A UNIVERSAL UPPER BOUND FOR THE BACKWARD DIFFUSION OF POLLUTION AND/OR FOR THE RE-SUSPENSION OF POLLUTION.

ALEXIS ZAGANIDIS

Abstract. The present article study the case of an object exposed to pollution by diffusion mechanisms during a unitary time. After a certain resting period without any pollution exposures, we derive a universal upper-bound for the remaining concentration levels of pollution within that object. There are only 6 parameters involved: the saturated concentration levels of pollution within the considered object immediately after being exposed to pollution during an arbitrary long time, the diffusion coefficients of that pollution, the spatial dimensions of the considered object, the pollution exposure time, the resting time and the concentration levels of pollution within the considered object. A universal upper bound for the remaining concentration levels of pollution after backward diffusion can be found and can hold for any diffusion coefficients. This universal upper bound for the remaining concentration levels of pollution is particularly useful in the case of disinfection procedures with disinfecting toxic volatile fluids having unknown diffusion coefficients. Indeed, a too short duration of the disinfection procedures would not decontaminate well enough the considered object while a too long duration of the disinfection procedures would contaminate the considered object too much for a too long time. In addition, the toxicity of disinfecting volatile fluids is often not well known precisely and may vary under various circumstances. Therefore, this universal upper bound for the remaining concentration levels of pollution can be used to figure out the optimal duration for the disinfection procedures and the optimal resting time immediately after these disinfection procedures without needing to know the diffusion coefficients of the involved toxic disinfecting volatile fluids. For the convenience of calculations, we consider a unitary time for the pollution exposure time, we consider unitary dimensions for the considered object and we consider unitary saturated concentration levels of pollution. In the present article, the universal upper bound for the remaining pollution after backward diffusion and/or for the remaining pollution after re-suspension, are derived in the 1D case and in the 3D spherical case.

1. Introduction

The present article study the case of an object exposed to pollution by diffusion mechanisms during a unitary time. After a certain resting period without any pollution exposures, we derive a universal upper-bound for the remaining concentration levels of pollution within that object. There are only 6 parameters involved: the saturated concentration levels of pollution within the considered object immediately after being exposed to pollution during an arbitrary long time, the diffusion coefficients of that pollution, the spatial dimensions of the considered object, the pollution exposure time, the resting time and the concentration levels of pollution

Date: April 14, 2025.

within the considered object. A universal upper bound for the remaining concentration levels of pollution after backward diffusion can be found and can hold for any diffusion coefficients. This universal upper bound for the remaining concentration levels of pollution is particularly useful in the case of disinfection procedures with disinfecting toxic volatile fluids having unknown diffusion coefficients. Indeed, a too short duration of the disinfection procedures would not decontaminate well enough the considered object while a too long duration of the disinfection procedures would contaminate the considered object too much for a too long time. In addition, the toxicity of disinfecting volatile fluids is often not well known precisely and may vary under various circumstances. Therefore, this universal upper bound for the remaining concentration levels of pollution can be used to figure out the optimal duration for the disinfection procedures and the optimal resting time immediately after these disinfection procedures without needing to know the diffusion coefficients of the involved toxic disinfecting volatile fluids. For the convenience of calculations, we consider a unitary time for the pollution exposure time, we consider unitary dimensions for the considered object and we consider unitary saturated concentration levels of pollution. In the present article, the universal upper bound for the remaining pollution after backward diffusion and/or for the remaining pollution after re-suspension, are derived in the 1D case and in the 3D spherical case.

2. Theoretical framework of the standard diffusion equation.

We use the following standard diffusion equation in the 1D case to calculate the concentration levels of pollution within the considered object at $t \geq 0$ (the resting time is $t-1$) :

$$D_i \frac{\partial^2 u_i\left(t,x\right)}{\partial x^2} - \frac{\partial u_i\left(t,x\right)}{\partial t} = 0 \tag{1}$$

$$u_i\left(0,x\right) = \left(2x\right)^{16} \tag{2}$$

$$u_i\left(t,-1/2\right) = H\left(1-t\right) \tag{3}$$

$$u_i\left(t,+1/2\right) = H\left(1-t\right) \tag{4}$$

$$Q\left(t\right) = \sum_i \left(\omega_i\ Q_i(t)\right) = 2\ \sum_i \left(\omega_i \int_0^{1/2} u_i\left(t,x\right) dx\right) \tag{5}$$

Remark : the true initial conditions at time $t=0$ immediately before the exposure to pollution should be $u_i\left(0,x\right)=0$ instead of $u_i\left(0,x\right) = \left(2x\right)^{16}$ but it is not convenient at all for solving numerically the above standard diffusion equation.

We use the following standard diffusion equation in the 3D spherical case to calculate the concentration levels of pollution within the considered object at $t \geq 0$ (the resting time is $t-1$) :

$$(6) \qquad D_i \frac{\partial^2 \psi_i(t,x)}{\partial x^2} - \frac{\partial \psi_i(t,x)}{\partial t} = 0$$

$$(7) \qquad \psi_i(0,x) = x^{17}$$

$$(8) \qquad \psi_i(t,0) = 0$$

$$(9) \qquad \psi_i(t,1) = H(1-t)$$

$$(10) \qquad \tilde{Q}(t) = \sum_i \left(\tilde{\omega}_i \ \tilde{Q}_i(t) \right) = 3 \ \sum_i \left(\tilde{\omega}_i \int_0^1 \frac{\psi_i(t,x)}{x} \ x^2 dx \right)$$

$$(11) \qquad \tilde{\tilde{Q}}(t) = \frac{4\pi}{3} \tilde{Q}(t)$$

$$(12) \qquad \tilde{\tilde{Q}}(t) = \sum_i \left(\tilde{\omega}_i \ \tilde{\tilde{Q}}_i(t) \right) = 4\pi \ \sum_i \left(\tilde{\omega}_i \int_0^1 \frac{\psi_i(t,x)}{x} \ x^2 dx \right)$$

Remark : the true initial conditions at time $t = 0$ immediately before the exposure to pollution should be $\psi_i(0,x) = 0$ instead of $\psi_i(0,x) = x^{17}$ but it is not convenient at all for solving numerically the above standard diffusion equation.

3. A universal upper bound for the backward diffusion of pollution.

In the 1D case, we have found the following universal upper bound for the remaining concentration levels of pollution after backward diffusion that holds for any diffusion coefficients D_i:

(13)

$$\frac{Q(t)}{\sum_i \omega_i} < f_{1D}(t) = \left(\frac{1}{10} + \frac{1}{t} \right) Max \left(1 - \frac{t-1}{7}, 0 \right) + \left(2 - \frac{1}{e^3} \right) \frac{1}{e \ t} Min \left(\frac{t-1}{7}, 1 \right)$$

In the 3D spherical case, we have found the following universal upper bound for the remaining concentration levels of pollution after backward diffusion that holds for any diffusion coefficients D_i:

(14)

$$\frac{\tilde{Q}(t)}{\sum_i \tilde{\omega}_i} < f_{S^2}(t) = \left(\frac{1}{9} + \frac{1}{t} \right) Max \left(1 - \frac{t-1}{4}, 0 \right) + \left(2 + \frac{1}{\pi^2} \right) \frac{1}{e \ t} Min \left(\frac{t-1}{4}, 1 \right)$$

In both cases, we can notice the factor $1/(e \ t)$ which come from the minimization of the quantity $D_i \ e^{-D_i \ t}$ with respect to the diffusion coefficient D_i.

We can also notice that the universal upper bound in the 1D case is slightly smaller than the universal upper bound in the spherical 3D case when the resting time $t-1$ is large enough.

In the 1D case, we found the following numerical lower bounds on the specific time interval $1 < t < 60$:

$$f_{1D}\left(t\right)-Q\left(t\right)<0.09901616 \tag{15}$$

$$\frac{f_{1D}\left(t\right)-Q\left(t\right)}{Q\left(t\right)}<0.3224447 \tag{16}$$

In the spherical 3D case, we found the following numerical lower bounds on the specific time interval $1<t<60$:

$$f_{S^2}\left(t\right)-\tilde{Q}\left(t\right)<0.10159583 \tag{17}$$

$$\frac{f_{S^2}\left(t\right)-\tilde{Q}\left(t\right)}{\tilde{Q}\left(t\right)}<0.2190139 \tag{18}$$

4. Simple numerical example

Let consider that a single tomato with a spherical shape of radius 3.50 cm is disinfected with a 65% ethanol solution during 90 seconds and having a resting time of 36 hours immediately after its disinfection. Let consider that the disinfection protocol uses a closed tank containing that single tomato and that ethanol solution. Let consider the saturated concentration level of that ethanol solution within that single tomato is approximately 25% by volume. Let consider that the ethanol density is $\rho = 798\ kg/m^3$, let consider that the ventilation of the room is 300 m^3/s and let consider that the human inhalation rate is 3 m^3/s about. By using the universal upper bound for the backward diffusion of pollution, the remaining ethanol weight within that single tomato after the resting time $t-1$ has the following upper bound :

$$m_{Pollution} = 0.25 \times 0.65 \times 798 \times \frac{4\pi}{3} \times (0.035)^3 \times \tag{19}$$

$$\left(\frac{1}{9} + \frac{1}{\tilde{t}}\right) Max\left(1 - \frac{\tilde{t}-1}{4}, 0\right) + \left(2 + \frac{1}{\pi^2}\right) \frac{1}{e\,\tilde{t}} Min\left(\frac{\tilde{t}-1}{4}, 1\right) \tag{20}$$

$$\tilde{t} = \frac{3600 \times 36}{90} = 1\ 440 \tag{21}$$

$$m_{Pollution} = 12.50\ mg \tag{22}$$

$$m_{Inhalation} = \frac{3}{300} m_{Pollution} = 125.0\ \mu g \tag{23}$$

The ethanol weight inhaled by the human body is calculated directly from the remaining ethanol weight within that single tomato after the resting time $t-1$.

In the 1D case with the same equivalent volume than the spherical 3D case, the remaining ethanol weight within that single tomato after the resting time has the following upper bound :

$$m_{Pollution} = 0.25 \times 0.65 \times 798 \times (0.035)^3 \times \tag{24}$$

$$\left(\frac{1}{10} + \frac{1}{\tilde{t}}\right) Max\left(1 - \frac{\tilde{t}-1}{7}, 0\right) + \left(2 - \frac{1}{e^3}\right) \frac{1}{e\,\tilde{t}} Min\left(\frac{\tilde{t}-1}{7}, 1\right) \tag{25}$$

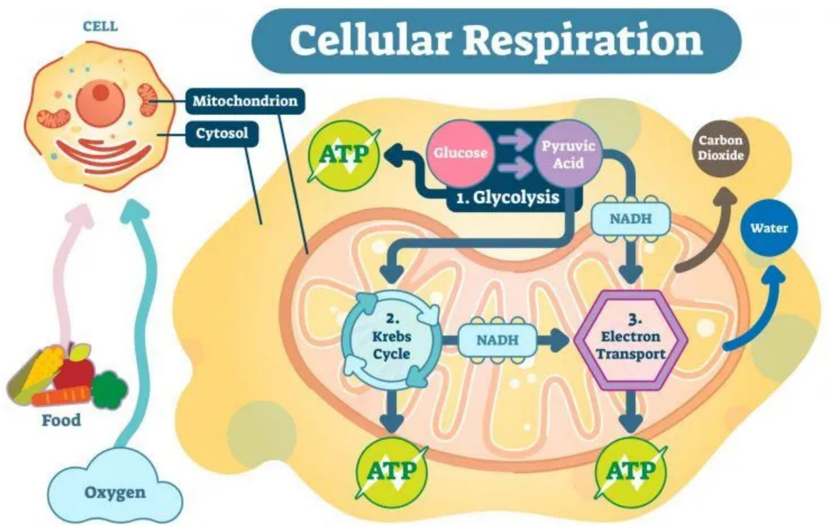
$$\tilde{t} = \frac{3600 \times 36}{90} = 1\ 440 \tag{26}$$

$$m_{Pollution} = 2.770\ mg \tag{27}$$

$$m_{Inhalation} = \frac{3}{300} m_{Pollution} = 27.70\ \mu g \tag{28}$$

The ethanol weight inhaled by the human body is calculated directly from the remaining ethanol weight within that single tomato after the resting time $t-1$.

Ethanol, methanol, formaldehyde, paraformaldehyde, formic acid, formate vapors or any other disinfecting toxic volatile fluids can efficiently cross the blood brain



barrier thanks to large diffusion coefficients and they can also disturb/reduce very significantly the cellular respiration, the mitochondrial function and the intracellular concentration levels of adenosine triphosphate. Therefore, it is particularly important to minimize as much as possible the weight of any disinfecting toxic volatile fluids that are inhaled by the human body. On the one hand, to achieve this minimization at practical level, the disinfection time must be carefully planned and timed to avoid any unnecessary excess diffusion of pollution within the considered object. On the other hand, to achieve this minimization at practical level, the resting time should be planned long enough with the help of an additional small fridge or with the help of an additional large cooler.

By combining the two previous requirements, the maximization of the ratio between the resting time ($t-1$ in arbitrary units) and the exposure time (1 in arbitrary units) plays a crucial role for the weight minimization of the disinfecting toxic volatile fluid inhaled by the human body.

To conclude with a practical consideration, the diffusion of ethanol within tomatoes and/or within cucumbers can undergo certain chemical reactions and produce little amounts of more toxic volatile fluids and/or more toxic pollutants.

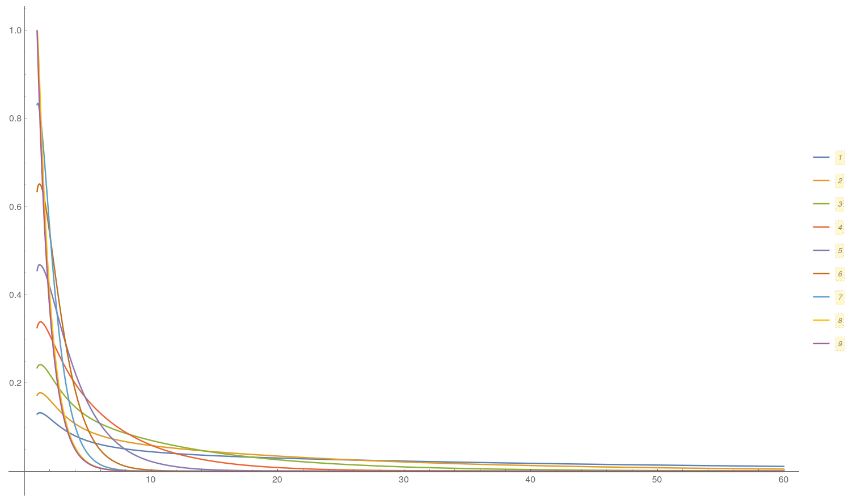


FIGURE 1. The remaining pollution $Q_i(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

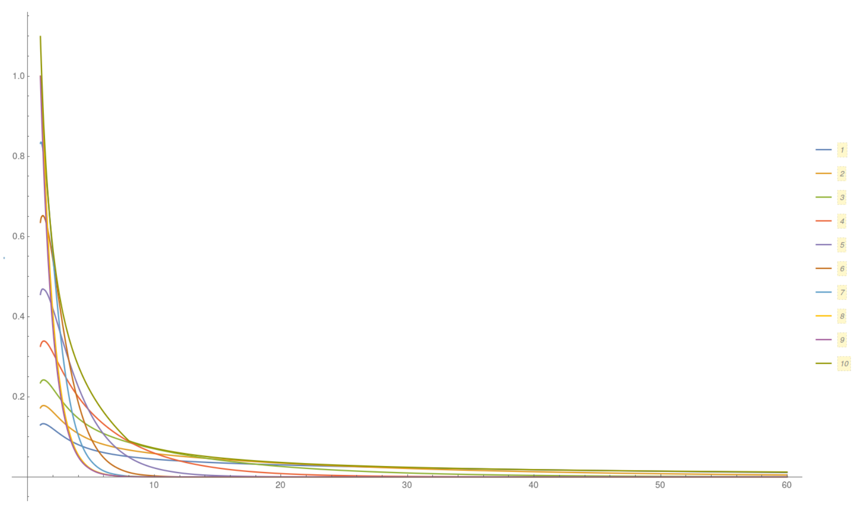


FIGURE 2. The remaining pollution $Q_i(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400. The universal upper bound is also included in the above plot.

5. PLOTS OF THE STANDARD DIFFUSION EQUATION IN THE 1D CASE.

On the figure 1, 2, 8 and 9, we can notice the following numerical artifact : a very short increase immediately after the beginning of the resting time.

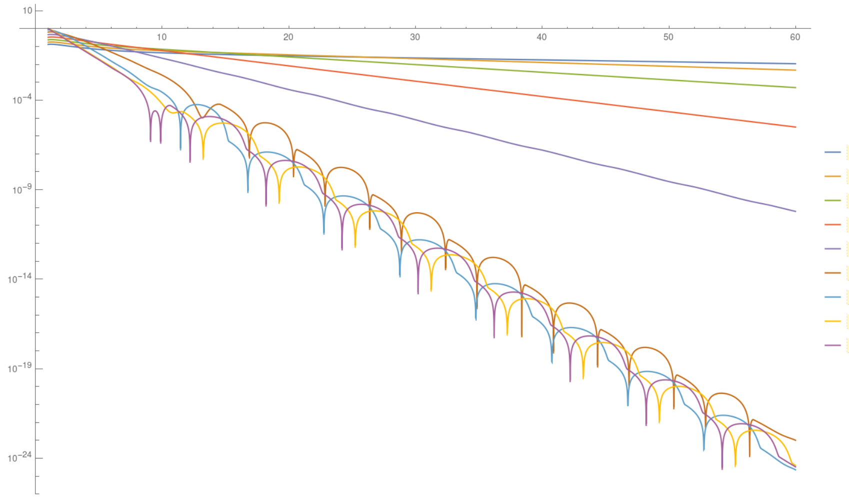


FIGURE 3. Logarithm scale : The remaining pollution $Q_i(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

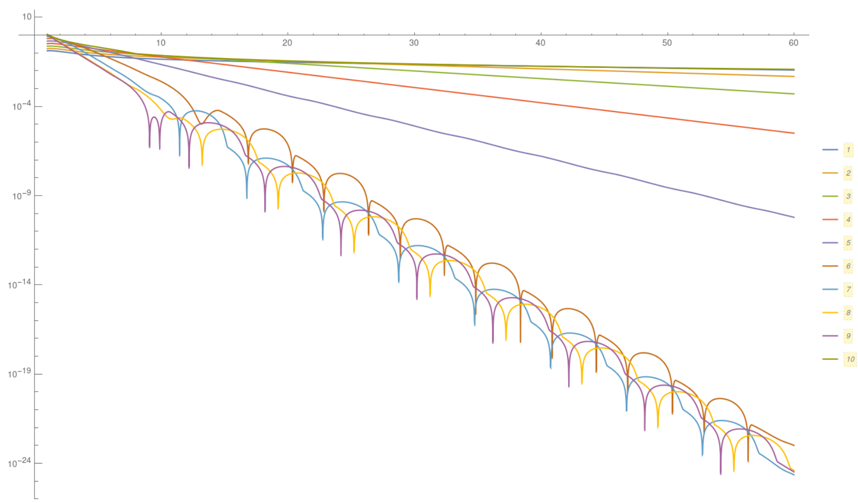


FIGURE 4. Logarithm scale : The remaining pollution $Q(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400. The universal upper bound is also included in the above plot.

6. Plots of the standard diffusion equation in the spherical 3D case.

On the figure 1, 2, 8 and 9, we can notice the following numerical artifact : a very short increase immediately after the beginning of the resting time.

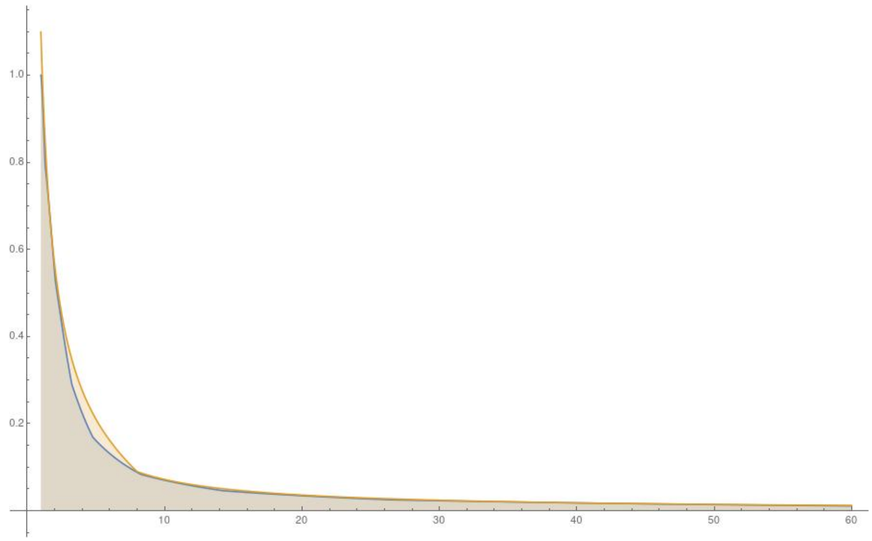


FIGURE 5. The universal upper bound and the maximal remaining pollution $Q(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

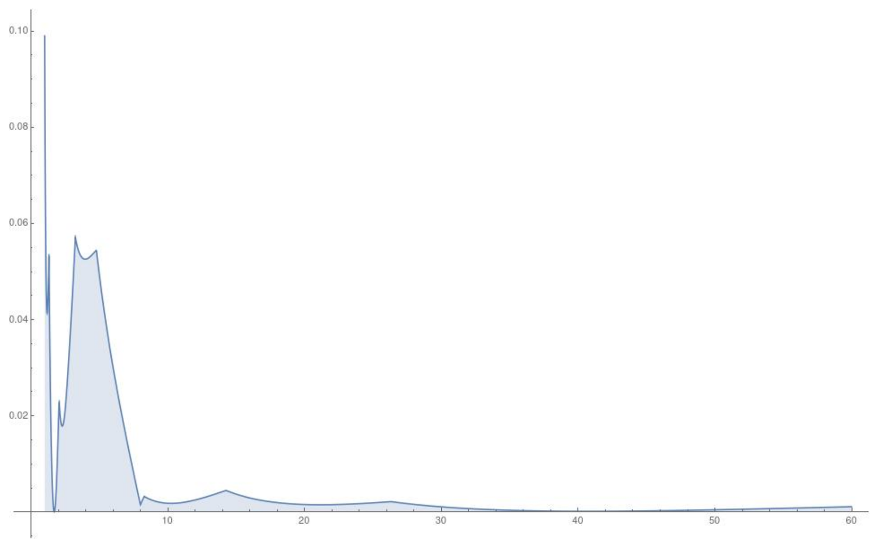


FIGURE 6. The difference between the universal upper bound and the maximal remaining pollution $Q(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

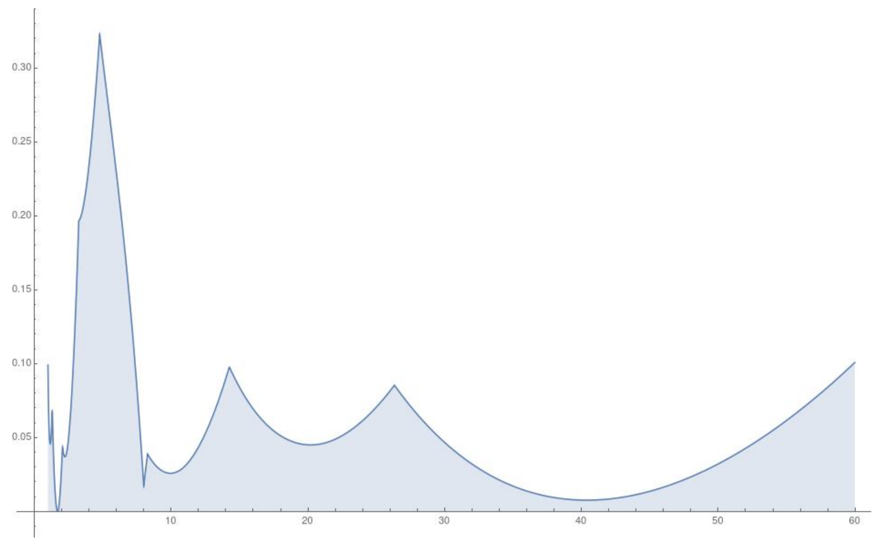


FIGURE 7. The percentage difference between the universal upper bound and the maximal remaining pollution $Q(t)$ after backward diffusion in the 1D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

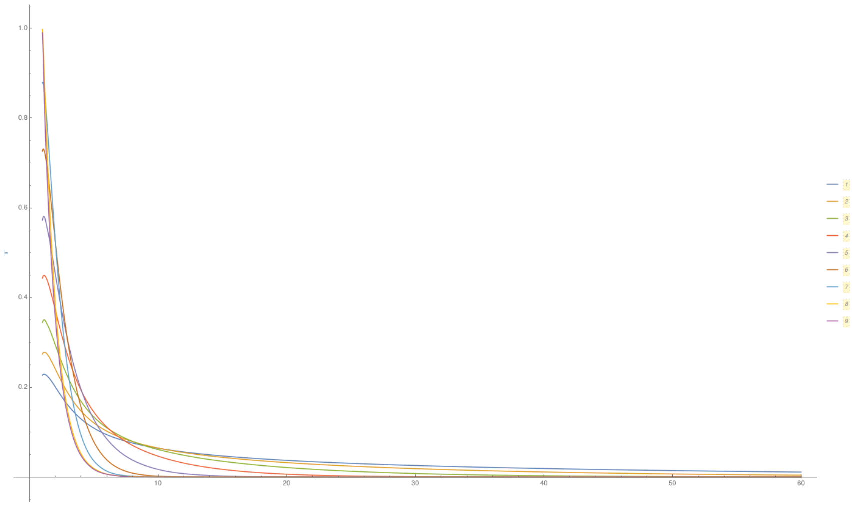


FIGURE 8. The remaining pollution $\tilde{Q}_i(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

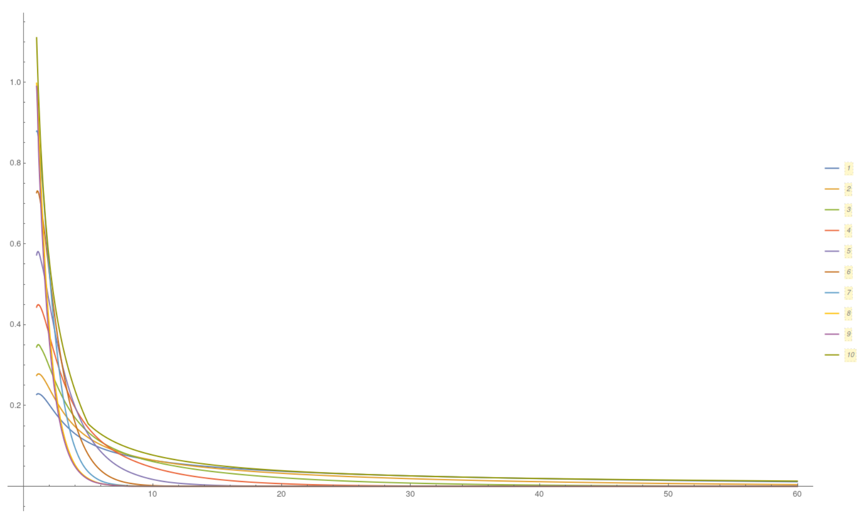


FIGURE 9. The remaining pollution $\tilde{Q}_i(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400. The universal upper bound is also included in the above plot.

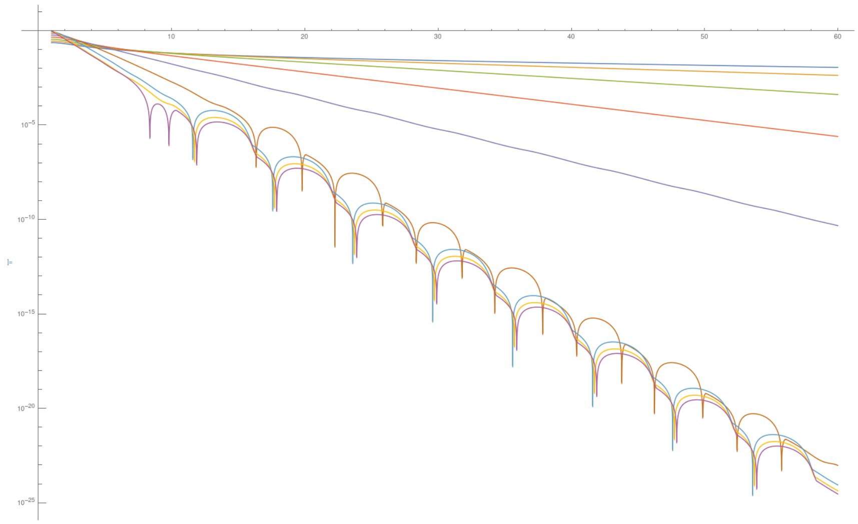


FIGURE 10. Logarithm scale : The remaining pollution $\tilde{Q}_i(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

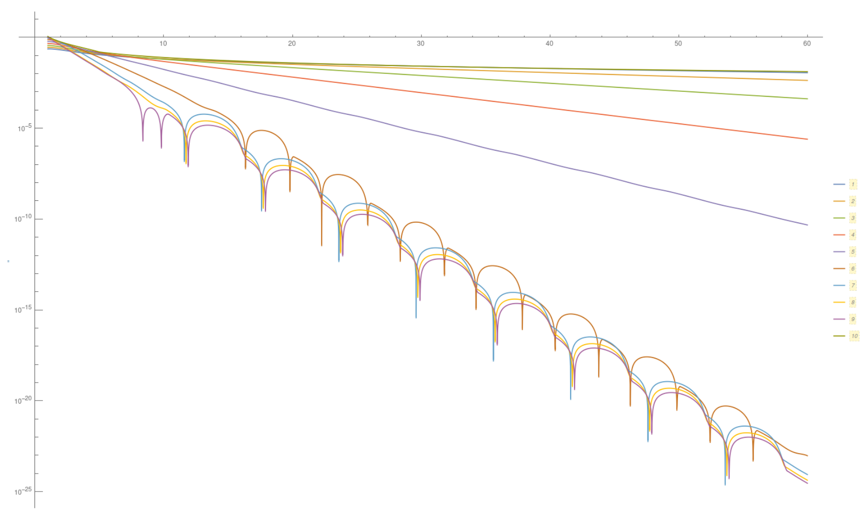


FIGURE 11. Logarithm scale : The remaining pollution $\tilde{Q}_i(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400. The universal upper bound is also included in the above plot.

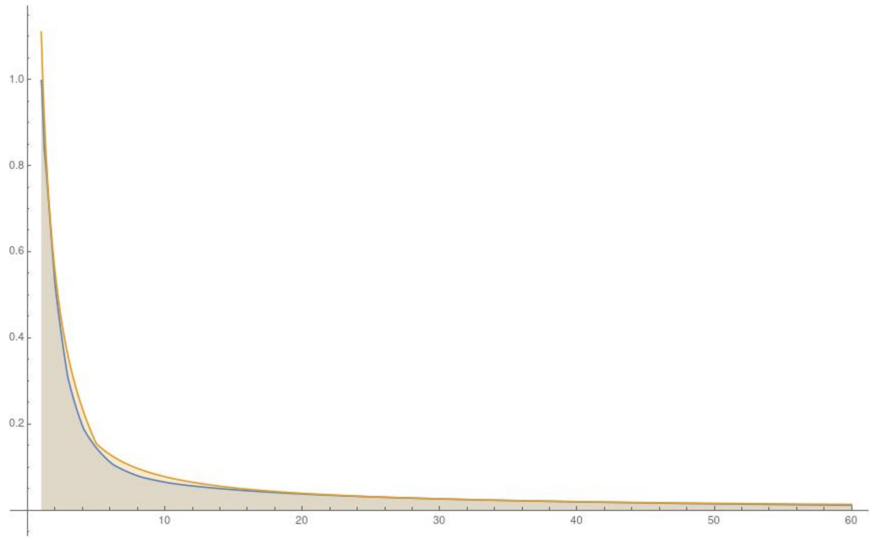


FIGURE 12. The universal upper bound and the maximal remaining pollution $\tilde{Q}_i(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

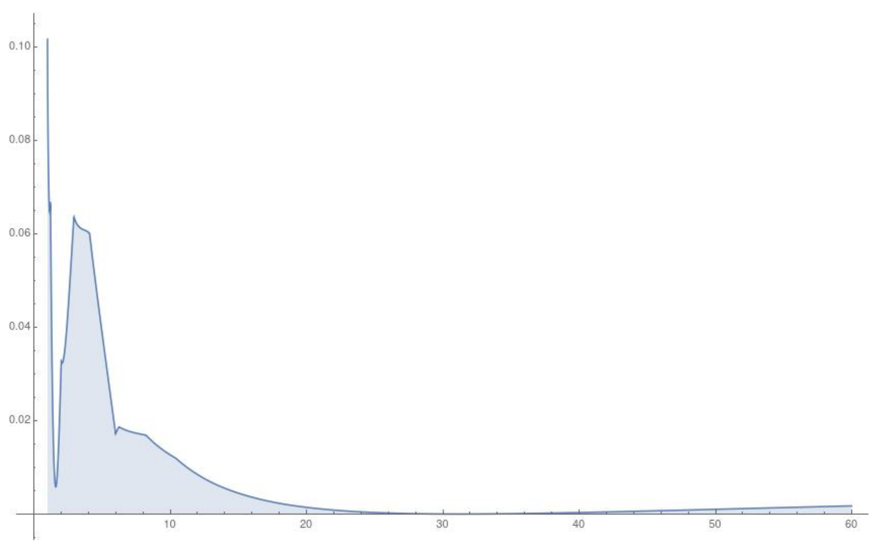


FIGURE 13. The difference between the universal upper bound and the maximal remaining pollution $\tilde{Q}(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

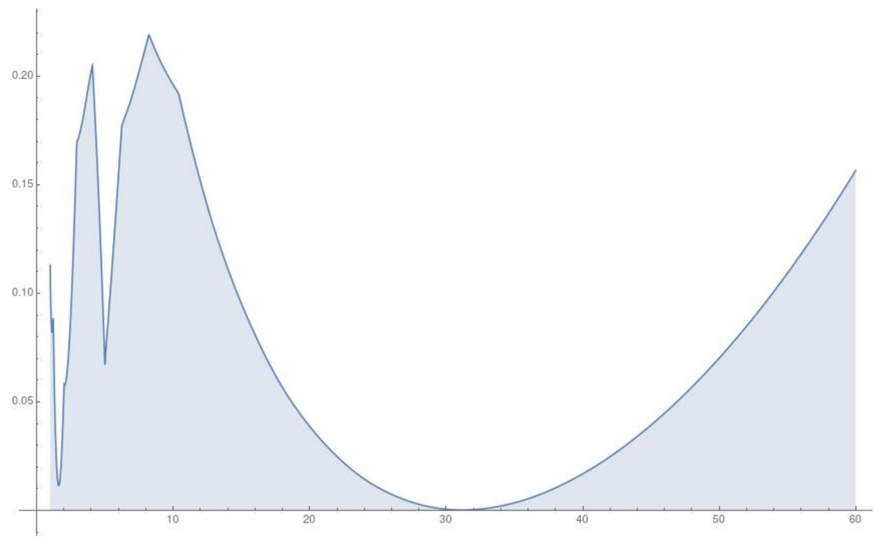


FIGURE 14. The percentage difference between the universal upper bound and the maximal remaining pollution $\tilde{Q}(t)$ after backward diffusion in the spherical 3D case with respect to the resting time at the following diffusion coefficients : 1/400, 2/400, 4/400, 8/400, 16/400, 32/400, 64/400, 1 and 400.

References

[1] A. Zaganidis, "A universal upper bound for the backward diffusion of pollution and/or for the re-suspension of pollution." https://drive.google.com/drive/folders/1Y3QEjQ3t6lcMr2wO_zQPVwPK3pzVoqRv?usp=sharing.

[2] Wikipedia. https://en.wikipedia.org/wiki/Disinfectant.

[3] Wikipedia. https://en.wikipedia.org/wiki/Fluid.

[4] Wikipedia. https://en.wikipedia.org/wiki/Volatility_(chemistry).

[5] Wikipedia. https://en.wikipedia.org/wiki/Diffusion.

[6] Wikipedia. https://en.wikipedia.org/wiki/Diffusion_equation.

[7] Wikipedia. https://en.wikipedia.org/wiki/Upper_and_lower_bounds.

[8] Wikipedia. https://en.wikipedia.org/wiki/Toxicity.

[9] Wikipedia. https://en.wikipedia.org/wiki/Pollution.

[10] Wikipedia. https://en.wikipedia.org/wiki/Ethanol.

[11] Wikipedia. https://en.wikipedia.org/wiki/Methanol.

[12] Wikipedia. https://en.wikipedia.org/wiki/Formaldehyde.

[13] Wikipedia. https://en.wikipedia.org/wiki/Paraformaldehyde.

[14] Wikipedia. https://en.wikipedia.org/wiki/Formic_acid.

[15] Wikipedia. https://en.wikipedia.org/wiki/Formate.

[16] Wikipedia. https://en.wikipedia.org/wiki/Cellular_respiration.

[17] Wikipedia. https://en.wikipedia.org/wiki/Mitochondria.

[18] Wikipedia. https://en.wikipedia.org/wiki/Adenosine_triphosphate.

[19] K. Bukacova, J. Mana, J. Klempíř, I. Lišková, H. Brožová, K. Poláková, I. Žák, D. Pelclová, S. Zakharov, E. Růžička, and O. Bezdicek, "Cognitive changes after methanol exposure: Longitudinal perspective," *Toxicology Letters*, vol. 349, p. 101–108, Oct. 2021.

[20] T. Zerin, J.-S. Kim, H.-W. Gil, H.-Y. Song, and S.-Y. Hong, "Effects of formaldehyde on mitochondrial dysfunction and apoptosis in sk-n-sh neuroblastoma cells," *Cell Biology and Toxicology*, vol. 31, p. 261–272, Dec. 2015.

[21] A. Zaganidis, "The Key to Unlock & Demultiply the Human Intelligence is the Effective Enhancement of the Brain Blood Barrier by the Practical Technologies & Protocols & Knowledge." https://drive.google.com/drive/folders/1gIvBFxavefHhENl_yBE771wuSeMTThEU?usp=drive_link.