Droplet Evaporation

by

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Background

I am an incoming third-year mathematics student at the University of Warwick. I conducted a summer research project in the field of fluid dynamics under the supervision of Dr. Radu Cimpeanu through the URSS (Undergraduate Research Support Scheme) offered by the University of Warwick. My research was about droplet evaporation, focusing on the relationship between advection and diffusion.

Acknowledgement

I would like to thank Dr. Radu Cimpeanu for his supervision throughout the duration of this URSS project. He was very helpful in providing relevant and useful resources for me. He was also being very patient with me even though I was new to the field. His insight has taught me a great deal for this project and beyond that. I would also like to thank Sebastian Dooley for helping me with the code for the time dependent advection-diffusion equation. He also helped me understand the theory behind it.

Contents

1 Introduction

Droplet evaporation is a natural phenomenon that happens all the time in the real world, especially in the fields of engineering and medicine. The process of liquid droplet evaporating on a substrate can be seen in applications such as in the drying of paints, in spray cooling, in inkjet printing, in the creation of DNA spot arrays etc [1]. Hence, it is vital to understand the process by using various methods and approaches.

Firstly, we will provide some mathematical background and notations that will be used. After that, we will discuss the governing equations related to the problem and provide a big picture on how researchers tend to approach the problem. We will then discuss a method to simplify the problem, which is called nondimensionalization. In the last section, we will then give an example of using finite difference method to solve the advection-diffusion equation in 1D, which will be introduced below.

2 Useful Mathematical Background

2.1 Definitions

- **Newtonian flow** refers to flow with constant viscosity.
- **Incompressible flow** refers to flow with constant density.
- **Laminar flow** refers to flow which is smooth and streamlined.
- **Turbulent flow** refers to flow which undergoes irregular fluctuations.
- **Advection/Convection** refers to the transport mechanism of a substance (or conserved property i.e. mass) by a fluid due to the fluid's bulk motion (i.e. to the flow).
- **Diffusion** refers to another transport mechanism which occurs without any motion of the fluid´s bulk.
- **Marangoni effect** refers to surface tension gradient driven flow inside the droplet.
- **Rayleigh effect** refers to buoyancy (and hence gravity) driven flow inside the droplet.
- **Contact angle** refers to the angle where a liquid-vapor interface meets a solid surface.
- **Contact line** refers to the line where a liquid-vapor interdace meets a solid surface.
- **Contact line pinning** refers to the phenomenon where the contact line of the droplet becomes stuck, permanently or temporarily, on a substrate. [2, p. 4]

2.2 Types of Evaporation Models

In general, evaporation models are categorised as one of the following: [3, p. 16]

- Diffusion-limited models

  In this model, the process of evaporation is controlled by the diffusion of the vapour molecules in the atmosphere. We usually consider this model when the droplet evaporates in an equilibrium state.

- Non-equilibrium models

  In this model, the process of evaporation is controlled by non-equilibrium thermal effects acting on the free surface of the droplet. We usually consider this model when the droplet is heated.

2.3 Parameters & Units

Now, we introduce some useful parameters and their respective units:
ρ = density $[kg\, m^{-3}]$, γ = surface tension $[kg\, s^{-2}]$, μ = viscosity $[kg\, m^{-1}\, s^{-1}]$,
c_p = specific heat capacity $[m^2\, s^{-2}\, K^{-1}]$, k = thermal conductivity $[kg\, m\, s^{-3}\, K^{-1}]$,
$D = \frac{k}{\rho c_p}$ = thermal diffusivity $[m^2\, s^{-1}]$, T = temperature $[K]$,
h = height $[m]$, t = time $[s]$, g = acceleration due to gravity $[m\, s^{-2}]$,
$\mathcal{L}$ = latent heat of vaporisation $[m^2\, s^{-2}]$, $l_c = \sqrt{\frac{\gamma}{\rho g}}$ = capillary length $[m]$,
θ = contact angle $[°]$, R = contact radius $[m]$, p = pressure $[kg\, m^{-1}\, s^{-2}]$,
c = variable of interests (vapour concentration for mass transfer) $[kg\, m^{-3}]$.

3 Governing Equations

Now, we state a few equations that describe the modelling of droplet evaporation. Note that bold letters denote vectors.

1. **Continuity Equation**: Describes the transport of some quantity.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{1}$$

   where $\vec{u}$ = velocity field of the fluid.

   If we assume incompressible flow, then we can simplify the Continuity Equation:

$$\nabla \cdot \boldsymbol{u} = 0 \tag{2}$$

2. **Navier-Stokes Equation**: Describes the motion of fluids.

   If we assume Newtonian and incompressible flow, we can write the equation in the form:

$$\rho \cdot \left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \right) = -\nabla p + \rho \boldsymbol{F} + \mu \cdot \nabla^2 \boldsymbol{u}, \tag{3}$$

   where $\vec{F}$ = external forces such as gravity, electromagnetic forces etc, p = pressure.

3. **Advection-Diffusion Equation**: Describes the physical phenomena where particles, energy, or other physical quantities are transferred inside a physical system due to two processes: advection and diffusion.

$$\frac{\partial c}{\partial t} + \nabla \cdot (\boldsymbol{u} c) = \nabla \cdot (D \nabla c), \tag{4}$$

   where $\boldsymbol{u}$ = velocity field of the fluid.

4 Main Idea

The main idea of a droplet evaporation problem can be solved in the following way:

1. First, we solve the heat conduction equation inside the substrate to obtain local temperature at the substrate-liquid interface.

2. Then, we solve equations inside the droplet (Continuity equation and the Navier-Stokes equation) to obtain flow field and temperature field, giving us the local temperature at the liquid-vapour interface.

3. Lastly, we solve equations outside the droplet, i.e. the surrounding atmosphere (Continuity equation, Navier-Stokes Equation and the Advection-Diffusion equation) to obtain flow field, temperature field and vapour concentration field, giving us the local evaporation rate at the liquid-vapour interface.

4. Now, depending on whether we consider contact line pinning, we can determine how the contact angle and radius of the droplet change over time.

Clearly, the steps are interchangeable and some steps can even be ignored depending on the context (i.e. which parameters are we focusing on etc.). A more in depth explanation and algorithm can be found in [1].

5 Nondimensionalization

The equations are too complicated to be solved analytically, thus mathematicians have been trying various methods to simplify the equations. The most common one is nondimensionalization.

Nondimensionalization is the partial or full removal of physical dimensions from an equation involving physical quantities by a suitable substitution of variables [4]. This is a method to reduce the number of free parameters in the equation, thus making it easier to solve. From now onwards, use carets to denote dimensional quantities.

5.1 Navier-Stokes Equation

For example, consider the dimensional Navier-Stokes equation for the flow inside a droplet, i.e. equation (3): [3, p. 22]

$$\begin{aligned} \hat{\rho} \cdot \left(\frac{\partial \hat{\boldsymbol{u}}}{\partial \hat{t}} + (\hat{\boldsymbol{u}} \cdot \hat{\nabla}) \hat{\boldsymbol{u}} \right) &= -\hat{\nabla} \hat{p} + \hat{\rho} \hat{\boldsymbol{F}} + \hat{\mu} \cdot \hat{\nabla}^2 \hat{\boldsymbol{u}} \\ \implies \qquad \frac{\partial \hat{\boldsymbol{u}}}{\partial \hat{t}} + (\hat{\boldsymbol{u}} \cdot \hat{\nabla}) \hat{\boldsymbol{u}} &= -\frac{\hat{\nabla} \hat{p}}{\hat{\rho}} + \hat{\boldsymbol{F}} + \frac{\hat{\mu}}{\hat{\rho}} \cdot \hat{\nabla}^2 \hat{\boldsymbol{u}} \end{aligned}$$

and by considering $\hat{\boldsymbol{F}} = -g e_z$ to be the gravitational force, we obtain:

$$\hat{\rho} \cdot \left(\frac{\partial \hat{\boldsymbol{u}}}{\partial \hat{t}} + (\hat{\boldsymbol{u}} \cdot \hat{\nabla}) \hat{\boldsymbol{u}} \right) = -\hat{\nabla} \hat{p} - \hat{\rho} g \hat{e}_z + \hat{\mu} \cdot \hat{\nabla}^2 \hat{\boldsymbol{u}}$$

Now, by scaling $\hat{\boldsymbol{u}} = \hat{U} \boldsymbol{u} = \frac{(\hat{L} \boldsymbol{u})}{\hat{\tau}}$, $\hat{t} = \hat{\tau} t$, $\hat{L} \hat{\nabla} = \nabla$, $\hat{p} = \left(\frac{\hat{\gamma}}{\hat{L}} \right) p$, $\hat{\boldsymbol{F}} = \hat{g} \boldsymbol{F}$, where $\hat{U} = \frac{\hat{L}}{\hat{\tau}}$ is the characteristic velocity scale, $\hat{L}$ is the characteristic length scale and $\hat{\tau}$ is the characteristic time scale, we obtain the following equation:

$$\mathrm{We} \left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} \right) = -\nabla p + \mathrm{Bo} \boldsymbol{F} + \mathrm{Ca} \nabla^2 \boldsymbol{u}, \tag{5}$$

where we have introduced the following dimensionless groups: [3, pp. 21–22]

- **Capillary Number** (Ca)

  $$\mathrm{Ca} = \frac{\hat{\mu} \hat{U}}{\hat{\gamma}}$$

  A dimensionless number which characterises the ratio of the magnitude of viscous forces to the magnitude of surface tension acting across the interface.

- **Weber Number** (We)

  $$\mathrm{We} = \frac{\hat{L} \hat{\rho} \hat{U}^2}{\hat{\gamma}}$$

  A dimensionless number which characterises the ratio of the magnitude of inertial forces to the magnitude of capillary forces inside the fluid.

- **Bond Number** (Bo)

  $$\mathrm{Bo} = \frac{\hat{L}^2 \hat{\rho} \hat{g}}{\hat{\gamma}}$$

  A dimensionless number which characterises the ratio of the magnitude of the force of gravity to the magnitude of the capillary forces acting on the droplet.

By doing this, we can now make further simplification of the equation. For example, if we consider the case where surface tension γ dominates (over viscous force), then $\mathrm{Ca} \ll 1$. In this case, equation (5) becomes

$$\mathrm{We} \left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} \right) = -\nabla p + \mathrm{Bo} \boldsymbol{F}. \tag{6}$$

By using different scales depending on the types of forces that are dominant (in different cases we consider), i.e. focusing on different parameters, we can introduce a few more dimensionless number such as:

- **Reynolds Number** (Re)

$$\mathrm{Re} = \frac{\hat{\rho}\hat{U}\hat{L}}{\hat{\mu}}$$

  A dimensionless number which helps predict flow patterns in different situations, i.e. it determines whether the flow is dominated by laminar flow or turbulent flow.

- **Froude Number** (Fr)

$$\mathrm{Fr} = \frac{\hat{u}}{\sqrt{\hat{g}\hat{L}}}$$

  A dimensionless number which characterises the ratio of the flow inertia to the external field (e.g. gravity). [5]

5.2 Advection-Diffusion Equation

Similarly, for the dimensional (Time Dependent) Advection-Diffusion equation, i.e. equation (4), we can also apply nondimensionalization:

$$\begin{aligned} \frac{\partial \hat{c}}{\partial \hat{t}} &= \hat{\nabla} \cdot (\hat{D}\hat{\nabla}\hat{c}) - \hat{\nabla} \cdot (\hat{\boldsymbol{u}}^a \hat{c}) \\ \implies \frac{1}{\mathrm{Fo}_m}\frac{\partial c}{\partial t} &= \nabla^2 c - \mathrm{Pe}_m \nabla \cdot (\boldsymbol{u}^a c), \end{aligned} \tag{7}$$

where $\hat{D}$ denotes the diffusivity of vapour through the atmosphere and $\boldsymbol{u}^a$ denotes the velocity field of vapour in the atmosphere.

This gives us the following dimensionless groups: [3, p. 26]

- (mass) **Péclet Number** (Pe_m)

$$\mathrm{Pe}_m = \frac{\hat{L}\hat{U}}{\hat{D}}$$

  A dimensionless number which characterises the ratio of the magnitude of diffusive transport of mass to the magnitude of advective transport of mass.

- (mass) **Fourier Number** (Fo_m)

$$\mathrm{Fo}_m = \frac{\hat{\tau}\hat{D}}{\hat{L}^2}$$

  A dimensionless number which characterises the ratio of magnitude of the evaporative timescale to the magnitude of the mass diffusion timescale.

For example, in the paper [6] where they discuss about the relationship between Marangoni and Rayleigh convection in evaporating binary droplets, they assume Péclet Number in the gas phase to be sufficiently small [6, p. 4] to consider only diffusive vapour transport. This leads to the Laplace equation:

$$\nabla^2 c = 0. \tag{8}$$

For more examples, see [7].

6 Finite Difference Method

Sometimes, after applying the nondimensionalization technique, we are still unable to solve the equations analytically. Hence, we introduce the concept of finite difference method. The basic idea is to approximate the differential operator by replacing the derivatives in the equation using differential quotients. The first step is to discretize the domain in space and in time. After that, we can use Taylor series to find the required approximation. For simplicity, we will just state the results that we will use here:

1. Suppose u is a C^2 continuous function on an interval $[x - h_0, x + h_0]$, $h_0 > 0$. Then, for all $h \in (0, h_0)$, the differential quotient $\frac{u(x+h)-u(x-h)}{2h}$ is a consistent second-order approximation of the first derivative u' of u at point x.

2. Suppose u is a C^4 continuous function on an interval $[x - h_0, x + h_0]$, $h_0 > 0$. Then, for all $h \in (0, h_0)$, the differential quotient $\frac{u(x+h)-2u(x)+u(x-h)}{h^2}$ is a consistent second-order approximation of the second derivative u'' of u at point x.

We will show two examples here, for the time independent advection-diffusion equation [8] and the time dependent advection-diffusion equation.

6.1 Time Independent Advection-Diffusion Equation

First, we consider the general case of 1D time independent advection-diffusion equation, which writes:

$$\hat{v}\frac{\partial \hat{c}}{\partial \hat{x}} = \hat{D}\frac{\partial^2 \hat{c}}{\partial \hat{x}^2}, \quad \hat{x} \in [0, \hat{L}], \quad \hat{L} \in \mathbb{R} \tag{9}$$

where $\hat{c}$ denotes the variable of interests (species concentration for mass transfer, and temperature for heat transfer), $\hat{D}$ denotes diffusivity/diffusion coefficient (mass diffusivity for particle motion, and thermal diffusivity for heat transport), $\hat{v}$ denotes velocity field of the fluid, $\hat{x}$ denotes the direction considered.

The boundary conditions that we will consider are

$$\hat{c}(0) = \hat{c}_0 \quad \text{and} \quad \hat{c}(\hat{L}) = \hat{c}_{\hat{L}}.$$

6.1.1 Analytical Solution

In order to simplify the problem, we apply scaling as follows:

$$x = \frac{\hat{x}}{\hat{L}} \quad \text{and} \quad c = \frac{\hat{c} - \hat{c}_0}{\hat{c}_{\hat{L}} - \hat{c}_0}.$$

Substitution yields:

$$\hat{v}\frac{\hat{c}_{\hat{L}} - \hat{c}_0}{\hat{L}}\frac{dc}{dx} = \hat{D}\frac{\hat{c}_{\hat{L}} - \hat{c}_0}{\hat{L}^2}\frac{d^2c}{dx^2}$$

with the boundary conditions

$$c(0) = 0 \quad \text{and} \quad c(1) = 1.$$

We then obtain the simplified equation:

$$\frac{dc}{dx} = \epsilon\frac{d^2c}{dx^2}, \quad c(0) = 0,\ c(1) = 1. \tag{10}$$

By inspection, we see that the expression

$$c_\epsilon(x) = \frac{e^{x/\epsilon} - 1}{e^{1/\epsilon} - 1} \tag{11}$$

solves the equation analytically. This can be represented by Figure 1 below (for 5 different values for ϵ):

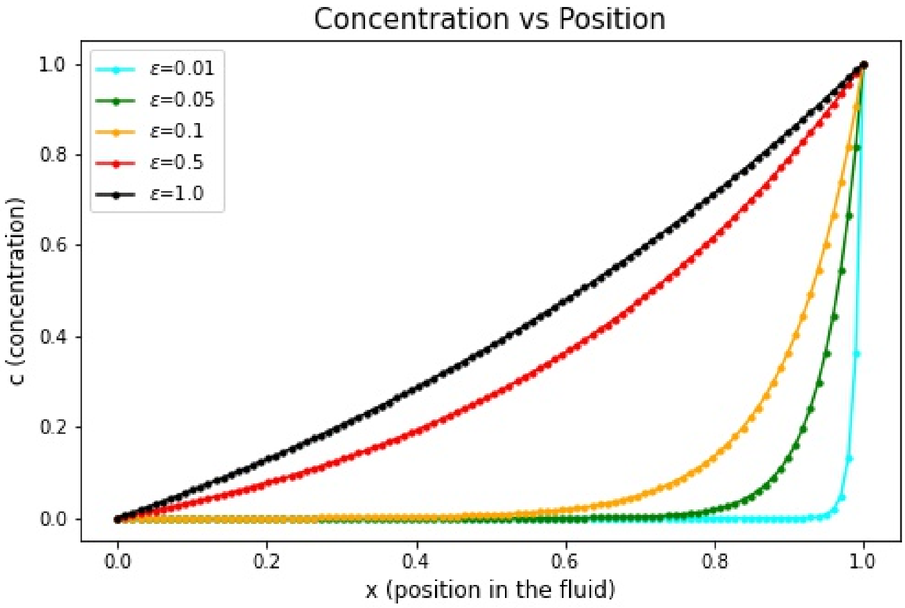


Figure 1: Concentration vs position for analytical solution of equation (10), i.e. expression (11).

6.1.2 Numerical Solution

Next, we want to solve the same equation after scaling (10) using finite difference method and compare the results to the analytical solution (11) from section 6.1.1.

There are two finite difference scheme, namely the **centered finite difference scheme** and the **upwind finite difference scheme**. We first apply the former scheme.

Firstly, we discretize the domain $[0,1]$ by introducing equidistributed grid points corresponding to a spatial step size $dx = \frac{1}{(N_x-1)}$, where $N_x \in \mathbb{Z}^+$. Next, we discretize the original equation (by the two results in section 6) to see that:

$$\frac{dc}{dx} \approx \frac{c_{i+1} - c_{i-1}}{2\Delta x} \qquad \frac{d^2c}{dx^2} \approx \frac{c_{i+1} - 2c_i + c_{i-1}}{(\Delta x)^2}$$

In this case, substitution yields:

$$\left(\frac{c_{i+1} - c_{i-1}}{2\Delta x}\right) = \epsilon \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} \qquad \forall i \in \{1, \dots, N_x - 1\}$$

$$\implies \left(\frac{1}{2\Delta x} - \frac{\epsilon}{\Delta x^2}\right)(c_{i+1}) + \left(\frac{2\epsilon}{\Delta x^2}\right)(c_i) + \left(-\frac{1}{2\Delta x} - \frac{\epsilon}{\Delta x^2}\right)(c_{i-1}) = 0,$$

with initial conditions $c_0 = 0$ and $c_{N_x} = 1$.
This can be written in a tridiagonal system as follows:

$$A_{i,i+1}c_{i+1} + A_{i,i}c_i + A_{i-1,i}c_{i-1} = 0 \qquad \forall i \in \{1, \dots, N_x - 1\}$$

where

$$\begin{aligned} A_{0,0} &= 1, \\ A_{i,i+1} &= \frac{1}{2\Delta x} - \frac{\epsilon}{\Delta x^2}, \\ A_{i,i} &= \frac{2\epsilon}{\Delta x^2}, \\ A_{i-1,i} &= -\frac{1}{2\Delta x} - \frac{\epsilon}{\Delta x^2}, \\ A_{N_x,N_x} &= 1 \end{aligned}$$

with the initial data

$$b_j = 0 \qquad \forall j \in \{1, \dots, N_x - 1\} \quad \textit{and} \quad b_{N_x} = 1.$$

Now, we can compare the difference between the analytical solution and the solution obtained by using finite difference method. We will consider 5 different values for ϵ and 2 different values for N_x and represent the results in Figure 2 on the next page.

Next, we apply the latter scheme, i.e. **upwind finite difference scheme**. We will use similar discretization of the domain as the former scheme. However, the discretization of the original equation changes:

$$\frac{dc}{dx} \approx \frac{c_i - c_{i-1}}{\Delta x} \qquad \frac{d^2c}{dx^2} \approx \frac{c_{i+1} - 2c_i + c_{i-1}}{(\Delta x)^2}$$

when $\hat{v} > 0$ ($\hat{v}$ in the equation (9)); and

$$\frac{dc}{dx} \approx \frac{c_{i+1} - c_i}{\Delta x} \qquad \frac{d^2c}{dx^2} \approx \frac{c_{i+1} - 2c_i + c_{i-1}}{(\Delta x)^2}$$

when $\hat{v} < 0$ ($\hat{v}$ in the equation (9)). Here, we only focus on the case where $\hat{v} > 0$, i.e. $\epsilon > 0$.
In this case, substitution yields:

$$\left(\frac{c_i - c_{i-1}}{\Delta x}\right) = \epsilon\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} \qquad \forall i \in \{1, \dots, N_x - 1\}$$

$$\implies \left(-\frac{\epsilon}{\Delta x^2}\right)(c_{i+1}) + \left(\frac{1}{\Delta x} + \frac{2\epsilon}{\Delta x^2}\right)(c_i) + \left(-\frac{1}{\Delta x} - \frac{\epsilon}{\Delta x^2}\right)(c_{i-1}) = 0,$$

with initial conditions $c_0 = 0$ and $c_{N_x} = 1$.
This can be written in a tridiagonal system as follows:

$$B_{i,i+1}c_{i+1} + B_{i,i}c_i + B_{i-1,i}c_{i-1} = 0 \qquad \forall i \in \{1, \dots, N_x - 1\}$$

where

$$\begin{aligned} B_{0,0} &= 1, \\ B_{i,i+1} &= -\frac{\epsilon}{\Delta x^2}, \\ B_{i,i} &= \frac{1}{\Delta x} + \frac{2\epsilon}{\Delta x^2}, \\ B_{i-1,i} &= -\frac{1}{\Delta x} - \frac{\epsilon}{\Delta x^2}, \\ B_{N_x,N_x} &= 1 \end{aligned}$$

with the initial data

$$b_j = 0 \qquad \forall j \in \{1, \dots, N_x - 1\} \quad \text{and} \quad b_{N_x} = 1.$$

We can once again compare the difference between the analytical solution and the solution obtained by using upwind finite difference method. Similarly, we will consider 5 different values for ϵ and 2 different values for N_x and represent the results in Figure 3 on page 12.

Figure 2: Analytical Solution vs Centered Finite Difference Method to Solve Equation (10)

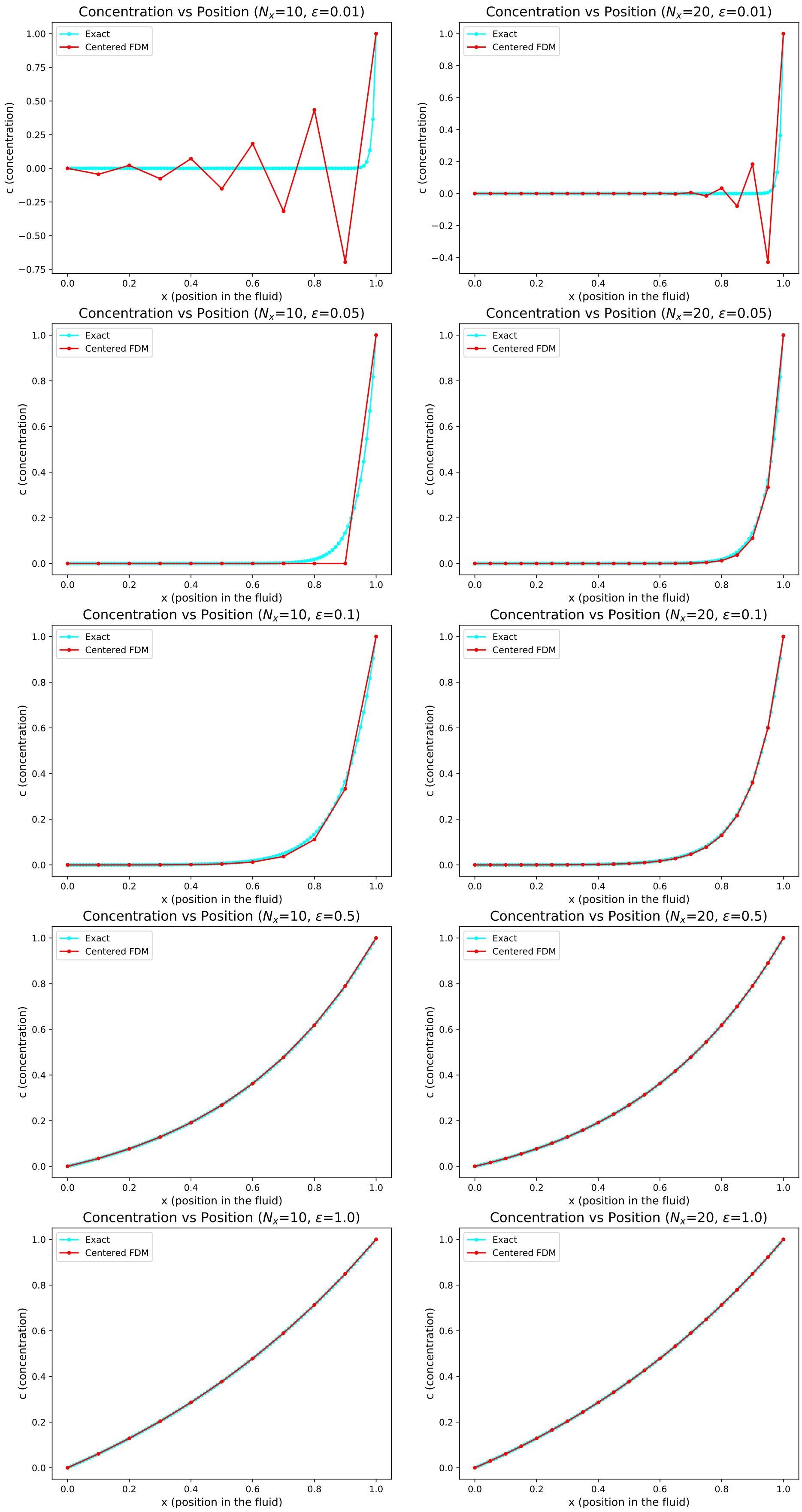
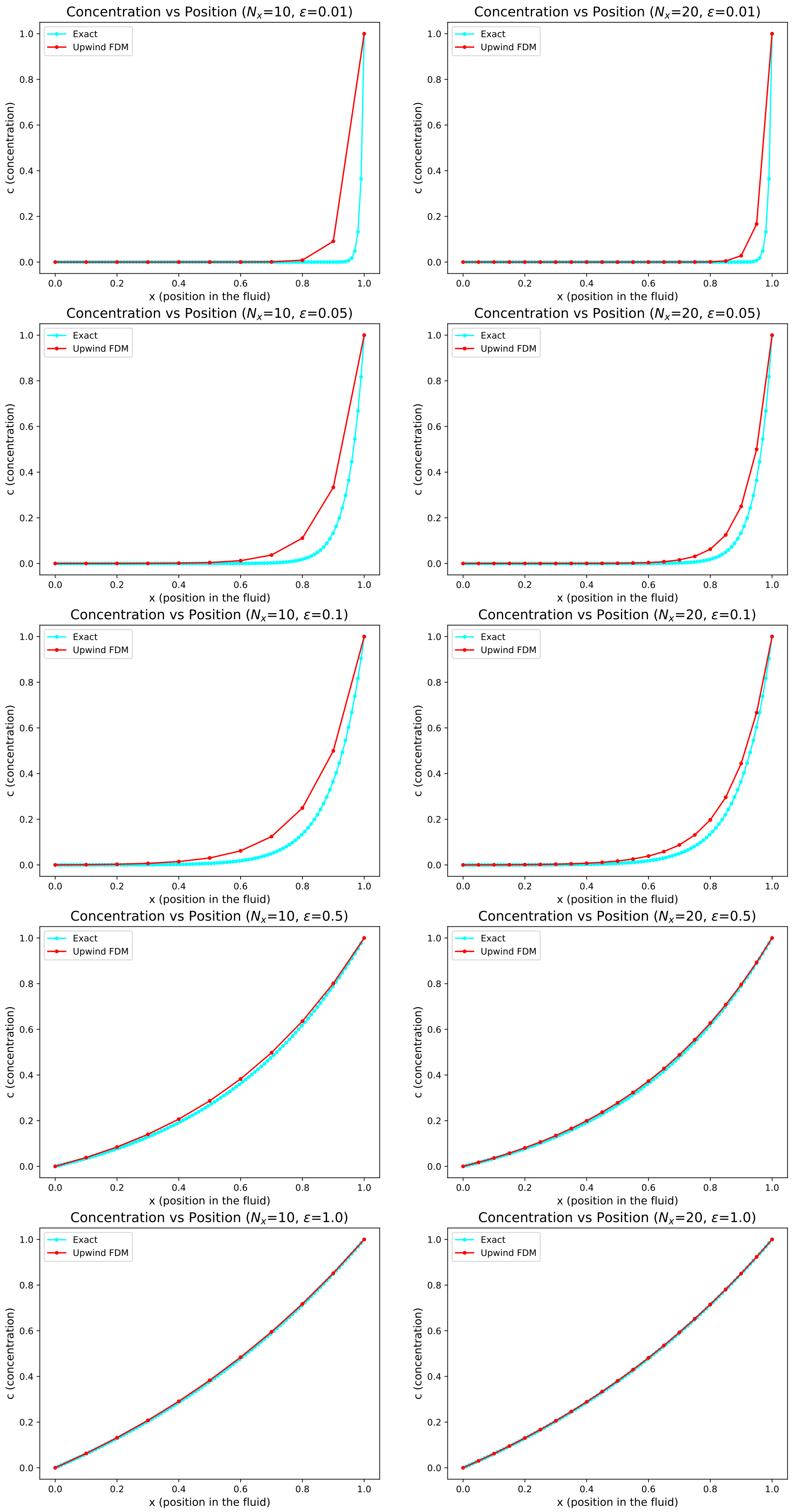


Figure 3: Analytical Solution vs Upwind Finite Difference Method to Solve Equation (10)



6.1.3 Comparison

By observing Figure 2 and 3, we see that the interesting case arises when $\epsilon = 0.01$. Notice that there are oscillations occured when using the centered finite difference method. This is a typical phenomenon when solving this type of problems. In order to avoid oscillations, we need a condition where

$$\Delta x \leq \frac{1}{\epsilon},$$

which explains why there are less oscillations when $N_x = 20$ compared to when $N_x = 10$.

Otherwise, we can also stabilize the scheme by making the dominant term (which is the advective term in this case since $\epsilon = 0.01$) collect its information in the flow direction, which precisely means using the upwind finite difference scheme. This is the reason that the behaviour of the solution is stable according to Figure 3.

6.2 Time Dependent Advection-Diffusion Equation

Lastly, we consider the general case of 1D time dependent advection-diffusion equation, which writes:

$$\frac{\partial \hat{c}}{\partial \hat{t}} + \hat{v}\frac{\partial \hat{c}}{\partial \hat{x}} = \hat{D}\frac{\partial^2 \hat{c}}{\partial \hat{x}^2}, \quad \hat{x} \in [0, L],\ \hat{t} \in [0, T], \quad L, T \in \mathbb{R} \tag{12}$$

with the same notations used as section 6.1 where t = time.

For simplicity, we drop the bars and assume D and v to be constants. Furthermore, we consider periodic boundary condition:

$$c_1^j = c_{N_x}^j$$

and take $c_0^j = c_{N_x-1}^j$ and $c_{N_x+1}^j = c_2^j$;

we also consider gaussian initial conditions:

$$c_x^0 = exp\left(\frac{-(x-\mu)^2}{2a^2}\right)$$

with $a = 2.5$ and $\mu = \frac{L}{2}$, which looks like the plot below (peak centered at the middle of spatial domain with amplitude 1):

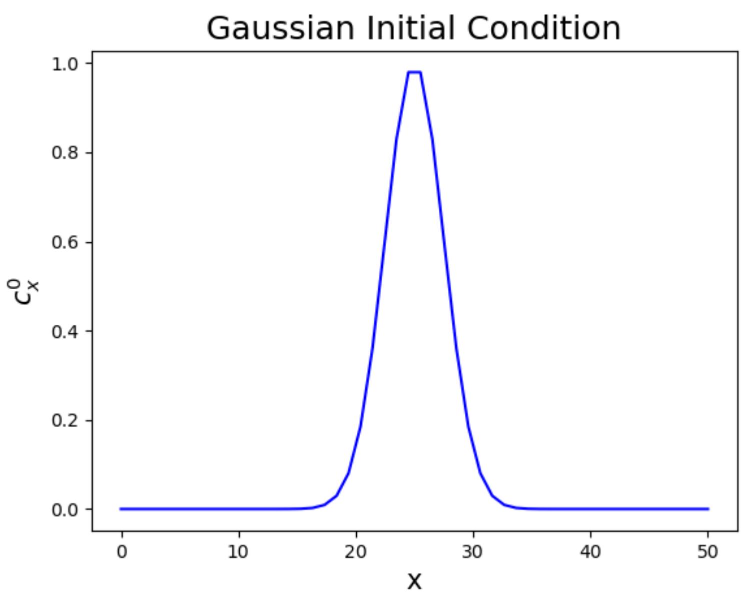


Figure 4: Gaussian initial condition when $a = 2.5$ and $L = 50$, i.e. $\mu = 25$.

6.2.1 Numerical Solution

We now apply the finite difference scheme. We will use the Crank-Nelson method, which is a semi-implicit method called the central time central space (CTCS) method [9]:

Firstly, we discretize the domain $[0, L] \times [0, T]$ by introducing equidistributed grid points corresponding to a spatial step size $dx = \frac{L}{(N_x-1)}$ and to a time step $dt = \frac{T}{(N_t-1)}$.

Next, we discretize the original equation to see that:

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{j+1} - c_i^j}{\Delta t} \qquad \frac{\partial c}{\partial x} \approx \frac{c_{i+1}^j - c_{i-1}^j}{2\Delta x} \qquad \frac{\partial^2 c}{\partial x^2} \approx \frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{(\Delta x)^2}$$

In this case, substitution yields:

$$\frac{c_i^{j+1} - c_i^j}{\Delta t} = \theta\left(D\frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{(\Delta x)^2} - v\frac{c_{i+1}^j - c_{i-1}^j}{2\Delta x}\right) + (1-\theta)\left(D\frac{c_{i+1}^{j+1} - 2c_i^{j+1} + c_{i-1}^{j+1}}{(\Delta x)^2} - v\frac{c_{i+1}^{j+1} - c_{i-1}^{j+1}}{2\Delta x}\right)$$

where $\theta = 0.5$.

This equation can then be written in vector form of $Ax = b$ as:

$$\begin{aligned} & c_{i+1}^{j+1}\left(\frac{v}{4\Delta x} - \frac{D}{2(\Delta x)^2}\right) + c_i^{j+1}\left(\frac{1}{\Delta t} + \frac{D}{(\Delta x)^2}\right) + c_{i-1}^{j+1}\left(-\frac{v}{4\Delta x} - \frac{D}{2(\Delta x)^2}\right) = \\ & = c_{i+1}^j\left(\frac{D}{2(\Delta x)^2} - \frac{v}{4\Delta x}\right) + c_i^j\left(\frac{1}{\Delta t} - \frac{D}{(\Delta x)^2}\right) + c_{i-1}^j\left(\frac{v}{4\Delta x} + \frac{D}{2(\Delta x)^2}\right), \end{aligned}$$

Now, define some variables to simplify the equation:

$$\alpha = \frac{v}{4\Delta x} - \frac{D}{2(\Delta x)^2},\ \beta = \frac{1}{\Delta t} + \frac{D}{(\Delta x)^2},\ \gamma = -\frac{v}{4\Delta x} - \frac{D}{2(\Delta x)^2},\ \beta_b = \frac{1}{\Delta t} - \frac{D}{(\Delta x)^2}.$$

Thus, we can now express the equation in tridiagonal form as follows:

$$Ax = b \implies \begin{bmatrix} \beta & \alpha & 0 & \cdots & 0 & \gamma & 0 \\ \gamma & \beta & \alpha & 0 & \cdots & 0 & 0 \\ 0 & \gamma & \beta & \alpha & 0 & \cdots & 0 \\ \vdots & 0 & \gamma & \beta & \alpha & 0 & \cdots \\ 0 & \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \ddots & 0 & \ddots & \ddots & \alpha \\ 0 & \alpha & 0 & \cdots & 0 & \gamma & \beta \end{bmatrix} \begin{bmatrix} c_1^{j+1} \\ c_2^{j+1} \\ \vdots \\ \\ \vdots \\ c_{N_x}^{j+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ \\ \vdots \\ b_{N_x} \end{bmatrix}$$

where

$$b_1 = -\gamma c_{N_x-1}^j + \beta_b c_1^j - \alpha c_2^j,$$

$$b_i = -\gamma c_{i-1}^j + \beta_b c_i^j - \alpha c_{i+1}^j \quad for \quad i = 2, \ldots, N_x - 1$$

and

$$b_{N_x} = -\gamma c_{N_x-1}^j + \beta_b c_{N_x}^j - \alpha c_2^j.$$

Finally, we can do some coding to solve the problem and generate a plot to visualise the behaviour of the solution (concentration c) at different points at different times. For example, we can use the *scipy.sparse.linalg.spsolve* function in python etc.

In [9], the author considers the case when $v = 1.4$, $D = 1.0$, $L = 32$, $T = 40$, $N_x = 256$ and $N_t = 2048$. This can be represented in the plot below (taken from [9, p. 22]):

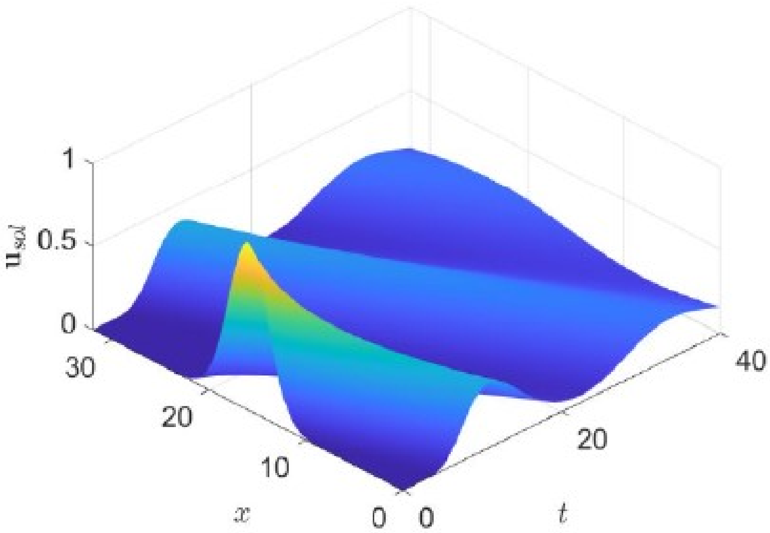


Figure 5: The solution data to the time dependent advection-diffusion equation that was produced.

7 Summary

In this review paper, we have given a rough summary on how researchers approach droplet evaporation problem, focusing on the case of a sessile droplet by using numerical methods. However, there are actually a lot of different ways to think about the problem.

From a more general perspective, we can consider pre-impact and post-impact effects on the evaporation rate of a droplet. To name a few, consider a droplet falling with a high velocity onto a solid substrate. This might cause spreading or bouncing which complicates the problem. We might also consider pattern formation in drying drops [10]. A real life example would be ring-like residue that is left when coffee dries on a table [11].

From a problem solving perspective, we can approach the problem analytically, numerically and experimentally. For example, there are experimentalists working on similar types of problems ([12], [13] etc), sometimes even involving mixture droplets. For instance, [6] focuses on binary droplet (liquid constituted by two components), which gets more complicated because the particle concentration affects the evaporation rate of the droplet. There are also papers focusing on analysing the results obtained in real life experiments vs the results obtained in theory such as [14].

In conclusion, we can now appreciate that the seemingly simple droplet evaporation problem turns out to be very complicated. Hence, researchers from all around the world are currently still attempting to come out with new ideas and different methods to better understand the behaviour of this natural phenomenon.

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