A Computational Fluid Dynamics Simulation of Anthrax Diffusion in a Subway Station

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Abstract— Anthrax endospores were used in the past to attempt to the life of civilians, just think about the failed attack in Tokyo in 1993 or the 22 cases, including five deaths, occurred in USA in 2001. Because of the high case-fatality rate (CFR around 50% for respiratory form of anthrax), to the strong resistance to environmental adverse conditions and to their high mobility in the air, anthrax endospores represent the ideal agent to perpetrate a spread with offensive purposes. Subway stations are densely frequented places, and are therefore a highly worthy objective for terrorists. The aim of this work is to determine, by means of Computational Fluid Dynamics simulations of the airflow blowing anthrax endospores dropped on the platform of a subway station, the temporal evolution of their concentration, and to estimate the related health risk. COMSOL Multiphysics™ software was used to simulate the so-produced multiphase flow.

Keywords— Anthrax, Bioterrorism, CBRNe, Computational Fluid Dynamics, Multiphase flow.

I. INTRODUCTION

According to the opinions of analysts and scientists, the harmful effects that could be achieved by the use of microorganisms in an attack against the population would be extremely a hazardous, even more damaging than an attack with nuclear weapons [1, 2, 3]. Biological agents used for purposes such as biological warfare and bio-terrorism (Biological Warfare Agents, BWA), can be divided into biological microorganisms and substances derived directly from them (e.g. toxins); when deliberately dispersed, they can be used to cause deaths or serious harm to the population, animals or plants [4]. To be efficient as BWA, a biological agent must possess several peculiarities, including high mortality and transmissibility, ability to survive for as long as possible in an environment without host and to possess excellent resistance to agents that could disable it [5]. Among the various microorganisms that could be used as BWA, pathogenic bacteria constitute a serious threat to public health, especially for being easy to be transported and disseminated.

The largest part of all currently known bacteria, if the environmental conditions are favorable to their metabolism, are present in the form called vegetative; in this condition they are able to grow and reproduce. In contrast, when environmental conditions become adverse, such as in case of extreme heat, cold, toxic chemicals, lack of nutrients and UV radiation, the bacteria begin to lyse [6]. Nevertheless, if conditions become adverse, some bacterial species shown the ability to survive becoming endospores, a bacterial form extremely resistant and metabolically inert; the endospore structure provides the protection required for survival over long time, even in the face of harsh environmental conditions [7, 8]. If compared to the vegetative bacterial form, endospores contain many coat layers both chemically and structurally more complex; the resistance of endospores to adverse environmental conditions may be mediated by dipicolinic acid, a calcium ion chelator found only in endospores [9]. Subsequently, if the appropriate conditions arise (i.e. availability of water and nutrients) spores germination occurs, forming vegetative cells [10]. Examples of spore-forming bacteria are widespread in the group of gram-positive bacteria, such as aerobic (Bacillus spp.) and anaerobes (Clostridium spp.) [6].

Among the family of Bacillaceae, the most important and dangerous, considered as one of the most important biological agents for use as BWA, is Bacillus anthracis [11].

*B. anthracis is a large (1–1.5 mm by 4–10 mm), Gram-positive, non-motile, rod-shaped and facultative anaerobic endospore (generally oval) forming bacteria and it is the etiological agent of anthrax [12, 13]. Anthrax name derives from the Greek word for coal “anthracis”, and refers to the coal-black skin lesions it causes infecting the skin [4]. Anthrax infection starts when the spores enter into the body of the victim, through skin lesion (cutaneous anthrax), lungs (pulmonary anthrax), or gastrointestinal route (gastrointestinal anthrax) and germinate, forming the vegetative form [11, 14]. The pathogenic effect is due to a toxin produced by the vegetative bacillus, which consists in three components: protective antigen (PA), edema factor (EF) and lethal factor (LF) [13]. Another anthrax virulence factor is the D-glutamic acid polypeptide capsule of the vegetative form [15].

*B. anthracis has become notorious as BWA, because thanks to the resistance of endospores that form, it is able to resist for decades in the environment compared to other pathogenic
bacteria [16]. Unlike the vegetative form, more susceptible to any type of agents, *B. anthracis* endospores, in addition to being more stable, have a higher ease of transport and storage, which is crucial for their potential use as BWA. If suitably prepared, endospores of anthrax may be the main agents for biological warfare and bioterrorism, because they can be produced in large quantities in a form that can be aerosolized and then inhaled. All these factors, in addition to the high mortality of the disease by inhaling spores derived, make a serious military threat anthrax and bioterrorism, as history has taught us [17].

In fact, anthrax has always been associated with the human history, because it was already known in Europe (1200-1500 BC) and in China (3000 BC). In recent times, both during the I and II world war, anthrax was studied as possible BWA. British Army, in 1942-1943, used Gruinard Island to evaluate the potential use of airborne spores of *B. anthracis* as a biological weapon, contaminating the soil of the island and some sheep used as test subjects [18]. After various remediation works, only in 1997 the island was declared remediated and habitable. Even an accidental release of aerosolized *B. anthracis* at a former Soviet military facility in Sverdlovsk in 1979 resulted in scores of infections and many humans and animals deaths [19]. Another case occurred in 1979-1980 when, during the civil war in Zimbabwe, the largest outbreak of anthrax in the world was observed: in two years, about 9400 cutaneous anthrax cases, including 182 fatalities were reported. Before the war anthrax was endemic in Zimbabwe, however only a few cases were reported [11]. Most recently, in July 1993, *B. anthracis* spores were aerosolized by Aum Shinrikyo cult from their headquarters building in Kameido, near Tokyo, Japan [20]. Fortunately, the use of an attenuated strain, low concentrations of spores, an ineffective dispersion and the inactivation of a part of the spores due to the sun UV rays probably contributed to the lack of human cases of anthrax [21].

Finally, contextually with the attacks occurred to World Trade Center in NYC in September 2001, there was a bioterrorist attack the United States of America. Through the US postal system, spores of *B. anthracis* were released through letters addressed to the government and press officials. There were 22 confirmed cases of anthrax contamination, consisting in 12 cutaneous and 10 inhalational cases. The 12 cutaneous patients responded positively to antibiotic treatment, while of the 10 inhalational cases, four were fatal [13, 22]. It appears evident then that the use of biological agents has moved, in recent times, to terrorist groups. This creates strong concerns that the use of bioweapons by terrorists can create unexpected scenarios characterised by massive destructive potential [13]. The CFD (Computational Fluid Dynamics) is the branch of the computational physics which studies, by means of numerical simulations, various kinds of flows. Independently on the problem, a simulation is carried out following three steps. First of all, the computational domain must be discretised in small sub-domains (called cells), in order to solve in each of them the discretised equations coming from the fluid chosen models. In this first step, the numerical schemes have to be set, as well as the materials properties, the boundary conditions and the initial conditions [23].

Secondly, the calculation has to be run. In order to be reasonably sure that the results are physically meaningful, the convergence has to be achieved, and the operator has to check out that there are no zones in the domain where some quantities assume wrong values (for example, a negative density). Furthermore, the results have to be grid-independent, i.e. the results mustn’t be influenced by the accuracy of the mesh, so a convergence study on the grid has to be carried out. Once the first two steps have been brought to an end, the last one consists in post-processing, i.e. elaborating the results, analysing them and creating graphs, videos and plots of the quantities of interest.

In the last decades, thanks to the increase in the computer performances, CFD simulations have become one of the main tools in fluid dynamics. The numerical approach to this field of physics enables the engineers to predict with a good accuracy the behaviour of the flow, without have to physically create the studied device. This virtual technique makes the researchers avoid expensive and sometimes dangerous experimental campaigns. That is the reason why CFD simulations are extensively use in aerospace and automotive field [24]. Recently, this approach is gaining popularity in other fields, as biomedical research. It was so thought to perform a CFD analysis an anthrax diffusion problem.

II. AIM OF THE STUDY

The aim of this work was to simulate with a CFD code, COMSOL Multiphysics™, the dispersion of anthrax endospores in a subway station. The considered diffusion was performed in a simple way: less than a cubic centimetre of anthrax is dropped on the platform near subway border (yellow star), as shown in Fig. 1 (all the reported dimensions are in metres). The simulation of releases plays an essential role in the development of preparedness and management strategies in CBRNe events [25, 26, 27].

When the train arrives, it generates a flow that blows the powder, making it disperse in the air. The people waiting on the platform are therefore contaminated by both inhalation and skin contact. In this paper, the inhalation route only was considered for the health effects, due to the much greater infectious effectiveness of the inhalation with respect to the skin contact. This diffusion does not require to access to the ventilation system, so it is much easier to bring to an end.

![Fig. 1 Computational domain](image)
III. SIMULATION SETTINGS

The anthrax endospores features are reported in Table 1.

<table>
<thead>
<tr>
<th>Diameter (µm)</th>
<th>Density (kg/m³)</th>
<th>Shape</th>
<th>Number of spores per cluster*</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1100</td>
<td>Spherical</td>
<td>10</td>
</tr>
</tbody>
</table>

Tab. 1 Anthrax endospores features (*Due to the presence of humidity, single spores tends to form little clusters).

In order to simulate the flow, a multiphase turbulent model (Euler-Euler) has been used to take into account the interaction between the solid dispersed particles and the surrounding air (continuous phase). The full set of equations governing the flow is:

\[ \rho = \rho_c \cdot (1 - \varphi_d) + \rho_d \cdot \varphi_d \] (1.1)

\[ \frac{\partial \varphi}{\partial t} + \vec{V} \cdot (\rho \vec{V}) = 0 \] (1.2)

\[ \rho \left( \frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \nabla) \vec{V} + \rho \vec{V} \right) = \nabla - \left( \rho_c \cdot (1 - \varphi_d) \left( \vec{u} \cdot - \frac{D_c}{1 - \varphi} \cdot \overline{\vec{v}} \right) \right) \]

\[ + \rho_c \cdot \vec{V} \cdot \vec{V} = 0 \] (1.4)

\[ \vec{u}_d = \vec{V} + (1 - \varphi_d) \cdot \overline{\vec{u}}_{slip} - D_{md} \cdot \vec{V} \varphi_d \frac{\varphi_d}{\varphi_d} \] (1.5)

\[ c_d = \frac{\rho_d \cdot \varphi_d}{\rho} \] (1.6)

\[ D_{md} = \frac{\mu_c}{\rho \cdot \sigma_c} \] (1.7)

\[ 3 \cdot \frac{c_d \cdot \rho_c}{4d_c} \left| \overline{\vec{u}}_{slip} \right| \cdot \overline{\vec{u}}_{slip} = - (\rho - \rho_d) \cdot \left( \frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot (\overline{\vec{V}}) + \overline{\vec{g}} \right) \] (1.8)

\[ \mu = \frac{\mu_c}{\left( 1 - \frac{\varphi_d}{\varphi_{\text{max}}} \right)^{2.5 \varphi_{\text{max}}}} \] (1.9)

\[ c_d = \begin{cases} 24 \cdot (1 + 0.15 \cdot R_{ep}^{0.687}) & \text{for } R_{ep} < 1000 \\ 0.44 & \text{for } R_{ep} > 1000 \end{cases} \] (1.10)

\[ R_{ep} = \frac{d_c \cdot \rho_c \cdot \overline{\vec{u}}_{slip}}{\mu} \] (1.11)

\[ \rho \left( \frac{\partial k}{\partial t} + (\overline{\vec{V}} \cdot \nabla) k \right) = \nabla \left[ \left( \mu + \frac{\mu_c}{\sigma_c} \right) \nabla \vec{V} \right] + P_k - \rho \epsilon \] (1.12)

\[ \rho \left( \frac{\partial \epsilon}{\partial t} + (\overline{\vec{V}} \cdot \nabla) \epsilon \right) = \nabla \left[ \left( \mu + \frac{\mu_c}{\sigma_c} \right) \nabla \vec{V} \right] + \frac{C_{c1} \epsilon}{k} P_k - \frac{C_{c2} \rho \epsilon^2}{k} \] (1.13)

\[ \mu_T = \rho C_{\mu} \frac{k^2}{\epsilon} \] (1.15)

(1.1) average density equation; (1.2) continuity equation; (1.3) Navier-Stokes equation; (1.4) mass balance between the two phases equation; (1.5) dispersed phase velocity vector; (1.6) dispersed phase mass fraction; (1.7) dispersed phase turbulent diffusion coefficient; (1.8) momentum balance between the two phases equation; (1.9) effective viscosity equation; (1.10) drag coefficient calculation (Schiller-Naumann model); (1.11) particle-based Reynolds number; (1.12) turbulent kinetic energy production rate; (1.13) turbulent kinetic energy dissipation rate conservation equation; (1.14) turbulent kinetic energy production rate; (1.15) turbulent viscosity calculation.

\[ \rho : \text{density}; \vec{V} : \text{velocity vector}; p : \text{pressure}; \mu : \text{molecular viscosity}; \mu_T : \text{turbulent viscosity}; \epsilon : \text{turbulent kinetic energy}; \kappa : \text{turbulent kinetic energy dissipation rate}; P_k : \text{turbulent kinetic energy production term}; C_{c1}, C_{c2}, C_{\mu} : \text{turbulence model constants}; v_T : \text{turbulent kinematic viscosity}; \varphi_d : \text{dispersed particles volume fraction}; c_d : \text{dispersed phase mass fraction}; \rho_c : \text{continuous phase density}; \varphi_d : \text{dispersed phase density}; d_d : \text{dispersed phase particles diameter}; \overline{\vec{u}_c \vec{u}_c} : \text{continuous phase velocity vector}; \overline{\vec{u}_d} : \text{dispersed phase velocity vector}; \overline{\vec{u}_{slip}} : \text{slip velocity}; \overline{\vec{g}} : \text{gravity acceleration vector}; \varphi_{\text{max}} : \text{maximum particles volume fraction}; C_{\mu} : \text{particles drag coefficient}; Re : \text{particle-based Reynolds number}; Q : \text{breath volumetric flow rate}; N_b : \text{number of spores in each endospore}; n_s : \text{number of spores per volume unit}; \psi : \text{number of inhaled spores}; \xi : \text{infection}
probability; \( l \): lethality of the infection; \( CBRNe \): Chemical, Biological, Radiological, Nuclear, explosive; \( BWA \): Biological Warfare Agents; \( CFD \): Computational Fluid Dynamics.

It has been assumed that the air has a density of 1.29 kg/m\(^3\) and that its viscosity is 1.78e-5 Pa·s.

Initially, the air is at rest and a t a pressure of 1 atm; the anthrax endospores are put on the platform in the marked point. The powder deposit has a cylindrical shape, with a radius equal to 0.5 cm and a thickness equal to 0.25 cm. The endospores have a maximum volume packing factor of 0.62.

The wind enters at 20 km/h, and the pressure at the exit of the domain is set to 1 atm.

The actual volume of the anthrax clusters is therefore:

\[
V_a = \varphi_m \cdot \pi R^2 \cdot h = 0.196 \text{ cm}^3
\]

The number of endospores contained in the deposit is:

\[
N_a = \frac{V_a}{\frac{4}{3} \pi \cdot \left(\frac{d_e}{2}\right)^3} = \frac{6\varphi_m \cdot R^2 \cdot h}{d_e^3 \cdot N_b} = 1.86 \cdot 10^6
\]

IV. SIMULATION RESULTS AND DISCUSSION

The number of anthrax endospores per volume unit, \( n \), is derived from their volume fraction as follows:

\[
v_a = \varphi_m \cdot \pi R^2 \cdot h = 0.196 \text{ cm}^3
\]

\[
n = \frac{N}{V_{tot}} = \frac{V_a \cdot \rho_d}{V_{tot} \cdot \rho_a} = \frac{\phi_d \cdot m_d}{m_d}
\]

where \( N \) is the number of particles, \( V_{tot} \) is the volume of the air-particles mixture, \( V_a \) is the volume of the dispersed phase and \( m_d \) is the mass of each particle. As \( m_d \) is calculated as follows:

\[
m_d = \rho_d \cdot \frac{4}{3} \pi \cdot \left(\frac{d_e}{2}\right)^3
\]

we finally get:

\[
n = \frac{6\varphi_d}{\pi d_e^3}
\]

As each endospore contains \( N_b \) spores, the number of bacteria per volume unit is:

\[
n_b = N_b \cdot n = N_b \cdot \frac{6\varphi_d}{\pi d_e^3}
\]

It is assumed that \( N_b = 10 \).

In Figure 2, the spatial distribution of the spores concentration (in logarithmic scale) and the streamlines are shown after 0.6, 1.2, 1.8, 2.4 and 3 s. As it can be seen, the formation of a trapped vortex behind the wall occurs just after the wind has started blowing. The powder is entrained by this vortex, which inseminates the main flow.

In order to evaluate the local effect of the attempt, the number of inhaled endospores during the simulation time was calculated in each point of the computational domain. It was assumed that a person breathes at a flow rate \( Q=10 \text{ L/min} \) and that all the endospores which entered in the lungs remain inside them. The number of inhaled endospores is therefore:

\[
\psi(x, y, z) = \int_0^{\Delta t} n_b(x, y, z, \tau) \cdot Q \cdot d\tau = \frac{6Q \cdot N_b}{\pi d_e^3} \int_0^{\Delta t} \varphi_d(x, y, z, \tau)d\tau
\]

In Figure 3, the number of inhaled anthrax endospores during 3 sec is shown in logarithmic scale. In order the determine the local effectiveness of the attempt, the infection probability, \( p \), has to be correlated to \( \psi \). An empirical law (the equation was obtained by linear regression from the graph reported by [28]) has been used to calculate the local probability of an infection:

\[
\xi(x, y, z) = p(\psi) = e^{-a} \exp \left[ \frac{-a}{6Q \cdot N_b} \int_0^{\Delta t} \varphi_d(x, y, z, \tau)d\tau \right]
\]

where a=6694. Now, assuming the lethality \( l \) of an infection is meanly about 50% [29], the local mortality will be:

\[
\omega(x, y, z) = l \cdot \xi(x, y, z) = \exp \left[ \frac{-a}{6Q \cdot N_b} \int_0^{\Delta t} \varphi_d(x, y, z, \tau)d\tau \right]
\]
simple air flow generated by the incoming train is fully sufficient to deadly harm many people staying on the platform in the surroundings of the deposited anthrax endospores powder. The simulation was carried out only for a 3-second duration, but, as it can be imagined, the endospores continue moving (and infecting people) even after the train has stopped.

![Image](Fig. 2. $n_b$ at 0.6 sec (A), 1.2 sec (B), 1.8 sec (C), 2.4 sec (D) and 3.0 sec (E) with streamlines ($\log_{10}(n_b \cdot 1 m^3)$)

![Image](Fig. 3. $\psi$ ($\log_{10} \psi$)

It is so possible to have an idea of how much an area is dangerous for the people staying there. To determine the risk distribution over space, $\omega$ has been evaluated on three horizontal planes, 0.8, 1.3 and 1.8 m above the platform (nose level for children, adolescents and adults), as shown in Figure 4.

As it can be seen, the mortality is very high in the first 10 m, i.e. in the part of the subway station which is blown by the wind in the first 3 seconds, and especially near the platform, that means that the zone below 1 meter above the platform is the most dangerous. The simulation demonstrates that the

![Image](Fig. 4. $\omega$ at z=0.8 m (A), z=1.3 m (B) and at z=1.8 m (C)

V. CONCLUSIONS

The CFD approach has led to the determination of the endospores mobilisation speed. It has been found that, due to the extremely small diameter of the anthrax endospores, the slow wind generated by a train approaching to the station is fast enough to disperse almost all endospores initially put on the platform. That means that such a diffusion can easily be made with discretion and is likely to be fully successful in spite of its simple realisation. Further refinements of the model can take into account the moisture influence on the solid particles mobilisation, in order to predict in a more realistic way the actual consequences of this kind of attempt.

ACKNOWLEDGMENT

Special acknowledgments for the realization of this work go the International Master Courses in “Protection against CBRNe events” (www.mastercbnr.com).

REFERENCES


