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Mathematical Model for Calculating the Dispersion Flow Rate of Decontamination Solutions for Chemical and Radiological Agents When Sprayed from Nozzles

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***Abstract*—The mathematical model for calculating the flow rate of fluids when dispersed from nozzles is based on the principles of fluid mechanics, using equations for the velocity of the fluid and the effects of nozzle diameter, pressure, and the dynamic properties of the fluid (density, viscosity). The model includes calculations of the flow rate based on the theoretical exit velocity from the nozzle, along with corrections for pressure losses associated with friction and turbulence. The Reynolds number is used to assess the flow characteristics (laminar or turbulent), which is crucial for optimizing the fluid dispersion. In MATLAB, various plots are generated to show the dependencies between the flow rate, nozzle diameter, and pressure, enabling a deeper understanding of the fluid behaviour during dispersion. The model is applicable to different types of fluids, including solutions with surfactants and hypochlorites, used for disinfection purposes.**

***Keywords*— decontamination, fluid dispersion, CBRN devices, dynamic properties of the fluid, spraying systems.**

I. Introduction

The development of Chemical, Biological, Radiological, and Nuclear (CBRN) machine decontamination systems is a critical aspect of military, emergency response, and industrial safety. These systems are designed to neutralize, remove, or contain hazardous contaminants from military vehicles, equipment, and infrastructure after exposure to CBRN threats. The advancement of CBRN decontamination technologies has been driven by the increasing risks posed by chemical warfare, bioterrorism, radiological threats, and nuclear incidents. [1] - [10]

Modern decontamination efforts focus on speed, efficiency, material compatibility, and environmental safety. These systems use a variety of chemical agents, physical cleaning methods, and advanced materials to ensure thorough decontamination while minimizing damage to sensitive equipment.

Innovations in dispersing solutions for the decontamination of nuclear, chemical, and biological (NBC) agents are essential to improving response capabilities in defence, emergency response, and industrial safety. [11] - [13]

Current methods are slow and resource-intensive: Many decontamination processes require large amounts of water, chemicals, or time to be effective. Innovations in dispersing solutions can significantly reduce response time and improve efficiency. Speed is crucial to minimizing casualties and environmental contamination, especially in high-risk areas such as military operations or urban centres. New solutions allow faster targeted decontamination without excessive liquid waste or secondary contamination. Many chemical-based decontaminants are toxic, corrosive, or leave harmful residues that further contaminate the environment. [14]

Traditional decontamination requires high-pressure water systems that generate hazardous runoff. Modern autonomous spraying systems, drones, and robotic decontamination units reduce the need for human operators to enter contaminated areas.

Wearable decontamination solutions (e.g., self-decontaminating fabrics) provide real-time protection.

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Traditional decontamination equipment is bulky and difficult to transport.

Advanced dispersing solutions (e.g., lightweight decontamination sprays, self-activating gels) enhance mobility. Decontaminants must work on a variety of surfaces (e.g., vehicles, weapons, infrastructure, sensitive electronic components). Innovations allow for more even distribution and effectiveness on porous and non-porous surfaces.

Advanced dispersing solutions can neutralize chemical, biological, and radiological threats simultaneously, reducing the need for multiple systems.

The flow rate (Q) of fluids when sprayed from nozzles can be calculated using fluid dynamics formulas that account for the nozzle diameter, the pressure of the fluid, the density of the fluid, and the efficiency coefficients.

Basic Formula (1) for Calculating the Flow Rate:

$$Q = C_d * A * \sqrt{\frac{2*\Delta P}{\rho}} \quad (1)$$

Where:

- Q – flow rate of the fluid, in m^3/s or l/s;
- C_d – discharge coefficient (dimensionless value, usually between 0.6 and 0.9 depending on the nozzle);
- A – cross-sectional area of the nozzle opening, in m^2;
- ρ – density of the fluid, in kg/m^3;
- ΔP – pressure difference, in Pa. This is the difference between the pressure of the fluid before the nozzle and the atmospheric pressure. [15]

Discharge Coefficient (C_d) reflects the efficiency of the nozzle in converting pressure energy into kinetic energy. It varies depending on the nozzle design and condition. Nozzle Diameter of the nozzle significantly impacts the flow rate. Larger nozzles allow more fluid to pass through, increasing the flow rate. The pressure difference is the force driving the fluid through the nozzle. It's the difference between the pressure inside the pipe or reservoir and the pressure at the nozzle exit. Higher pressure differences result in higher flow rates. The density of the fluid affects its ability to flow. Higher-density fluids require more energy to move through the nozzle.

For round nozzles (2) [16]:

$$A = \pi * \frac{d^2}{4} \quad (2)$$

Where d – diameter of the nozzle opening, in meters.

Spraying nozzles can have different shapes, which affect the discharge coefficient (C_d). When creating a mathematical model for a specific case, the value of C_d that is provided in the manufacturer's documentation should be used. If the fluid is viscous, instead of the standard formula, correction factors should be applied to account for the fluid's viscosity.

If there is more than one nozzle, as is common in machines used for the decontamination of nuclear, chemical, and biological agents, the total flow rate (Q_{total}) is calculated using the following formula (Formula 3):

$$Q_{total} = N * Q \quad (3)$$

Where:

- N – the number of nozzles.
- Q – the flow rate per nozzle (as calculated using the formula previously mentioned).
- Q_{total} – the total flow rate for the system.

This approach helps account for multiple nozzles and gives a comprehensive understanding of the system's performance, ensuring that the total volume of fluid required for the decontamination process is accurately calculated. The flow rate from a nozzle is directly influenced by the nozzle diameter, the pressure driving the fluid, the density of the fluid, and the efficiency of the nozzle (C_d). For accurate calculations, each of these factors should be considered, as they impact the volume of fluid sprayed over time.

To calculate the flow rate of a fluid being sprayed from a nozzle, we can use Torricelli's equation and empirical coefficients. The general formula for the flow rate $Q_{through}$ a nozzle is given by the following formula (Formula 4):

$$Q = C_d * A\sqrt{2 * g * h} \quad (4)$$

Where:

- Q – the flow rate (m^3/s or l/s)
- C_d – the discharge coefficient (dimensionless), which accounts for the efficiency of the nozzle
- A – cross-sectional area of the nozzle (m^2)
- ΔP – pressure difference (Pa), which is the difference between the pressure before the nozzle and the atmospheric pressure
- ρ – density of the fluid (kg/m^3)

This formula is derived from Torricelli's law, which is based on the principles of fluid dynamics. It assumes that the flow of the fluid is caused by the pressure difference between the inlet and the nozzle outlet, and the velocity of the fluid is related to the square root of the pressure difference. This formula considers both the pressure difference and the fluid density, along with the nozzle's characteristics (size and discharge coefficient), to calculate how much fluid will pass through the nozzle in each time.[15]

The model is based on Bernoulli's equation, considering:

- Hydrodynamic losses (friction, discharge coefficient)
- Flow regime
- Nozzle friction – modelled using the Darcy-Weisbach equation
- Viscous losses – accounted for through the Reynolds number and empirical turbulence models
- Cavitation and vapor pressure are not included in the model. If the pressure drops below the liquid's vapor pressure, cavitation may occur, leading to a decrease in flow rate. However, this is not characteristic of the developed model.

II. MATERIALS AND METHODS

A. Deactivating solutions based on surfactants

Surfactants are used to neutralize and remove hazardous substances such as chemical, biological, or radioactive contaminants. They work by emulsifying, dissolving, or breaking down harmful agents, making them less dangerous and easier to wash away.

These solutions typically contain:

- Anionic, non-ionic, or cationic surfactants – help degrade contaminants.
- Oxidizers – such as sodium hypochlorite (NaClO) or hydrogen peroxide (H_2O_2), which break down toxic substances.
- Buffer systems – maintain an optimal pH for neutralization.
- Complexing agents – help bind heavy metals.

Some deactivating substances used for military purposes include:

- DS2 solution – military standard for decontamination. DS2 is a highly alkaline solution with strong solvent and emulsifying properties.
- Oxidizing mixtures based on sodium percarbonate.
- Solutions with Triton X-100 or Tween-80 – used in laboratories. Triton X-100 and Tween-80 are widely used non-ionic surfactants with applications in research, pharmaceuticals, and industrial settings.

They are primarily used for solubilization, emulsification, and protein stabilization.

B. Decontamination Solutions Based on Hypochlorite

Decontamination is the process of neutralizing and breaking down toxic chemical agents (CWAs) like mustard gas (HD), sarin (GB), VX, and other nerve agents. Solutions based on sodium hypochlorite (NaOCl) or calcium hypochlorite ($Ca(OCl)_2$) are commonly used for decontamination, as hypochlorites act as strong oxidizers that break down the molecules of toxic agents. Known hypochlorite-based solutions include: Alkaline Hypochlorite Solutions and Calcium Hypochlorite ($Ca(OCl)_2$) Solution – "Bleaching Lime".

Table 1 shows the main differences between the two solutions.

TABLE 1 COMPARISON OF THE TWO SOLUTIONS

Property	NaOCl Solution	$Ca(OCl)_2$ Solution
Decontamination of VX, HD	Yes	Yes
Decontamination of biological agents	Partial	Yes
Stability during storage	High	Low
Corrosiveness	Moderate	High
Application on equipment	Suitable	Limited

III. RESULTS AND DISCUSSION

A. Definition of Input Parameters:

- Nozzle dimensions, d or l;
- Fluid characteristics ρ, μ;
- Pressures: P_{in}, P_{out}.

B. Flow Rate Calculation (Theoretical and Actual):

- Calculate the theoretical velocity $V_{theoretical}$;
- Compute the Reynolds number to determine the flow regime.
- Identify the flow regime (laminar or turbulent) and determine the friction factor, f.
- Calculate frictional losses.
- Adjust the actual flow rate based on the calculated losses.

C. Specific Effects of Solutions on the Model

a) Surfactants

- Reduce surface tension – can affect the dispersion process
- Change viscosity (μ) – increased viscosity can lead to higher pressure losses
- Affect the Reynolds number (Re) – increased viscosity reduces the Reynolds number (Re), which can alter the flow regime

b) Hypochlorite Solutions

- Higher density (ρ) compared to pure water (~1100–1200 kg/m³)
- Can cause corrosion, increasing nozzle roughness
- Chemical activity can change the discharge coefficient due to interaction with the walls

D. How do we adapt the mathematical model?

- To account for these factors, we make the following modifications in the model - Adjusting the Reynolds number
- The Reynolds number changes because, the density of hypochlorite solutions is higher
- The viscosity of surfactant solutions may be higher

E. Visualization:

- Plot of flow rate vs. nozzle diameter.
- Plot of flow rate vs. inlet pressure.
- Plot of Reynolds number.

With this mathematical model, we can accurately predict the flow rate under different conditions.

The following modifications have been made to the model:

- We corrected the Reynolds number.

The Reynolds number changes because the density of hypochlorite solutions is higher. The viscosity of surfactant solutions may be greater. [15], [16]

$$R_e = \frac{\rho_{solution*V*d}}{\mu_{solution}} \quad (5)$$

Where:

- $\rho_{solution}$ is the density of the solution, kg/m³.
- V is the velocity of the fluid or solution, m/s.
- d is the diameter of the pipe or characteristic length, m.
- $\mu_{solution}$ is the dynamic viscosity of the solution, Pa.s or N.s/m^2.
- Re is the Reynolds number.

We have adjusted the discharge coefficient (Cd), as it depends on the properties of the liquid. Typically:

- Pure water – Cd ≈ 0.98
- Viscous surfactant solutions – Cd ≈ 0.92 – 0.96
- • Hypochlorite solutions – Cd ≈ 0.90 – 0.94 [15]

We introduce the corrected formula (6):

$$C_d = C_{d\ whater} - \Delta C_{d\ viscosity} - \Delta C_{d\ corrosion} \quad (6)$$

$\Delta C_{d\ viscosity}$ – decreases at high μ;

$\Delta C_{d\ corrosion}$ – decreases with a damaged surface.

The flow rate of the liquid passing through a nozzle increases with the nozzle diameter. This is because a larger diameter increases the cross-sectional area available for the liquid to pass through, allowing a greater volume of liquid to flow through the nozzle per unit time. The relationship is linear, meaning that as the nozzle diameter increases, the flow rate also increases.

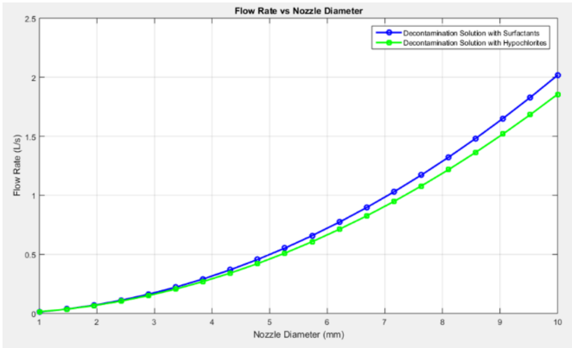

Fig. 1. Flow rate of decontamination solutions versus nozzle diameter.

For disinfection solutions containing surfactants and hypochlorite solutions, the flow rate increases in a similar manner. However, the actual volume of liquid passing through the nozzle will differ due to variations in the density and viscosity of the two solution types. Larger nozzles enable a higher flow rate, which is crucial for applications requiring rapid disinfection of large surfaces or volumes.

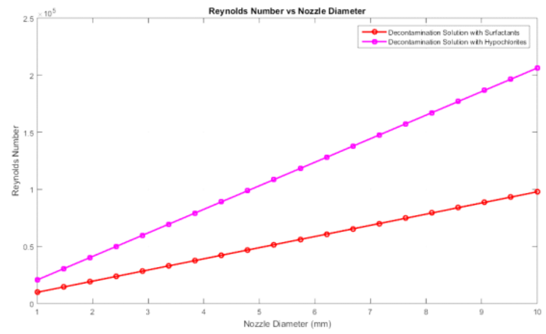

Fig. 2. Flow rate of decontamination solutions versus inlet pressure.

Increasing the inlet pressure will raise the flow rate, but to a lesser extent than increasing the nozzle diameter. Higher inlet pressure results in a greater liquid flow rate, which is beneficial for applications requiring faster dispersion of disinfectant solutions. However, the effect of pressure increase on flow rate is limited compared to the impact of nozzle diameter. This is due to the quadratic relationship between flow rate and pressure.

Since surfactant solutions typically have a higher density than hypochlorite solutions, their flow rate may be lower under the same pressure conditions.

The Reynolds number (R_e) measures the turbulence of the flow. It increases with the nozzle diameter because a larger diameter leads to a consistent increase in flow rate, which can cause the transition from laminar to turbulent flow. As the nozzle diameter increases, the Reynolds number also rises, indicating the potential transition from laminar to turbulent flow.

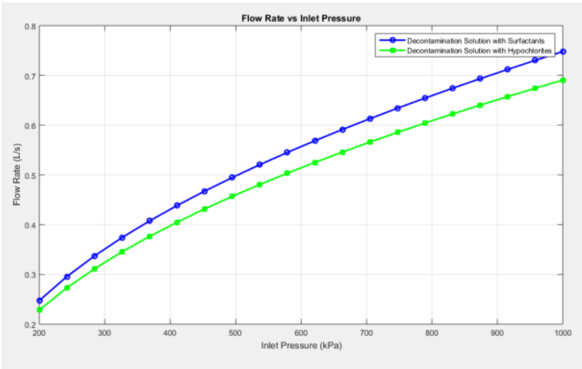

Fig. 3. The relationship between the Reynolds number and the nozzle diameter.

For surfactant solutions, which have a higher viscosity, the Reynolds number will be lower than for hypochlorite solutions, which have a lower viscosity. This suggests that higher pressure or larger nozzles may be necessary for surfactant solutions to achieve turbulent flow.

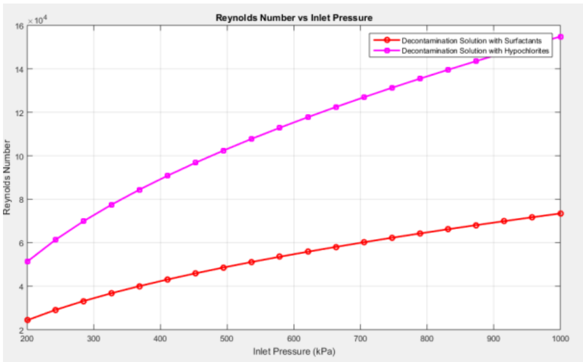

Fig. 4. Relationship between the Reynolds number and the inlet pressure.

The Reynolds number increases with rising pressure. Higher pressure leads to an increased flow velocity, which in turn enhances turbulence. As the inlet pressure increases, the flow becomes more turbulent for all liquids, which is crucial for effective spraying and disinfection.

Surfactant solutions will transition to turbulent flow at lower pressures compared to hypochlorite solutions because surfactants have higher density and viscosity.

IV. Conclusion

Increasing the nozzle diameter leads to a higher flow rate, which is important for effective dispersion of the liquid. Increasing the inlet pressure also raises the flow rate, but its effect is less significant compared to increasing the nozzle diameter. The Reynolds number indicates the transition from laminar to turbulent flow. For more viscous liquids (surfactants), higher pressure or a larger nozzle diameter is required to achieve turbulent flow. Surfactant solutions will require more effort for effective dispersion compared to hypochlorite solutions due to their higher density and viscosity. These relationships and conclusions can be useful for optimizing disinfection processes in industrial applications involving chemical or radiological substances.

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VI. Disclosure of Interests

The author has no competing interests.

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