COMPUTATIONAL FLUID DYNAMIC MODEL FOR ESTIMATING DROPLET NUMBER FLOW RATE THROUGH A LASER BEAM

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Abstract: *The current work is related to improving security by developing a new type of fog sensors and devices. We investigate fogs and their ability to absorb and clean various pollutants from air, including chemical, biological, radiological and nuclear (CBRN) agents. Fog can be used very effectively for counteraction to terrorist attacks and weapons of mass destruction, as well as for prevention of industrial accidents and disasters. It is crucial to study the specific sizes of fog droplets, which optimally collect dangerous substances. We present a computational fluid dynamic model for estimating droplet number flow rate through a laser beam. It shows, that we can make a quantitative assessment of both the number flow rate and the droplet diameter distribution. After we have confirmed that it is possible to monitor these parameters, we proceed and investigate how they are varied, when the laser beam's distance from the nozzle is changed. Thus, by selecting the distance between the laser beam and the nozzle, it will be possible to measure the diameters and the number of fog droplets. Different nozzles can be simulated easily by entering their output parameters (mass flow rate, diameter distribution, orifice diameter) in the setup.*

Keywords: SENSORS, FOG, DROPLETS, COMPUTATIONAL FLUID DYNAMIC MODEL, LASER BEAM, NOZZLE

1. Introduction

The development of aerosol analysis apparatus relies on a solid theoretical basis, but in practice it is always necessary to calibrate the final device with a standard aerosol with known parameters [1]. Due to the number of parameters which can affect the analytical signal, the calibration process is a strenuous task. For example, the scattering of a beam of light [2], which is the basis of most modern particle analysis techniques [3], is influenced by the particle number concentration, their chemical composition, size, velocity and the optical path length among others.

It is obvious that in order to distinguish the effective influence of the parameter of interest on the signal, all other parameters and their effect on the signal must be known. When only the investigated parameter is varied and the others are kept constant, the changes in the analytical signal can be related directly to it.

This can be achieved by using precise methods for particle generation which make it possible to create streams or clouds of particles with a high degree of control over chemical composition, size and number concentration. In cases where the particles are generated as a large stream, one cannot be certain of the number concentration of droplets as their generation rate is large - in the order of 10^9 or more droplets per second.

2. Prerequisites and means for solving the problem

We have done a fluid dynamics research on the change in the number flow rate of droplets as a function of the distance from the nozzle. More specifically, when a nozzle generates droplets with different diameters consecutively. Calculations show that if we know some of the parameters of the nozzle, the distance at which the number of droplets is approximately the same for different nozzles, can be determined. Thus, if we were to move the laser beam, ensuring that the number flow rate of droplets is identical, then the measured signal will be a function only of the diameter of the droplets. In this way, the devices we have developed can be used to measure the diameter of droplets.

During our investigations for developing a fog analysis system based on light extinction measurements, we have been using various atomizing nozzles that produce sprays with different mean droplet diameter for calibration. These include nozzles which generate large conical sprays with length between 1 and 2 meters.

This investigation is focused exclusively on 5 different nozzles that generate hollow cone sprays with distinct droplet diameter distributions. The manufacturer of the nozzles provided us with information regarding the size distribution of droplets generated using the nozzles at a constant pressure of 5 bar, which we use.

The chemical composition of the droplets can be easily kept constant, thus preventing it from affecting the extinction. In the absence of external force fields except for the gravitational, the velocity of the droplets is dependent on the atomizing pressure and their mass (respectively size) which are known. Therefore, the diameter distribution and the number concentration (flow rate in our case) of droplets passing through the laser beam will affect the extinction the most [2].

Initially, two possible ways of controlling these two parameters have been outlined – sampling a portion of the spray for analysis or filtering the droplets to reduce the flow rates and shrink the size spectra. Different methodologies have been reviewed with the purpose of isolating a relatively identical number of droplets.

2.1. Filtration/separation methods

The problem can be solved by filtering the flow and separating a group of particles, usually with regard to their size. The generation of monodisperse aerosols is difficult, therefore most precision particle generators have a separator/filter stage, which controls their output to produce aerosols with uniform properties.

Passing the aerosol through a high temperature area is one of the simplest ways to remove the smallest droplets, as their evaporation rate is much higher [4].

On industrial scale, particle removal from gas flows is often of crucial importance, either from technological or ecological point of view. For this purpose, various apparatus have been developed such as settling chambers, cyclones, scrubbers, electrostatic filters [5]. For smaller particles, filtering via porous material or fibers [6] is often employed. All these methods are used on a large scale, and their purpose is to separate all particles from the flow, therefore are not useful for our needs.

An interesting case is the cascade impactor, which is used for segregating groups of droplets with regard to size for further chemical analysis. Its construction consists of a series of orifices with baffles behind them, with decreasing orifice-baffle distance at each consequent stage. The flow passes through each orifice and around the baffle after it, but the heavier entrained particles possess more momentum and instead of following the flow, settle on the baffles. As the distance at each stage becomes shorter, lighter particles settle, until only the smallest or no particles are left in the stream [1]. This is an interesting way to separate particles, but its operation is quite complicated and it would be very difficult to apply it for our sprays, which consist of a large number of particles of high velocity.

2.2. Our approach

The research we have made on separation methods lead to the conclusion that most methodologies are either used at larger scale, or would have trouble separating droplets with higher inertia, such as ours.

Instead, we have chosen a different, simpler solution – the laser beam is placed at a specific distance from each nozzle, which ensures relatively identical droplet flow rates. This reduces the number of variable parameters to one – the droplet diameter distribution, which is determined by the nozzle. Hence, we can study the signal dependence on the droplet diameter distribution and calibrate our devices.

In this particular investigation we have created a numerical simulation model for studying the fluid dynamics of different sprays in order to predict their parameters in regions of interest.

3. Solution of the examined problem

3.1. A short overview on Computational Fluid Dynamics

Computational methods for investigation of fluid flows, regarded as Computational Fluid Dynamics (CFD), are becoming more and more popular. There are often cases where experimental studies are practically impossible due to the harsh process conditions. In other cases, computational methods are preferred to experimental methods as interrupting the process and altering its parameters would be technically challenging and result in a negative economic impact, for example in industrial-scale flows. CFD studies are also extensively used for nozzle optimization [7].

For our study, we have chosen to use the fluid analysis system CFX included in the software package ANSYS. It consists of a set of components used to define the case, solve the equations describing the process and output the solution results in a convenient form.

The stages of our investigation are:

- Creation of a geometrical model of the investigated domain.
- Discretizing the domain by generating a mesh of elementary volumes.
- Defining the boundary conditions and setting the solver parameters.
- Solving the process equations numerically.
- Exporting and analyzing the relevant data, drawing conclusions.

3.2. Presumptions

Several presumptions have been made, prior to the investigations, with the purpose of simplifying the model and reducing the computational load.

1) The model is considered to be stationary – the process parameters do not change in time and the results define the equilibrium state of the process. As the input parameters (water pressure, flow rate, environmental conditions, nozzle geometry) are either constant or vary insignificantly we conclude that the output parameters in a given point of interest (droplet flow rate, velocity, size distribution) will also be invariant of time. It should be mentioned that the size distribution in a different point will differ slightly due to evaporation.
2) The actual liquid atomization process is not modelled, even though ANSYS CFX supports primary and secondary liquid breakup models, because this would only increase the computational load tremendously. Hence, the droplets are injected from an injection point with a predefined diameter distribution, corresponding to the nozzle.
3) The flow of droplets is fully axisymmetric around the axis, normal to the nozzle orifice. As the nozzle is placed perpendicularly over the laser beam, almost all of the droplets will flow through the beam from above and only an insignificant number will flow through the sides.
4) The environmental surroundings are an infinite source of heat - the droplets receive heat and their temperature increases but the temperature of air remains constant.

3.3. Geometry

In accordance with presumption 1, the geometric model resembles a 30-degree slice of the volume of the spray (Fig. 1), as we are only interested in the flow through the laser beam and in the area close to it. The nozzle orifice is located where the central axis crosses the top face.

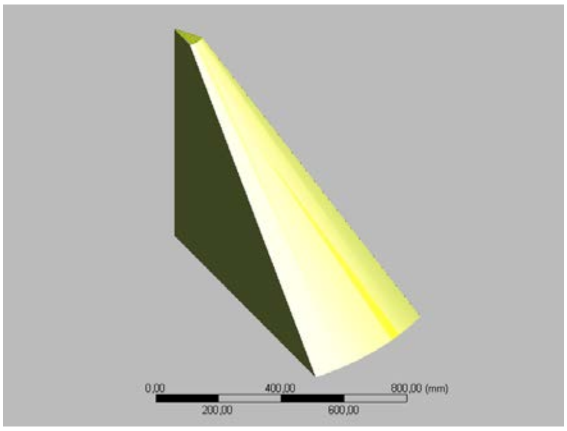

Fig. 1 *Geometry of the investigated volume*

The laser beam is directed radially from the central axis through the middle of the outer edge. It is simulated as a 2-mm wide rectangular boundary at the middle of the slice's bottom face. The beam's distance from the nozzle is varied by moving this face up or down, changing the height of the slice.

It should be noted that in this model the laser beam only passes through half of the spray until it reaches the central axis. Therefore, the resulting droplet flow rate must be doubled, again assuming that the other half is identical to the investigated one (presumption 1).

3.4. Elemental mesh

In order to obtain a relatively identical size of the elements in the mesh and consistency of the results when simulating different distances from the nozzle, the height of each element was set to be 4 mm. If the distance is not a multiple of 4, one layer of elements (usually at the top or bottom, as in Fig. 2) will have a different height.

As the shape of the spray resembles a hollow cone and most of the droplets flow closer to the edge of the volume, the element width is biased towards this area (can be seen in Fig. 2). This is done in order to increase the accuracy of the droplet trajectories.

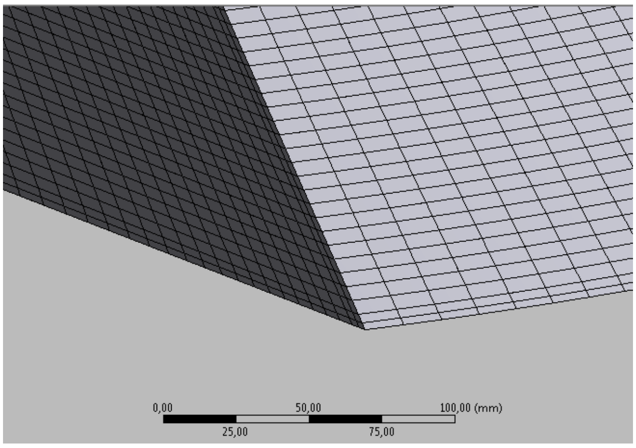

Fig. 2 *An enlarged view of the elemental mesh.*

3.5. Domain and boundary conditions

Two phases are present in the domain description – Air and Water. Water is defined as a pure substance (H_2O in liquid state) in the material description, while Air is a mixture of the materials Air Ideal Gas and H_2O (in gaseous state). The evaporation from water droplets is defined as a mass transfer of H_2O from Water to H_2O present in the Air mixture. The transfer rate is determined by the content of H_2O in Air and the heat transfer rate.

The entire volume is occupied by Air, while Water is injected from the injection region in the form of polydispersed particles. The two phases are fully coupled, meaning that any change in the velocity field of one will affect the velocity field of the other. Additional forces taken into account are drag, buoyancy and turbulent dispersion.

The injection parameters are defined using the data given by the manufacturer. The injection velocity is derived from the nozzle orifice diameter and the mass flow rate. The injection angle is 45 degrees from the central axis. Additionally, a deviation of 3 degrees from the injection angle was set. The particle diameter spectrum is defined using 4 values – minimum, maximum, mean diameters and standard deviation. The particle temperature is set to be 4°C, which is the temperature of tap water. The number of trajectories, used to represent the flow was set to 100 000.

The domain has two boundaries – the laser beam face and all other faces. They have identical conditions – openings to the environment with 0 relative pressure difference. The reason for defining them separately is to filter the droplet trajectories and isolate the ones which flow through the laser beam boundary. The number flow through the laser will be determined by these trajectories.

3.6. Solver settings

The main criterion for convergence of the solution is that the RMS (root-mean-square) value of the error in all elements is less than 10^{-6}. As convergence is too slow in some cases and the chosen RMS value may be reached after long, a secondary condition was defined – the maximum number of iterations is set to 1000. When either of these two conditions is fulfilled, the solution stops.

4. Results and discussion

The solution has converged when the main criterion was fulfilled after 225 iterations. The domain imbalances of several parameters (momentum in the 3 directions, mass fractions of the components and others) were taken as an initial numerical assessment of the accuracy, and it has been seen that the absolute value of the maximum imbalance is 0.0048%.

4.1. Particle flow trajectories

Two separate particle track objects were created – one which displays all generated tracks and one which isolates only the particle tracks which reach the laser beam boundary. The latter bears information regarding the diameter distribution and number flow rate of droplets which enter the laser beam volume.

The particle flow trajectories are shown in Fig. 3. On the left side, all trajectories are shown, and on the right side, only the trajectories that exit the domain through the laser beam boundary. The color indicates the mean diameter of the particles that travel the trajectory.

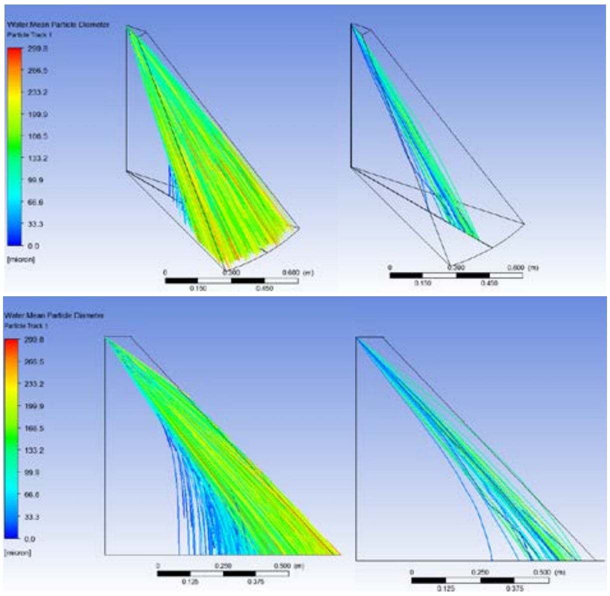

Fig. 3 *Particle trajectories, the images on the right side show only the isolated trajectories which cross the laser beam*

An interesting observation can be made – the smaller the droplets are, the closer to the central axis they settle. This phenomenon is known as droplet segregation. [6] Lighter droplets possess little momentum and lose it quickly due to drag, while heavier droplets possess more momentum and retain their velocity longer.

4.2. Flow rates

The number flow rate of droplets was calculated by taking the sum of the flow rates on each trajectory. This was done using the expression:

sum(Water.Particle Number Rate)@Particle Track

The expression was evaluated twice by changing the particle track identifier – once for the total flow rate of droplets generated by the nozzle and a second time to determine the flow rate of droplets through the laser beam. The following values were obtained:

- Total flow rate: $1.303*10^9$ [s^{-1}]
- Flow rate through laser: $4.665*10^6$ [s^{-1}]

Again, it must be noted that the value of the number flow rate through the nozzle must be doubled to obtain the expected value. In this case, the number of droplets crossing the beam per second should be $9.33*10^6$ [s^{-1}].

4.3. Diameter distribution

The diameter distribution of the spray as well as the diameter distribution of droplets which enter the laser beam were plotted in one graph for comparison (Fig. 4).

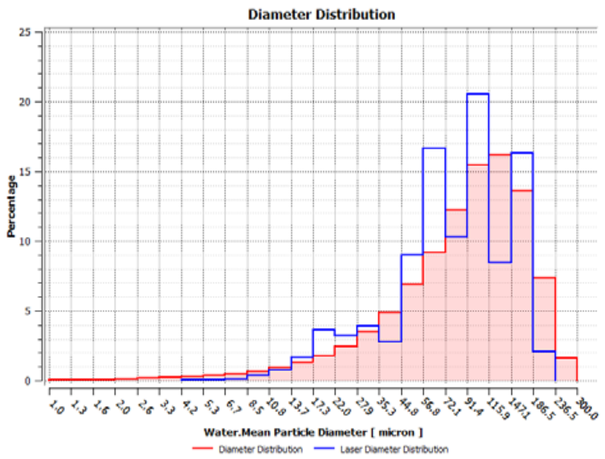

Fig. 4 *Overall droplet diameter distributions (red) and droplet diameter distribution in the volume of the laser beam (blue).*

The red plot represents the overall distribution and the blue one represents the diameter distribution of droplets that enter the laser beam. It can be seen that they are almost identical. The deviation of the blue distribution is due to the small number of trajectories that define it, compared to the overall distribution. By increasing the total number of trajectories, the plots would eventually coincide, but the increase in computational time would be great and it was decided that it is not necessary.

5. Conclusion

A spray segment model has been created and used for a computational fluid dynamics investigation of the spray's dynamics. It includes computational models that take into account the coupling of the phases, the turbulence, drag and buoyancy forces as well as evaporation of material from the disperse phase into the continuous. High accuracy was chosen for the solution (RMS < 10^{-6}) and the obtained results show very low relative domain imbalances of the main variables.

The number flow rate of droplets through a boundary, representing the laser beam has been investigated. As mentioned in the problem description, this parameter is our main concern. The results have shown that we can make a quantitative assessment of both the number flow rate and the droplet diameter distribution through the area of interest.

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