air of droplets having diameters in the range from 600 to 1100 μm by Ranz and Marshall [2]:

$$(8) \quad Sh_g = 2 + 0.6 Re_w^{1/2} Sc_g^{1/3}$$

$$(9) \quad Nu_g = 2 + 0.6 Re_w^{1/2} Pr_g^{1/3}$$

The drag coefficient C_D is obtained from the Oseen formulation [14] for hard spheres (i.e. impenetrable spheres that cannot overlap in space):

$$(10) \quad Re_w < 3 \quad C_D = 24 / Re_w \quad (\text{Stokes flow})$$

$$(11) \quad 3 < \text{Re}_w < 905 \quad C_D = \frac{24}{\text{Re}_w} \left(1 + \frac{\text{Re}_w^{2/3}}{6} \right) \text{(intermediate flow)}$$

$$(12) \quad \text{Re}_w > 905 \quad C_D = 0.44 \quad \text{(potential flow)}$$

Equations are solved on a fixed meshing by using an Forward Euler method.

3.1.3 Mass and energy balance

The gas composition and temperature are assumed to be homogeneous inside a given zone. The time evolution of the thermodynamics conditions in the room (pressure, temperature and relative humidity) due to the spray is determined from a mass and energy balance. This balance corresponds to the mass and enthalpy removed by the droplet spray during their fall. This one is determined from the results of the dynamics of droplets and the evolution of the droplet distribution function between the top and the bottom of each zone crossed by droplets:

$$(13) \quad \frac{dp_s}{dt} = - \frac{d}{dz} \left(\int f(r) \cdot m_w(r) \cdot v_w(r) \cdot dr \right)$$

$$(14) \quad \frac{dU}{dt} = - \frac{d}{dz} \left(\int f(r) \cdot m_w(r) \cdot H_w(r) \cdot v_w(r) \cdot dr \right)$$

3.2 Validation of the model against the CARAIDAS experiments

An experimental device named CARAIDAS [16] was designed and built at IRSN in order to determine the collection efficiency of aerosols and iodine absorption by droplet spray with representative conditions of nuclear post-accident atmosphere. CARAIDAS allows measuring experimental droplet diameter evolution as a function of different experimental conditions described hereafter.

3.2.1 *Experimental vessel*

The experimental vessel is a 5 meters high cylinder with an inner diameter of 0.6 meter as shown in Figure 1. The vessel is heated up by circulating a thermo-fluid through the double-walled stainless steel casing. Homogeneous thermodynamic conditions are obtained during the experiments by using an air-steam circulation. When operating conditions (pressure, temperature, relative humidity) are reached, the air handling system is stopped and the vessel is thermically insulated. The droplet generator is located at the top of the experimental vessel. In order to release monodispersed droplets, the generator is designed on a break-up process of a water jet to droplets by applying a periodic disturbance. This specific device can produce monodispersed water droplets with a diameter ranging from 200 to 700 μm . Droplets are injected at very low mass flow rate in an ambient atmosphere with steady and homogeneous conditions. Optical measurements of the droplet diameter are performed at three elevations: one at the upper part of the vessel where the droplets are released ($z = 0 \text{ m}$), a second one at about mid-height ($z = 2.51 \text{ m}$) and the last one at the lower part of the device ($z = 4.39 \text{ m}$).

3.2.2 *Results and discussion*

The experimental results obtained from the CARAIDAS device allow validating the modeling of dynamics of water droplets. During these tests, a wide range of experimental conditions was performed: pressure from 1 bar to 7 bar, ambient temperature from 20°C to 160°C, and relative humidity from few percent till 95%. For each test, measurements of the mean droplet diameter and standard deviation of droplets are determined at the three measurement levels. Only experiments performed at atmospheric pressure and low relative humidity (summarized in

Table 1) are used for the validation of the model, corresponding to gas conditions that could be met in the fire room prior the activation of a spray system. Comparison between

experimental data and SYLVIA simulations of droplet diameter evolution is reported in

Table 2. With the proposed formulation of the mass, momentum and heat transfer described previously in section 3.1.2, a very good prediction of the droplets dynamics is obtained on the CARAIDAS tests. Indeed, the difference between experimental data and SYLVIA simulations is typically less than 4%. An equilibrium between the heat flow rate transferred to the droplet and the heat flow rate lost by evaporation is quickly reached in the first meters of the droplet fall. Thus, the temperature inside the droplets can be considered thermically as homogeneous and steady (evaporation period) while its diameter decreases during its fall.

4 CALIBRATION OF SPRAY MODELING BASED ON FULL-SCALE FIRE TESTS IN DIVA FACILITY

4.1 Methodology for the calibration process

A numerical method for determining droplet size distribution and droplet initial velocity of a water spray system using the two-zone model SYLVIA is developed. This method is based on a calibration of spray modeling using full-scale fire tests carried out in the DIVA facility of IRSN. More precisely, a parametric study is firstly performed with the SYLVIA software to adjust the droplet size distribution at injection and droplet initial velocity on a given fire test. Indeed, the numerical technique [15] consists to keep the best inputs for minimizing the difference between some appropriate outputs (or responses) from experiments and simulations. In a second hand, the validation of the method is performed on other fire tests of the campaign with different operating conditions (water flow rate, heat release rate for the fire source, ventilation flow rate) using the same water spray system.

However, several prerequisites in using this method must be observed. First, the heat release rate of the fire source must be well controlled and known to reduced the uncertainties on the prediction of the droplet size distribution and initial velocity. Secondly, spray model used in the method must be relevant with the water spray system of interest. Thirdly, the aeraulic resistivity of the ventilation network must be well simulated by the predicting tool. Indeed, the aeraulic resistivity of the ventilation network plays a major role on the thermalhydraulic behavior in the fire room. Fourth, a minimum of two relevant outputs from the numerical results is required in the parametric study because a single output can lead to a good fit even if the spray model is weakly satisfactory. It is no more the case with several responses.

4.2 Propane gas fire tests

The Propane gas fire tests [11] used for the calibration of spray modeling were conducted in the large-scale DIVA facility of IRSN. The scenario consists of a fire in one room of the facility. This room is a 3.90 m meters high parallelepiped with a ground surface area of 42.3 m^2 ($4.88 \text{ m} \times 8.67 \text{ m}$). Walls are made of re-enforced concrete and the top of the room is covered with a false ceiling made of 100 mm of air, 10 mm of insulated fiber wool panels (Thermals ceramics, Board 607) and 12.7 mm of calcium silicate panels (Monalite M1-A). The ventilation configuration consists of one admission line and one exhaust line in the upper part of the room, at about 0.80 m from the ceiling. The ventilation lines are connected to an industrial ventilation network equipped with blowing and exhaust fans. For all tests, the ventilation is set to the same operating conditions, with a volumetric flow-rate of $2550 \text{ m}^3/\text{h}$ which corresponds to renewal rate of 15.4 h^{-1} . This level of ventilation maintains the fire source under well ventilated conditions. As shown in Figure 2, the fire source is located in a corner of the room in order to minimize water projection directly towards the fire source, fire suppression being not required in these tests. This fire source

is a propane gas burner apparatus that simulates the behaviour of a pool fire. Water spray system is made of two nozzles located at 2.97 m from the ground. The nozzles are connected to a piping system equipped with valves, pressure transducer and water flow rate device. The nozzles are activated manually by opening (or closing) valves on the water pipe. Nozzles are of the deluge type, Protectospray ® D3, HV with a coefficient k of 26 l/min/bar^{0.5} (see Figure 2).

Four fire tests are considered in this study as reported in Table 3. The varying parameters are the heat release rate (HRR) of the fire source (140, 210 and 290 kW) and the total water flow rate of the water spray system (80 and 110 l/min, which corresponds to an operating pressure head of 236 and 447 kPa). HRR is computed as the propane volumetric flow rate measurement multiplied by the gas density and the effective combustion enthalpy of propane (43 MJ/kg). For the four tests, the spray system is activated 8 min after fire ignition, for a 5-min period. The time period for the water spray system to reach the targeted water flow rate or to drop down to zero has a significant influence on the pressure variation inside the fire compartment. For all tests, the water flow rate increases from zero to the targeted value in about 5 s. Water spray is injected at 20 °C.

4.3 SYLVIA modeling of the ventilation network

A fully dataset of the ventilation network of the DIVA facility was used to simulate properly the experimental aeraulic resistivity of the ventilation network for the Propane gas fire tests. Indeed, the various nodes and branches of the modeled ventilation network (see Figure 3) correspond to aeraulic elements for which one or more experimental measurements were performed. In order to prevent some errors for the dataset of the ventilation network, the characteristic of the DIVA ventilation network is processed by means of the experimental data obtained from Propane gas fire tests in operating conditions, just before the fire ignition. Of course, the fire scenario definition is achieved in

SYLVIA by defining the compartment equipment (firebreak doors, fire-dampers, ...), the fire source and the walls properties (possible presence of insulation layers), these features being specific for each test.

4.4 Description of the calibration technique

The goal is to measure the effects of some input parameter variations on some output responses of interest. More precisely, since the uncertainty associated with each considered parameter is summarized by a range of variation, an uniform probability distribution is chosen to represent this information. The propagation through SYLVIA modeling is then achieved by Monte Carlo simulations: each uncertain parameter is randomly sampled according to the chosen probability distribution and then the output of interest is evaluated for each set of values of input parameters provided by the sampling matrix.

The uncertain input parameters of the study are the two parameters characterizing the log-normal distribution function of droplets and their initial velocity:

- Mass median diameter (MMD) of droplets, ranging between 700 and 1200 μm ;
- Geometric standard deviation of the distribution (σ_g), ranging from 1.4 and 1.6;
- Initial velocity of droplets (v), ranging between 5 and 10 m.s^{-1} .

The number of droplet size classes was set constant to 15.

The outputs of the study focus on two major parameters considered as the most influenced by the spray:

- Minimum value of the pressure in the fire room over the spray period;
- Minimum value of the mean gas temperature in the fire room over the spray period.

A first series of about one thousand runs was performed to determine the area of uncertain parameters satisfying in the best the expected responses. A second series was carried out to improve the accuracy of final values for the three input parameters (i.e. MMD, σ_g , v).

4.5 Pressure effect on droplets initial velocity

A change in the pressure at the nozzle head leads to a change in the droplets initial velocity. The sprinkler orifice is designed to provide a known water flow rate at a design water pressure. Sprinkler orifices verify the Bernoulli's orifice equation, which states that the velocity of the water through the orifice is proportional to the water pressure [7]. Since the volumetric flow rate is more suitable than the velocity for applications, the Bernoulli's orifice equation is rewritten as:

$$(15) \quad Q_w = k\sqrt{P}$$

The orifice flow coefficient, k , is nearly constant for the range of operating pressures used in sprinkler applications. This relationship will be used hereafter to take into account some changes in the pressure head compared to the initial characterization of the spray nozzle.

4.6 Pressure effect on droplets size

A change in the pressure at the nozzle head also leads to a change in the droplets size. The relationship proposed by Dundas [3] links the sprinkler orifice size to the characteristic droplet size. He shows that the ratio of the characteristic droplet size to the sprinkler orifice size is connected to the Weber number by the relationship:

$$(16) \quad \frac{d_w}{D_A} = \frac{\alpha}{W_e^{1/3}}$$

which can be written as:

$$(17) \quad d_w = \alpha \left(\frac{16\rho_w}{\pi^2 \sigma_w} \right)^{-1/3} D_A^2 Q_w^{-2/3}$$

Using this relationship, a reduction by half of the sprinkler flow rate contributes to a 60% increase in the droplet size. This relationship is widely used in sprinkler spray analysis because it allows the characteristic droplet size in the spray to be calculated using initial known parameters about the sprinkler. As previously for the water flow rate, this relationship will be used hereafter to take into account some changes in the pressure head compared to the initial characterization of the spray.

5 RESULTS AND DISCUSSION

5.1 Determination of droplets size distribution and droplets initial velocity on A2 test by means of the calibration technique

The droplets size distribution and droplet initial velocity of the deluge spray nozzle were fitted on A2 test (see Table 3 for the detailed description of test conditions). For this test, Figure 4 and Figure 5 show the time evolutions of pressure and mean gas temperature in the fire room. As a first comment, it can be observed that room atmosphere is strongly modified by the triggering of the water spray system during the fire. The kinetics of decrease of pressure and gas temperature at the start of the spray period are very sharp. Indeed, the temperature slope appears to be as high as 0.5 °C per second despite the heat release rate from the fire source and an under-pressure peak of -11 hPa is achieved. A stationary phase of the fire is then developed. At the end of the spray period, gas temperature increases significantly and a pressure peak is observed, the fire extinction not being reached during the spray period. Thanks to the calibration technique, the predicted droplets size distribution produced by the deluge spray nozzle for a volume flow-rate of 55 l/min is assessed by a mass median diameter of 920 μm and a geometric standard deviation of 1.5 (cf. Figure 6). The predicted droplets initial velocity is 7.0 m/s. The predicted time evolutions of pressure and mean gas

temperature obtained with the fitted droplets size distribution is reported in Figure 4 and Figure 5. It can be seen that droplets size distribution of the deluge spray nozzle appears to be well fitted by a log-normal distribution function. The under-pressure peak at the start of the spray period is correctly reproduced by SYLVIA and the difference of mean gas temperature between experimental data and prediction during the stationary phase of the fire is less than 10 °C, this result being considered as satisfactory.

5.2 Validation of the new technique on B2, C2 and C5 tests

The validation of the droplets size distribution and droplets initial velocity fitted on A2 test is performed on B2, C2 and C5 tests with other operating conditions (see Table 3). The B2 and C2 tests were performed with the same spray volume flow-rate as the one used in A2 test but with a lower HRR. This decrease of HRR leads to a reduction of the under-pressure peak at the start of the spray period and to a lower gas temperature in the fire room during the stationary phase of the fire as seen in Figure 7-a and Figure 7-b for B2 test and in Figure 7-c and Figure 7-d for C2 test. Predicted time evolutions of pressure and mean gas temperature in the fire room obtained with the droplets size distribution and initial droplets velocity fitted on A2 test are in good accordance with experimental data for both tests as seen in Figure 7-a through Figure 7-d. The under-pressure peak at the start of the spray period is correctly simulated by the SYLVIA software and the difference of mean gas temperature between experimental data and prediction during the stationary phase of the fire is kept less than 4 °C for both tests. With the reduction of the spray volume flow rate in C5 test, the adjustments discussed previously in this paper have been performed on droplet size distribution and droplet initial velocity. According to Eq. 15 and Eq. 16, the predicted droplets size distribution produced by the deluge spray nozzle for a volume flow-rate of 40 l/min is characterized by a mass median diameter of 1140 μm and a geometric

standard deviation of 1.5 (see Figure 6). The droplets initial velocity is estimated at 5.1 m/s. Using these spray characteristics in the simulation of C5 test, time evolutions of pressure and mean gas temperature in the fire room are well predicted by the SYLVIA software as seen in Figure 7-e and Figure 7-f. This good result shows that the adjustments on input parameters based on the previous correlations applied on size and velocity of droplets is a valuable and efficient approach.

6 CONCLUSION

A numerical method for determining droplet size distributions and droplets initial velocity of spray nozzles using a two-zone model has been developed. This method is based on a calibration of spray modeling on full-scale fire tests carried out in the DIVA facility of IRSN for which the fire was perfectly controlled. More precisely, a parametric study was performed with the SYLVIA software to fit the droplet size distribution at injection and the droplets initial velocity on a given test of the Propane gas fire test campaign. Since the uncertainty associated with each considered parameter is summarized by a range of variation, a probability distribution was chosen to represent this information and the propagation through SYLVIA modeling was achieved by Monte Carlo simulations. The validation of the method was then performed on other tests of the Propane gas fire test campaign, with other operating conditions. For all tests, a good agreement between experimental data and predictions was obtained on time evolutions of pressure and mean gas temperature in the fire room, even with the adjustments performed on droplets size and droplets initial velocity to take into account the change of operating conditions for the spray water flow-rate.

This alternative new technique is able to overcome some difficulties encountered in the experimental characterization of droplet size distributions and initial droplet velocity of large size sprays such as deluge or sprinkler spray nozzles, as discussed previously. Finally, experimental characterization of droplet size distributions and droplets velocities is performed at a given pressure head. An adjustment on droplet size distribution and droplets initial velocity is required in predictive simulations to take into account the change of droplet size distribution and initial velocity due to different operating conditions of water flow-rate.

The method that has been developed appears to be valuable and efficient in the frame of this work, and can be likely more widely applied to other water spray system for which some difficulties in the experimental characterization of such spray equipment are encountered.

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7 APPENDIX: OVERVIEW OF THE SYLVIA SOFTWARE

7.1 Main features

The SYLVIA software [25] is designed to predict the behaviors of mechanical/natural ventilation, growth fire, hot gas and smoke propagation, and airborne contamination transfer in confined and mechanically ventilated enclosures. Indeed, it is a simulation tool for calculating the consequences of multi-compartment fires in industrial and nuclear facilities, which are equipped with a full ventilation network (including ducts, room leaks, dampers, fans, horizontal/vertical openings, filters...).

The fire design of the SYLVIA software belongs to the well-known two-zone fire modeling ([17],[18]). In such software, each compartment is described with two Lagrangian control volumes, i.e. one lower and one upper gas layer separated by a thermal interface changing with time. The features of ambient quantities (pressure, temperature, gas concentration, etc.) in each control volume are assumed to be uniform at a given time. These control volumes can be connected by various ventilation components representing either natural or mechanical ventilation. The convective/conductive/radiative heat transfers inside the compartments and in the ventilation network (walls, gas phase) are fully modelled and play a major role for predicting temperature and pressure, especially in rooms and ventilation ducts near the fire. The fire itself is described by several correlations (plume, fire height, source point approach, chemical reaction, etc.) available in the literature ([17],[18],[19]). Furthermore, the SYLVIA software has additional specific models for simulating a water spray system, the condensation/adsorption of gaseous species (as water vapour) on walls, and the transport and deposition of aerosol particles (soot, dust) on solid surfaces (as ventilation ducts, room walls, High Efficiency Particulate Air filters).

The design of ventilation network is based on the node-and-branch method ([6],[20]). A node is a point (no volume) or a simple zone (with a fixed volume) in the ventilation network, where the different physical quantities (pressure, temperature, density, particle or gas species concentration and mass fraction, etc.) are considered uniform. A point can be considered as a simple junction between two or more ducts, or linked with an exterior environment (boundary condition). A zone, which leads to inertial effects under transient conditions due the fixed volume, may involve a single room (as the fire compartment) or a node between two branches. A branch represents a passive element of the network (for instance, pipe, filter, damper, leak, etc.) or an active element (for instance, fan, motor-driven valve, etc.). A mass flow rate is assumed to be uniform in 0D branches and is a function of the pressure difference at its boundaries (nodes) . A given branch is always connected to two nodes, but there is no limit on the number of branches connected to a given node. Pure aeraulic simulations in connection with the ventilation requirements (design of ventilation networks, aeraulic balancing, studies of the wind effect on airborne contamination transfer and their release to the environment...[28]) is possible with the SYLVIA software.

7.2 Technical review of SYLVIA software

The fire and ventilation network modeling in SYLVIA considers an initial value problem based on usual Ordinary Differential Equations (ODEs). The mathematical system of equations is derived mainly from the conservations of mass, species (gas and particles) and temperature (or enthalpy), and from the ideal gas law. Each equation can be written for a control volume as:

$$(18) \quad \gamma \frac{d\phi(t)}{dt} = \sum_l S_l(t) \quad (l = \text{index on the source terms})$$

The source term $S_l(t)$ is positive for increasing the term $\phi(t)$ with time (i.e. production term) and negative otherwise (i.e. sink term). The outputs ($\phi(t)$ as functions of time) are mainly pressure, layer height, temperatures and mass fraction of gas/particle species in the two (or one) layers for the fire modeling and for the node modeling of the ventilation network. The branch modeling allows predicting the mass flow rate between two successive nodes. The great challenge for simulating properly a compartment fire coupled with a ventilation network consists in describing all the source term sub-models of each equation of conservation ([17],[18]).

For the numerical aspect, the SYLVIA software solves a set of ODEs to calculate the thermodynamic states versus time in each compartment and in the ventilation network. The numerical algorithms to compute the ODE system is based on a BDF (Backward Differential Formula) method, which is an implicit, multistep method, well-suited to stiffness problems ([21]). The time step is managed automatically according to both the previous time step and the maximum number of iterations necessary to converge on the previous time step. The linear system is resolved by an iterative Newton-Raphson algorithm.

In order to assess the capability of SYLVIA software for simulating properly fire scenarios and ventilation network, a Verification and Validation process [26] is applied based on about 250 test cases. Moreover, SYLVIA code has also a statistic tool allowing especially to perform some sensibility analysis on scenarios of interest.

7.3 Modeling of the ventilation network

The SYLVIA software is able to model a comprehensive ventilation network of a nuclear facility by using the node/branch method (usually adopted by ventilation computer codes [6],[20]). This approach is based on the analogy of the ventilation network with an

electrical one. Hence, at each node (as described in

Table 4), the conservative equations of mass, enthalpy and species (gas/particles) are solved and the mass flow rate between two nodes is computed by means of the generalized Bernoulli equation taking into account the effect of branch length L on the mechanical inertia, which can be significant for a very long duct for instance. This latter relation can be written as:

$$(19) \quad \frac{L}{A} \frac{d\dot{m}}{dt} = P_{up} - P_{dn} + \rho g (z_{up} - z_{dn}) + h(Q_m, \rho, \dots)$$

The function $h()$ is the branch's characteristic function depending on the type of branch considered. Under normal operating conditions (i.e. when $Q_m > 0$), the function $h()$ is positive for an active element (as fans) and negative for a passive (or resistive) element. The scalar quantities (temperature, density and gas concentration) in the branches are determined by a donor cell technique. The upstream node quantities are used when the flow is positive and the downstream node quantities are used when the flow is negative. Each branch acts as a sink term for its donor node, and as a source term for its receiver one. The features of the ventilation network are introduced by the function $h()$ defined in the general case for passive elements as:

$$(20) \quad h(Q_m, \rho, \mu) = -R_{lin} \frac{\mu}{\mu_0} \frac{Q_m}{\rho} - \text{sgn}(Q_m) R_{quad} \frac{Q_m^2}{\rho}$$

A generic resistive element models are used for the airflow resistance defined as:

$$(21) \quad R = \frac{\Delta P}{\alpha \rho^\beta Q_v^\gamma}$$

Thus, all resistant elements (duct, valve, fire damper, filter, leak...) are described by the three parameters (α , β and γ). On other hand, the active elements (fans, PID controller...) have their specific modeling (for instance, an operating curve –flow rate/pressure- for fans) allowing also, among other possibilities, to simulate the opening of a fire break door due to the pressure effect.

7.4 Fire modeling

The fire modeling in SYLVIA software involves several sub-models (fire source, plume, combustion, radiative heat transfer, horizontal/vertical hot smoke propagation...) for simulating the fire compartments as summarized in Figure 8. The usual fire sources (gas burner, pool fire, fixed heat release rate) are modeled and some complex fuels can also be taking into account in fire engineering purposes as electrical cabinet (with open or closed door) and horizontal cable trays. As the heat conduction can be calculated by a 1D approach in walls and targets, the ignition of fire source is possible based on a temperature criteria. The fire sources can be limited due to the oxygen depletion (Peatross approach [24], Low Oxygen Limit law [27]) in the fire compartment until the possible fire extinction based on mass loss rate criterion [19], adiabatic flame temperature criterion ([22],[23]) or simply by lack of fuel. The combustion modeling allows defining a chemical reaction of two or more reactants but the stoichiometric coefficients for each product are kept constant.

LIST OF FIGURE CAPTIONS

Figure 1: Experimental device of CARAIDAS

Figure 2: Description of the facility for Propane gas fire tests and picture of the Deluge spray nozzle

Figure 3: Modeling of the ventilation network

Figure 4: Time evolution of pressure in the fire room for test A2

Figure 5: Time evolution of mean temperature in the fire room for test A2

Figure 6: Droplets size distribution function obtained from the calibration technique

Figure 7: Time evolutions of pressure and mean temperature in the fire room for tests B2, C2 and C5

Figure 8: Design of fire modeling in SYLVIA software

Figure 1: Experimental device of CARAIDAS

Figure 4: Time evolution of pressure in the fire room for test A2

Figure 5: Time evolution of mean temperature in the fire room for test A2

Figure 6: Droplets size distribution function obtained from the calibration technique

(a) Pressure in fire room

(b) Mean temperature in fire room

(c) Pressure in fire room

(d) Mean temperature in fire room

(e) Pressure in fire room

(f) Mean temperature in fire room

Figure 7: Time evolutions of pressure and mean temperature in the fire room for tests B2, C2 and C5

(a) Approach for fire compartments

(b) Overview of fire room modelings

Figure 8: Design of fire modeling in SYLVIA software

LIST OF TABLE CAPTIONS

Table 1 of the CARAIDAS program

Table 2

Table 3s performed in the DIVA facility

Table 4

	<i>Gas conditions</i>			<i>Spray droplets at injection</i>		
	P_g (Pa)	T_g (°C)	RH (%)	T_w (°C)	d_w (μm)	v_w (m.s ⁻¹)
EVAP4	10^5	47	12	25	387 ± 5	1.44
EVAP8	10^5	106	< 1	25	414 ± 7	1.55
EVAP11	10^5	147	< 1	28	423 ± 4	1.59

Table 1

	<i>d_w (μm) at $z = 2.51$ m</i>			<i>d_w (μm) at $z = 4.39$ m</i>		
	Test	SYLVIA	Diff.	Test	SYLVIA	Diff.
EVAP4	375 ± 4	375	0%	363 ± 6	365	+0.5%
EVAP8	393 ± 6	381	-3%	363 ± 5	352	-3%
EVAP11	393 ± 4	377	-4%	342 ± 7	333	-2%

Table 2

<i>Test</i>	<i>Gas burner</i>	<i>Deluge spray nozzle</i>	
	Flow-rate (l/min)	Flow rate (l/min)	Droplets size distribution
A2	210 (290 kW)	110	Fitted
B2	150 (210 kW)	110	Evaluated
C2	100 (140 kW)	110	Evaluated
C5	100 (140 kW)	80	Evaluated

Table 3

Type of nodes	Boundary condition	Point	1-zone node	2-zone node
Nber of zones	-	-	1	2
Main unknowns	-	P, T, Y_i	P, T, Y_i	P, T_{low} , $Y_{i,low}$, z_i , T_{up} , $Y_{i,up}$,
Volume	No	No	Yes	Yes

Table 4