A BIOLOGICAL MODEL DESCRIBING VAPOUR AND DROPLETS

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1 Introduction

Delay equations (i.e., Delay Differential Equations, Renewal Equations and coupled Renewal and Delay Differential Equations) are fundamental in many scientific areas such as biology, medicine, engineering and physics as the introduction of the delay can provide a more realistic mathematical model incorporating the information from the past in the evolution law. For this reason the interest for these equations is still growing. The theory of delay equations with finite delay is well established (see [1] and [5] for the theory of DDEs) and some examples can be found in [6], [1]. As regards the theory of delay equations with infinite delay see [7] in which the principle of linearized stability is proved with the sun-star calculus. The Daphnia model described in [2] is an instance of a population model described with a coupled RE/DDE with infinite delay.
Due to the complexity of the analytical investigation of the properties of delay equations with both finite and infinite delay, it is necessary to use suitable numerical methods such as the pseudospectral discretization approach. Whereas in the case of finite delay we have convergence results [1], in the case of infinite delay numerical evidences are achieved [4], but the proof of convergence is still ongoing.
This work is dedicated to a new biological model introduced by the professor Mats Gyllenberg of the University of Helsinki and currently studied by his PhD student Eugenia Franco. This model describes the evolution of water droplets in a vapour and it can be mathematically represented by a DDE with infinite delay. The latter has some features in common with the Daphnia model introduced in the paper [2].
After having briefly described the features of the model, we will introduce a new mathematical model which allows us to study numerically the properties of the original model. Moreover, we will show some simulations obtained with codes developed with the software MATCONT using the pseudospectral approach (we will focus only on the results and not on the description of this numerical method).

2 The model

We consider a finite mass of vapour which contains a finite number of water droplets of different sizes. There are only three phenomena: birth, growth and death of the droplets. Moreover, we assume that the growth of a droplet is determined by a growth function and that there is a unique size-at-birth. The model is described by

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t) = \frac{\alpha}{x_0}\int_0^{+\infty}\big[\mu\big(X(a;V_t)\big)\,X(a;V_t) - g\big(X(a;V_t),V(t)\big)\big]\,\mathcal{F}(a;V_t)\,V_t(-a)\,\mathrm{d}a - \alpha V(t) \tag{1}$$

where $V(t)$ is the mass of the vapour per unit of space at time t, V_t is the history of the vapour, α is the condensation rate, x_0 is the size-at-birth of a droplet, $X(a;V_t)$ is the mass of a droplet at age a, $g(X,V)$ is the growth rate, $\mu(X)$ is the death rate and $\mathcal{F}(a;V_t)$ is the survival probability until age a.
The first integral represents the vapour that originates from the death of the droplets at time t, the second term represents the vapour that becomes water increasing the droplets at time t and the last term represents the vapour that condenses producing new droplets at time t.

Proposition 1 *The mass conservation holds, i.e., the sum of the concentration of the vapour and of the droplets (that is the total mass concentration) is constant:*

$$V(t) + \frac{\alpha}{x_0}\int_0^{+\infty} X(a;V_t)\,\mathcal{F}(a;V_t)\,V_t(-a)\,\mathrm{d}a = constant$$

for every $t \geq 0$.

Proposition 2 *Every constant function $\bar{V}$ is an equilibrium of the DDE* (1), *i.e.,*

$$0 = \frac{\alpha}{x_0} \int_0^{+\infty} \left[\mu\big(X(a;\bar{V})\big)\, X(a;\bar{V}) - g\big(X(a;\bar{V}),\bar{V}\big)\right] \mathcal{F}(a;\bar{V})\,\bar{V}\,\mathrm{d}a - \alpha\bar{V}$$

for every constant $\bar{V}$.

In order to fix a finite number of equilibria and to study how an equilibrium changes when a parameter varies, we propose to add a term corresponding to the mass conservation law with a fixed value of the total mass concentration E into the equation (1):

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}V(t) = \frac{\alpha}{x_0} \int_0^{+\infty} &\left[\mu\big(X(a;V_t)\big)\, X(a;V_t) - g\big(X(a;V_t),V(t)\big)\right] \mathcal{F}(a;V_t)\cdot \\ &\cdot V_t(-a)\mathrm{d}a - \alpha V(t) + E - V(t) - \frac{\alpha}{x_0}\int_0^{+\infty} X(a;V_t)\,\mathcal{F}(a;V_t)\,V_t(-a)\,\mathrm{d}a\,,\end{aligned} \tag{2}$$

From now on we will call (1) the *original (mathematical) model* and (2) the *new (mathematical) model*.

3 An example

We assume that the growth rate is

$$g(x,V) = k\,x^{2/3}\,V$$

where $k > 0$. It follows that

$$X(a;V_t) = x(a) = \left(\sqrt[3]{x_0} + \frac{k}{3}\int_0^a V_t(-s)\,\mathrm{d}s\right)^3 \qquad a \geq 0$$

and

$$g(X(a;V_t),V(t)) = k\left(\sqrt[3]{x_0} + \frac{k}{3}\int_0^a V_t(-s)\,\mathrm{d}s\right)^2 V(t) \qquad a \geq 0\,, t \geq 0\,.$$

Furthermore, we assume that $\mu(X(a;V_t)) = \mu > 0$ is constant and so $\mathcal{F}(a;V_t) = e^{-a\mu}$. In this case, equation (2) becomes

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}V(t) = \frac{\alpha}{x_0}(\mu-1)\int_0^{+\infty} &\left(\sqrt[3]{x_0} + \frac{k}{3}\int_0^a V_t(-s)\,\mathrm{d}s\right)^3 e^{-a\mu}\,V_t(-a)\,\mathrm{d}a - \\ -\frac{\alpha}{x_0}kV(t)\int_0^{+\infty} &\left(\sqrt[3]{x_0} + \frac{k}{3}\int_0^a V_t(-s)\,\mathrm{d}s\right)^2 e^{-a\mu}\,V_t(-a)\,\mathrm{d}a + \\ &+ E - (1+\alpha)V(t)\end{aligned} \tag{3}$$

Proposition 3 *If the parameters μ, k, α, E and x_0 are fixed, then every equilibrium $\bar{V}$ of* (3) *satisfies the following equation*

$$2\alpha k^3\bar{V}^4 + 6\alpha\sqrt[3]{x_0}\,k^2\mu\bar{V}^3 + 9\alpha\sqrt[3]{x_0^2}\,k\mu^2\bar{V}^2 + 9x_0\mu^3(\alpha+\mu)\bar{V} - 9x_0\mu^4E = 0\,. \tag{4}$$

Moreover, let Λ_1 and Λ_2 be the set of the roots of the characteristic equation of the linearization at $\bar{V}$ of the original model and the new model (3) *respectively. Then*

1) $0 \in \Lambda_1$,
2) $-1 \in \Lambda_2$,
3) $\Lambda_1 \setminus \{0\} = \Lambda_2 \setminus \{-1\}$.

Remark 1 *The eigenvalue $0 \in \Lambda_1$ reflects the fact that the original model* (1) *has infinite equilibria. Hence it does not influence the stability of $\bar{V}$. Moreover, since -1 is the only different characteristic root, by the Principle of linearized stability, the stability properties of $\bar{V}$ are the same in the two models.*

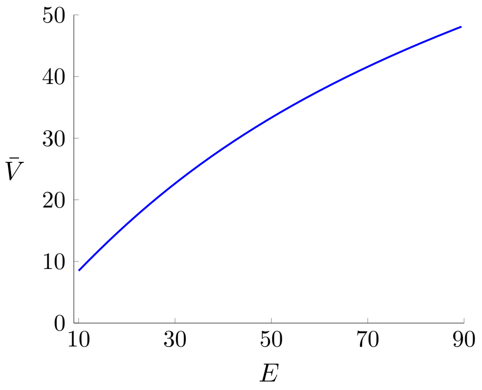

Figure 1: Continuation varying the parameter E from 10; $M = 10$, $\alpha = 0.5$, $\mu = 4$, $k = 0.2$, $x_0 = 2$, $\rho = 2$.

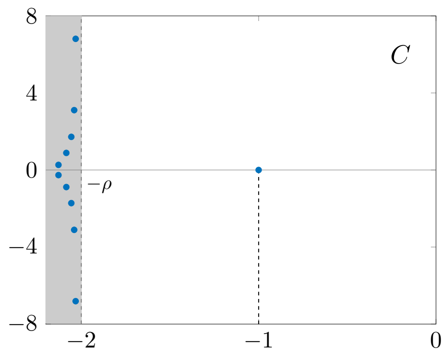

Figure 2: Computed spectrum with $M = 10$, $\alpha = 0.5$, $\mu = 4$, $k = 0.2$, $E = 10$, $x_0 = 2$, $\rho = 2$.

3.1 Simulations with MATCONT

We fix

$$\rho = \frac{1}{2}\mu \tag{5}$$

and we use the classical Laguerre-Gauss-Radau nodes as collocation nodes for the pseudospectral model.
Let $M = 10$, $\alpha = 0.5$, $\mu = 4$, $k = 0.2$, $E = 10$ and $x_0 = 2$. Then the equation (4), which solutions are the equilibria of the model, becomes

$$\frac{1}{125}\bar{V}^4 + \frac{12}{25}\sqrt[3]{2}\,\bar{V}^3 + \frac{72}{5}\sqrt[3]{4}\,\bar{V}^2 + 5184\,\bar{V} - 46080 = 0\,.$$

Using the function roots of the software MATLAB we can verify that the equation has four distinct solutions:

$$\begin{aligned}\bar{V}_1 &= -108.67\\ \bar{V}_2 &= 12.29 + 78.05i\\ \bar{V}_3 &= 12.29 - 78.05i\\ \bar{V}_4 &= 8.49\end{aligned}$$

In particular, only $\bar{V}_4$ is real and belongs to the interval $[0, E] = [0, 10]$. Figure 1 shows the continuation plot of the equilibrium $\bar{V}_4$ varying the total mass E from 10 to 90. Note that there are no bifurcation points.
Analysing the characteristic equation it is possible to prove that for $E = 10$ the characteristic roots are all negative, i.e., the equilibrium is asymptotically stable. The eleven eigenvalues computed by the pseudospectral method (λ_5 plus ten spurious) are illustrated in Figure 2.
Finally, Figure 3 shows that we have spectral accuracy and that the error is already 10^{-9} when we choose $M \approx 10$.

4 Conclusion

In the simulation the dynamics is very simple: there is one equilibrium which remain asymptotically stable when a parameter varies, i.e., there are no bifurcation points. We could probably get more complex dynamics considering other functions for the growth rate $g(x, V)$, considering a not constant death rate μ or adding other phenomena in the formulation of the model. For example, at the University of Helsinki a model with other two phenomena (*fragmentation* of a droplet and *coagulation* of two droplets) is currently studied.

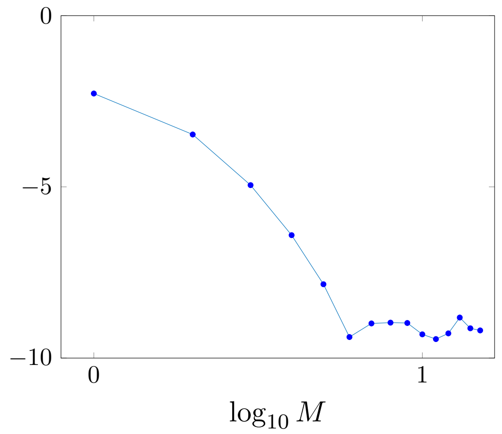

Figure 3: Log-log plot of the absolute error of the characteristic root -1; $\alpha = 10$, $\mu = 30$, $k = 0.5$, $E = 10$, $x_0 = 2$.

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