ANALYSE DE SENSIBILITÉ DE LA DISPERSION DE GOUTTELETTES AUX CONDITIONS D'ÉMISSION ET A L'AIR AMBIENT

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TITLE

Sensitivity of droplet dispersion to emission and ambient air properties

RESUME

Nous présentons une méthodologie pour analyser la sensibilité et quantifier l'incertitude des résultats de simulation numérique obtenus dans le contexte de la dispersion de gouttelettes dans l'air. La méthodologie se fonde sur les outils existants d'analyse de sensibilité (notamment la méthode de Sobol). L'intérêt de recourir à ces outils d'analyse de grands nombres de résultats est illustré à travers deux situations: un cas simplifié sans écoulement fluide environnant et un cas réaliste avec écoulement fluide. Les résultats préliminaires permettent d'identifier les paramètres influençant les résultats numériques mais montrent une forte sensibilité à l'observable choisie pour l'analyse.

ABSTRACT

This work presents a methodology to analyse the sensitivity of numerical simulations related to the dispersion of droplets in the air. The methodology is based on existing tools for sensitivity analysis (e.g. Sobol sensitivity index). This methodology is illustrated by analysing a large number of numerical results obtained in two situations: first a simple toy model (without underlying flow) and then a more realistic case (with underlying flow). The preliminary results allow to identify the parameters affecting the results but show a significant impact of the observable chosen for the analysis.

MOTS-CLÉS : dispersion, gouttelettes, analyse de sensibilité / **KEYWORDS:** dispersion, droplets, sensitivity analysis

1. INTRODUCTION & CONTEXT

The spreading of a disease/virus can occur through a number of pathways (Afsset committee, 2009), including:

- direct contact (physical contact with an infected patient);
- indirect contact (contact with contaminated surfaces);
- transmission via droplets (those emitted during coughing/sneezing/talking, i.e. at a rather short range);
- transmission via airborne aerosols (those emitted by an infected patient or droplet nuclei formed by droplet evaporation, i.e. at longer ranges than droplets).

Yet, it remains unclear what is the relative importance between these pathways, in particular between long-range airborne transmission and short-range large droplet transmission for many diseases (Bourouiba, 2014). This study aims at providing a new methodology to evaluate the relative importance between such transmission routes. This methodology is based on the analysis of the sensitivity of numerical results for droplet dispersion on a number of input parameters.

2. METHODOLOGY

In line with the objective of this study, we perform numerical simulations of droplets dispersion. We then analyse the sensitivity of the results to a number of parameters affecting the dispersion of such droplets. For that purpose, we first introduce the system studied together with a list of the input parameters that are varied and the observables defined here. Then, the models used for the numerical simulations are presented, as well as the tools used for sensitivity analysis.

2.1. System studied

The fate of droplets in the air depends on two mechanisms: the emission of droplets by a human being and their subsequent dispersion in the atmosphere. On the first hand, the emission of droplets varies with a number of aspects, including: the velocity of the expelled air, the duration of the cough, the mouth opening, the angle at which cough occurs, the droplet size and the droplet concentration. Moreover, the emission of droplets depends strongly on the way in which droplets are emitted: this can occur due to breathing, talking,

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sneezing or coughing. On the second hand, the dispersion of droplets in the air is a subtle balance between transport by the underlying airflow (which depends on the ambient air velocity), by the droplet condensation/evaporation (which is a function of the air humidity and temperature) and by the interaction between droplets or with surfaces (e.g. leading to their agglomeration/fragmentation or to surface deposition). Moreover, when dealing with the spread of virus by droplets, additional information is required (e.g. the concentration of virus in a droplet, its lifetime in the droplet and in the air, its contagiousness).

In this study, we consider a simplified case of droplets emitted during a cough and dispersed in the air. The methodology used here can be easily adapted to study other types of droplet emissions.

2.2. Numerical simulations of droplet dispersion

The numerical simulations are performed using existing approaches available in CFD (Computational Fluid Dynamics) software. More precisely, we have designed three simulation set-ups:

- Droplet emission in quiescent air: the dispersion of rigid droplets injected in a quiescent airflow (i.e. the cough airflow is neglected) is studied using the Lagrangian tracking module of *Code_Saturne* CFD, which includes a model for the transport of rigid particles in turbulent and laminar flows (Peirano et al, 2006).
- Droplet tracking in ambient air: the dispersion of rigid droplets in a constant ambient air (fixed wind velocity, cough airflow neglected) is studied using the Lagrangian module of *Code_Saturne*.
- Air & droplet emission in quiescent air: the airflow emitted during cough is simulated using CEDRE simulation platform (Refloch et al., 2011), which includes a model for dry air and water vapor concentrations. The results obtained on the air velocity, temperature and humidity are then coupled to the Lagrangian module of *Code_Saturne* to track the dispersion of droplets.

These three scenarios have been designed in a step-by-step manner: we start with a simple simulation to evaluate the robustness of the methodology and then increase the complexity/richness of the system studied incrementally to allow for a detailed understanding and analysis of the results obtained. As a result, the first system is used to evaluate the present methodology, to quantify the sensitivity of the results to droplet properties as well as to the observable chosen (see section 2.3 on sensitivity analysis). The second system is used to assess the role of an ambient airflow while the third system is used to assess the sensitivity to droplet evaporation and to the cough airflow.

2.3. Sensitivity analysis

Type of analysis: We rely here on existing variance-based methods to quantify the sensitivity of the observed outputs on certain observables. More precisely, we use the so-called “Sobol indices” or “variance-based sensitivity indices” (Sobol, 1993). It measures the effect of varying one input alone, but averaged over variations in other input parameters. It is normalized by the total variance to provide a fractional contribution. The index obtained has a value in the range [0,1]: the larger the index is, the more influential the input is. This means that, by comparing the index obtained for each input, we can sort these inputs in terms of their respective influence on the results (assuming that the inputs are independent of each other, or using extensions to the classical Sobol index method).

Uncertainty on inputs: sensitivity analysis is usually performed with some information on source of the uncertainties on the inputs. In the present case, we have opted to vary some of the inputs that can affect the fate of droplets in air (see Section 2.1) using existing measurements on cough airflow and emitted droplets.

Observables of interest: the use of sensitivity analysis tools also requires to identify an output of interest (or observable), together with the inputs on which there are uncertainties. When dealing with the fate of droplets emitted by a human, there is actually a wide range of possible observables, such as: the maximum time during which droplets remain suspended; the mean or minimum or maximum distance travelled by droplets after a given time; the number of droplets remaining above a certain height after some time; the number of droplets reaching a given target in a given time. The choice of one observable is often motivated by a given application and the objectives.

3. RESULTS

To illustrate the methodology, we present here the results obtained for the first case, i.e. droplet emission in quiescent air (only Brownian motion is considered). In that simple case, two observables are considered: the number of particles remaining above a given height after some time (here 1.5 m after 20 s) and the mean distance from the source after some time (here 20 s).

Numerical simulations are then performed using the Lagrangian tracking module of Code_Saturne. Droplets are injected in a box of size 4 x 3 x 2 m. The fluid is at rest with a temperature of 25°C. Droplets are injected in the domain at a given location (1 x 2 x1.7 m), respecting a typical human height. In adequacy with typical mouth geometry (Gupta, 2019), particles are emitted from a mouth with an ellipsoidal shape (width of 0.03 m and height of 0.015 m), with a vertical injection angle (uniformly distributed between 15 and 40°) and with a horizontal injection angle (uniformly distributed between -5 and 5°). Droplets are all injected with the same size and the same velocity. Simulations are run for 20 s (with a time step of 0.01 s).

To complete the simulation set-up, five additional input parameters are used as uncertainty sources:
- The droplet diameter (uniform distribution between 1 and 10 µm);
- The number of injected droplets (uniform distribution between 700 and 1 300);
- The head angle with respect to the vertical direction (uniform distribution between -15 and 50°);
- The cough velocity (Gaussian distribution, mean of 10 m/s and variance of 2 m/s);
- The cough duration (Gaussian distribution, mean of 75 ms and variance of 6 ms).

Typical results of such simulations are illustrated in Figure 1, which shows that droplets are dispersed in the flow at rest. Once injected in the simulation, these droplets undergo only Brownian motion and settling due to gravity. Due to their size and the fact that no evaporation is accounted for, the gravity is predominant and leads to their sedimentation on the ground within a finite time.

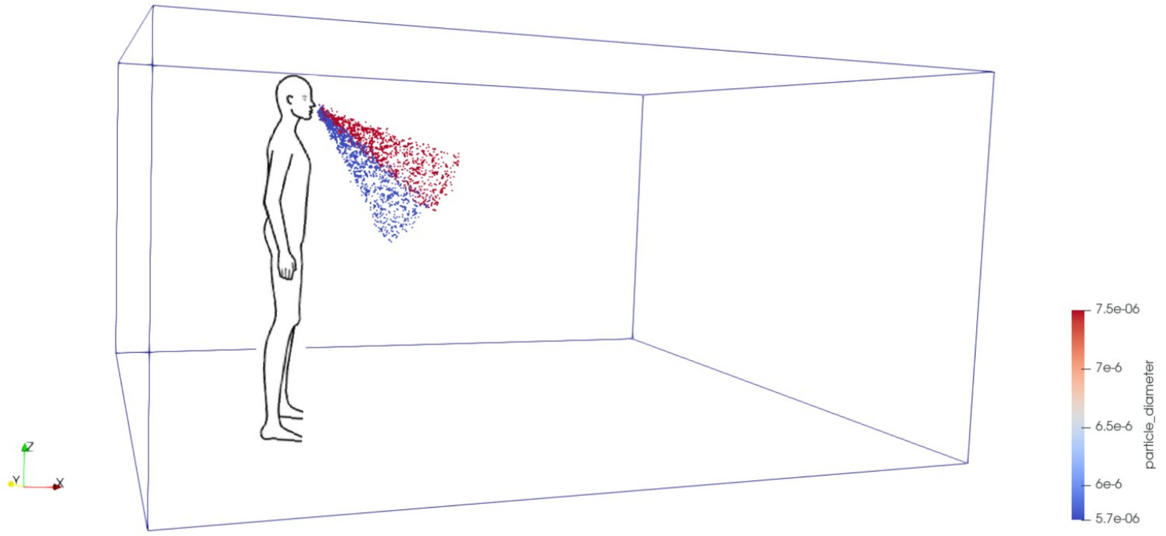

Figure 1. 3D plot of the droplets generated from two simulations:
997 droplets of 7.6 µm injected during a time of 705 ms and at a velocity of 12.4 m/s (red dots);
997 droplets of 5.7 µm injected during a time of 743 ms and at a velocity of 11.4 m/s (blue dots).
Note: the person's drawing was added for visualisation purposes only.

Using OpenTurns package (Baudin, 2016), 6.000 simulations are performed with various values of the five uncertainty sources (i.e. droplet diameter, number of droplets, head angle, cough velocity and cough duration). The results obtained with the first order Sobol indice are summarised in Table 1:

Table 1. First-order Sobol indices obtained from 6.000 simulations, with a column for each uncertainty source and two lines corresponding to the two observables (number of droplets remainng above a height of 1.5 m and the mean distance from the point source along the x-direction) .

Observable	Number of droplets	Droplet diameter	Cough velocity	Cough duration	Head angle
N_p (z>1.5 m)	0,252435	-0,0593705	0,0942603	-0,0427005	0,434486
$\langle X_p - X_0 \rangle$	0,0838429	0,084791	0,346216	0,123051	0,765763

As expected, it appears that the number of droplets remaining above a certain height (here 1.5~m) is mostly driven by the angle at which the head is tilted. The second parameter that affects the results is actually the number of droplets emitted during coughing, while the injection velocity is only the third most influential parameter (with a much lower importance).
Yet, if the observable of interest is taken to be the mean distance travelled by droplets along the x-direction, then the analysis changes. The results are again mostly affected by the angle at which the head is tilted, but

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the second input affecting the results is the velocity of injection of the droplets. The cough duration, the number of particles and the diameter of particles are less influential on the result.

4. CONCLUSION & PERSPECTIVES

This study shows the interest of using sensitivity analysis techniques to investigate the dispersion of droplets in the air. The first results show the robustness of the techniques as well as its limitations. In particular, in the simple case considered (first case), the cough angle is the key parameter driving the particles towards the ground. However, these results are expected to change significantly if another observable is used. Moreover, this result shows that, before using such sensitivity analysis techniques, a clear observable has to be defined.

Simulations in more complex cases are still under way due to the high numerical costs and size of data generated by such simulations. In the near future, we will pursue these developments towards more realistic simulations, including models for droplet evaporation/condensation as well as new models related to viral and biological properties (lifetime, contagiousness, etc.) that appear to be key in designing more efficient public health recommendations (Bourouiba, 2020).

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