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# Fractional derivative model for diffusion-controlled adsorption at liquid/liquid interface

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**Abstract.** The Ward-Tordai integral equation governs the diffusion-controlled surfactant adsorption at air/liquid interfaces. In this paper the Ward-Tordai equation is generalized in two directions. First, the adsorption is assumed to take place at a liquid/liquid interface, where the surfactant is soluble in both liquid phases. Second, the diffusion in the bulk phases is anomalous and is governed by time-fractional diffusion equations. For the computation of the change of adsorption with time two numerical techniques are proposed and compared. Numerical results are presented.

## INTRODUCTION

In the recent decades Fractional Calculus attracted the attention of many researchers [1]. For applications in Mechanics we refer to [2, 3, 4], to mention only few of many recent monographs.

The work of Ward and Tordai (1946) [5] on the dynamics of surfactant interfacial layers, is still the theoretical basis of all new models to describe the time dependence of interfacial properties [6]. In fact, the famous Ward-Tordai integral equation governing the diffusion-controlled adsorption of surfactants at air/liquid interfaces, is a remarkable example of a fractional-order equation (in this particular case of order 1/2) derived from a classical integer-order model. The problem leading to the Ward-Tordai equation concerns adsorption of an aqueous surfactant solution at the air/solution interface. The process consists of two steps: diffusion (transport of surfactant molecules from the bulk phase to the subsurface due to a concentration gradient) and adsorption (transport of molecules from the subsurface to the surface). If the rate of the diffusion step is much slower than that of the adsorption, the whole process is controlled by diffusion and is called diffusion-controlled adsorption [7, 8]. For completeness, a simplified derivation of the Ward-Tordai equation is given next.

The diffusion of surfactant in the bulk phase is governed by the equation

$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2}, \quad t > 0, \quad x > 0, \quad (1)$$

with initial and boundary conditions on the surface ( $x = 0$ ) and at infinity:

$$C(x, 0) = C_{eq}, \quad x > 0, \quad (2)$$

$$\lim_{x \rightarrow 0^+} C(x, t) = C_s(t), \quad \lim_{x \rightarrow +\infty} C(x, t) = C_{eq}, \quad t \geq 0. \quad (3)$$

Here  $C(x, t)$  is the surfactant concentration in the bulk phase,  $D$  is the diffusion coefficient,  $C_{eq}$  is the input concentration of surfactant in the bulk, and  $C_s(t)$  is the subsurface surfactant concentration.

For the surfactant concentration on the interface,  $x = 0$ , we use the standard notation  $\Gamma(t)$ . There is a relationship between  $C_s(t)$  and  $\Gamma(t)$  in the form  $KC_s(t) = f(\Gamma(t))$ , called “adsorption isotherm”. Here  $K$  denotes the adsorption constant. Different surfactants obey different adsorption isotherms. Typical adsorption isotherms are those of Langmuir, Frumkin, Van der Waals, Freundlich, etc. [9, 10].

The change of surfactant concentration on the interface is compensated by the diffusion flux from the bulk:

$$\frac{d\Gamma(t)}{dt} = D \left. \frac{\partial C(x, t)}{\partial x} \right|_{x=0}, \quad t > 0. \quad (4)$$

It is supposed that, initially, the interface contains a given amount of surfactants, i.e.

$$\Gamma(0) = \Gamma_0. \quad (5)$$

The aim is to determine the evolution of surfactant concentration  $\Gamma(t)$  on the interface.

The problem is conveniently treated applying the technique of Laplace transform with respect to time  $t$ , where the following notations are used

$$\mathcal{L}\{u(x, t)\}(s) = \widehat{u}(x, s) = \int_0^\infty e^{-st} u(x, t) dt.$$

Applying Laplace transform to the diffusion equation (1) and taking into account the initial condition (2), the following ODE is obtained

$$s\widehat{C}(x, s) - C_{eq} = D \frac{\partial^2 \widehat{C}}{\partial x^2}, \quad x > 0, \quad (6)$$

where  $s > 0$  is considered as a parameter. Equation (6), equipped with boundary conditions for  $\widehat{C}(x, s)$ , derived from conditions (3):  $\widehat{C}(0, s) = \widehat{C}_s(s)$ ,  $\widehat{C}(+\infty, s) = C_{eq}/s$ , admits the solution

$$\widehat{C}(x, s) = \frac{C_{eq}}{s} + \left( \widehat{C}_s(s) - \frac{C_{eq}}{s} \right) \exp\left(-\sqrt{\frac{s}{D}}x\right). \quad (7)$$

On the other hand, application of Laplace transform to equation (4) yields

$$s\widehat{\Gamma}(s) - \Gamma_0 = D \left. \frac{\partial \widehat{C}}{\partial x} \right|_{x=0} = \sqrt{Ds} \left( \frac{C_{eq}}{s} - \widehat{C}_s(s) \right), \quad (8)$$

where (5) and (7) have also been used. We divide both sides of equation (8) by  $s$  and take the inverse Laplace transform with the help of the convolution property for Laplace transform and the identity

$$\mathcal{L}^{-1}\left\{\frac{1}{\sqrt{s}}\right\} = \frac{1}{\sqrt{\pi t}}.$$

In this way, as a final result, the diffusion equation is transformed into the following space independent nonlinear Volterra integral equation with a weakly singular kernel:

$$\Gamma(t) = \Gamma_0 + \sqrt{\frac{D}{\pi}} \int_0^t \frac{C_{eq} - C_s(\tau)}{(t - \tau)^{1/2}} d\tau. \quad (9)$$

It was derived for the first time (in a different way) by Ward and Tordai in [5]. Since  $C_s(t)$  is a function of  $\Gamma(t)$  via an adsorption isotherm, we can define the function

$$F(\Gamma(t)) = \sqrt{D}(C_{eq} - C_s(t)) = \sqrt{D}(C_{eq} - f(\Gamma(t))/K)$$

and rewrite the Ward-Tordai integral equation (9) in the form:

$$\Gamma(t) = \Gamma_0 + \frac{1}{\sqrt{\pi}} \int_0^t \frac{F(\Gamma(\tau))}{(t - \tau)^{1/2}} d\tau. \quad (10)$$

Further, using the definitions of fractional integrals and derivatives, see Appendix, equation (10) can be rewritten in compact form as the following fractional-order integral equation

$$\Gamma(t) = \Gamma_0 + \mathbf{J}_t^{1/2} \{F(\Gamma(t))\}, \quad (11)$$

where  $\mathbf{J}_t^\alpha$  denotes the Riemann-Liouville fractional integral. Applying to both sides of (11) the fractional derivative in Caputo sense  $\mathbf{D}_t^{1/2}$ , the following fractional-order differential equation is deduced

$$\mathbf{D}_t^{1/2}\Gamma(t) = F(\Gamma(t)), \quad \Gamma(0) = \Gamma_0. \quad (12)$$

The derived equations (9)-(12) are usually nonlinear due to the nonlinearity of the adsorption isotherms. Therefore, numerical techniques for the solution are necessary.

Interpretation of the Ward-Tordai equation in the light of Fractional Calculus can be found in [11, 12]. In [13] fractional-order generalizations to the diffusion-controlled adsorption problem are proposed and studied. In this work memory effects are introduced into the processes of diffusion and adsorption by replacing the first derivatives in time in equations (1) and (4) by fractional derivatives of orders between 0 and 1. In general, anomalous diffusion through non-homogeneous media is studied in a vast amount of papers, e.g. [14, 15] and the very recent survey paper [16]. Numerical techniques for the solution of the Ward-Tordai equation and its generalizations are discussed in [11, 17, 13]. For the general theory of interfacial transport processes we refer to [9].

In this work we consider diffusion-controlled adsorption of surfactants at a liquid/liquid interface, where the surfactants are soluble in both phases. Anomalous diffusion is assumed in both bulk phases, governed by time-fractional diffusion equations. We derive a generalization of the Ward-Tordai integral equation for the surfactant concentration  $\Gamma(t)$  on the interface. Two methods for the numerical computation of  $\Gamma(t)$  are presented and some numerical experiments are performed. Definitions and basic properties of the Riemann-Liouville fractional integral and Caputo fractional derivative, as well as details on the Fractional Adams method for numerical solution of nonlinear fractional-order integral equations, are given in an Appendix.

## FRACTIONAL DIFFUSION-CONTROLLED ADSORPTION AT LIQUID/LIQUID INTERFACE

Consider surfactant that is soluble in two liquid phases which are in contact at an interface. Such system is in general not in equilibrium and processes of diffusion of surfactant in the bulk phases and adsorption on the interface take place.

Schematic sketch of the problem for diffusion-controlled adsorption at liquid/liquid interface is given in Fig. 1, where  $C^+(x, t)$  and  $C^-(x, t)$  denote the surfactant concentrations in phase 1 ( $x > 0$ ) and phase 2 ( $x < 0$ ), respectively;  $\Gamma(t)$  is the concentration of surfactant on the interface at  $x = 0$ ;  $K^\pm$  are adsorption constants. Fig. 1 corresponds to a practically important particular case, in which initially one of the phases is free of surfactants.

The mathematical formulation of the problem for adsorption at liquid/liquid interface controlled by anomalous diffusion contains two time-fractional equations for anomalous diffusion of surfactant in the bulk phases:

$$\mathbf{D}_t^\mu C^-(x, t) = D^- \frac{\partial^2 C^-(x, t)}{\partial x^2}, \quad x < 0, \quad \mathbf{D}_t^\nu C^+(x, t) = D^+ \frac{\partial^2 C^+(x, t)}{\partial x^2}, \quad x > 0; \quad t > 0, \quad (13)$$

where  $\mu$  and  $\nu$  are parameters of anomalous diffusion,  $0 < \mu \leq 1$ ,  $0 < \nu \leq 1$ , and  $D^\pm$  are the diffusion coefficients in the corresponding phases. The diffusion equations are complemented with the initial conditions:

$$C^-(x, 0) = C_{eq}^-, \quad x < 0; \quad C^+(x, 0) = C_{eq}^+, \quad x > 0; \quad (14)$$

and boundary conditions

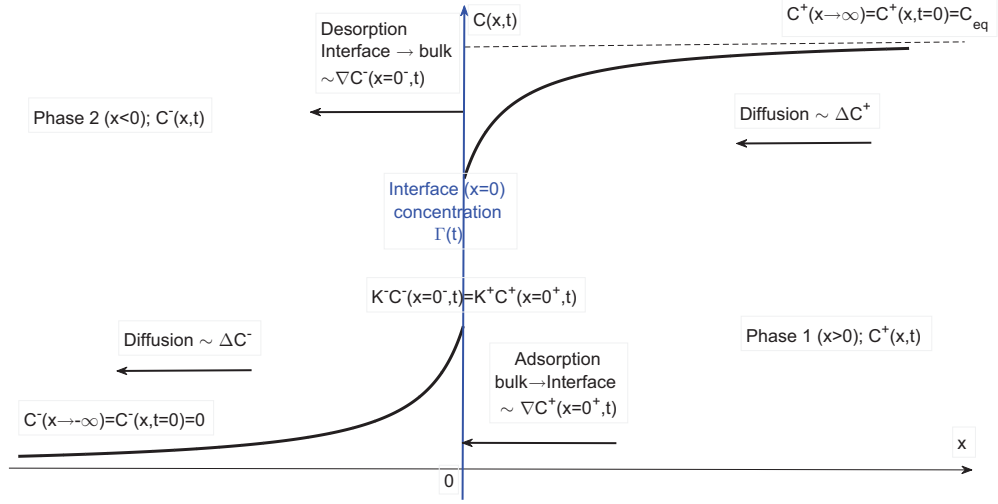
$$\lim_{x \rightarrow -\infty} C^-(x, t) = C_{eq}^-, \quad \lim_{x \rightarrow \infty} C^+(x, t) = C_{eq}^+, \quad t > 0, \quad (15)$$

$$\lim_{x \rightarrow 0^-} C^-(x, t) = C_s^-(t), \quad \lim_{x \rightarrow 0^+} C^+(x, t) = C_s^+(t), \quad t > 0, \quad (16)$$

where  $C_s^\pm(t)$  are the subsurface surfactant concentrations and  $C_{eq}^\pm$  are the input concentrations of surfactant in the bulk phases. Recall that in Fig. 1 a particular case is depicted, in which initially one of the phases is free of surfactants:  $C_{eq}^- = 0$ ,  $C_{eq}^+ = C_{eq}$ . In addition, the following identity for the two subsurface surfactant concentrations is satisfied

$$K^- C_s^-(t) = K^+ C_s^+(t) = f(\Gamma(t)), \quad t > 0, \quad (17)$$

where  $f(\Gamma)$  is the adsorption isotherm.



**FIGURE 1.** Schematic sketch of the problem for diffusion-controlled adsorption at liquid/liquid interface.

The change of the surfactant concentration  $\Gamma(t)$  on the interface is compensated by the diffusion fluxes from the both bulk phases, which results in the equation:

$$\frac{d\Gamma(t)}{dt} = -D^- \left. \frac{\partial C^-(x,t)}{\partial x} \right|_{x=0^-} + D^+ \left. \frac{\partial C^+(x,t)}{\partial x} \right|_{x=0^+}, \quad t > 0; \quad \Gamma(0) = \Gamma_0. \quad (18)$$

Here again  $\Gamma_0$  is the initial surfactant concentration on the interface.

To find an equation for the surfactant concentration on the interface  $\Gamma(t)$ , we first apply Laplace transform with respect to  $t$  to the diffusion equations (13) in the bulk phases using (26). Taking into account the initial conditions (14) and boundary conditions (15) and (16) we deduce the solutions of the obtained ODEs

$$\widehat{C}^-(x,s) = \frac{C_{eq}^-}{s} + \left( \widehat{C}_s^-(s) - \frac{C_{eq}^-}{s} \right) \exp \left( x \sqrt{\frac{s^\mu}{D^-}} \right), \quad x < 0; \quad (19)$$

$$\widehat{C}^+(x,s) = \frac{C_{eq}^+}{s} + \left( \widehat{C}_s^+(s) - \frac{C_{eq}^+}{s} \right) \exp \left( -x \sqrt{\frac{s^\nu}{D^+}} \right), \quad x > 0. \quad (20)$$

On the other hand, application of Laplace transform to equation (18) yields by the use of equations (19) and (20)

$$s\widehat{\Gamma}(s) - \Gamma_0 = -D^- \left. \frac{\partial \widehat{C}^-}{\partial x} \right|_{x=0^-} + D^+ \left. \frac{\partial \widehat{C}^+}{\partial x} \right|_{x=0^+} = \sqrt{D^-} s^\mu \left( \frac{C_{eq}^-}{s} - \widehat{C}_s^-(s) \right) + \sqrt{D^+} s^\nu \left( \frac{C_{eq}^+}{s} - \widehat{C}_s^+(s) \right),$$

which implies

$$\widehat{\Gamma}(s) = \frac{\Gamma_0}{s} + \sqrt{D^-} s^{\mu/2-1} \left( \frac{C_{eq}^-}{s} - \widehat{C}_s^-(s) \right) + \sqrt{D^+} s^{\nu/2-1} \left( \frac{C_{eq}^+}{s} - \widehat{C}_s^+(s) \right).$$

We take the inverse Laplace transform and deduce with the help of the identity (26) for the Riemann-Liouville integral and relation (17) the following integral equation for the surfactant concentration on the interface:

$$\Gamma(t) = \Gamma_0 + \mathbf{J}_t^{1-\mu/2} \{F^-(\Gamma(t))\} + \mathbf{J}_t^{1-\nu/2} \{F^+(\Gamma(t))\}, \quad (21)$$

where

$$F^\pm(\Gamma(t)) = \sqrt{D^\pm} \left( C_{eq}^\pm - f(\Gamma(t))/K^\pm \right).$$

In the case of classical diffusion in the bulk phases,  $\mu = \nu = 1$ , the equation governing the surfactant concentration on the liquid/liquid interface is deduced from (21):

$$\Gamma(t) = \Gamma_0 + \mathbf{J}_t^{1/2} \{F^-(\Gamma(t)) + F^+(\Gamma(t))\}. \quad (22)$$

Equations (22) and (21) are generalizations of the Ward-Tordai equation (11).

## NUMERICAL RESULTS

For numerical computation of the function  $\Gamma(t)$  two different numerical methods are applied.

- Fractional Adams method for numerical solution of the Ward-Tordai equation (11) and its generalizations (22) and (21). The numerical scheme is described in the Appendix. This scheme can be directly applied to solve equations (11), (22), and (21) with  $\mu = \nu$ . For the solution of (21) for  $\mu \neq \nu$  a straightforward modification of the fractional Adams method can be used, adding to the terms corresponding to  $\mathbf{J}_t^{1-\mu/2} \{F^-(\Gamma(t))\}$  in the predictor and corrector equations (29) and (30) analogous terms corresponding to  $\mathbf{J}_t^{1-\nu/2} \{F^+(\Gamma(t))\}$ .

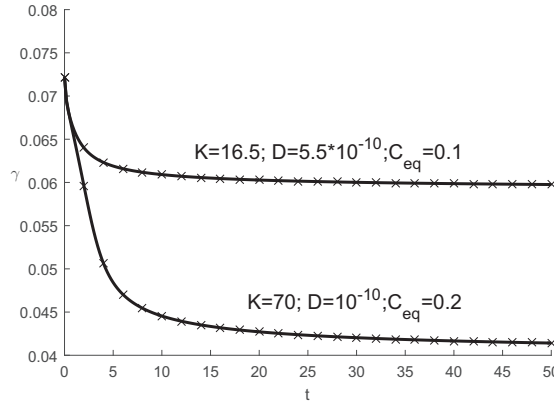
- Finite difference method (FDM) for the diffusion-adsorption problem. The proposed finite difference scheme uses a nonuniform mesh in space. The spatial step  $h_i$  increases as a geometric progression with common ratio  $q$ :  $\bar{\omega}_h = \{x_{i+1} = x_i + h_i, x_0 = 0, i = \overline{0, n}; h_{i+1} = h_i q, i = \overline{2, n-3}\}$ , with an exception that the first three and the last two steps are constant,  $h_0 = h_1 = h_2$  and  $h_{n-1} = h_n$ . Thus, keeping the ratio  $q$  close to 1 the mesh is locally almost uniform. The time step is constant as in the previous scheme.

In the tests performed in this paper  $h_0 = 2.5 \times 10^{-7}$  and  $h_n = 2.5 \times 10^{-4}$  at  $q = 1.2, n = 40$  and time step  $\tau = 10^{-5}$ .

For the approximation of the spatial terms  $\frac{\partial^2 C}{\partial x^2}$  third order finite differences are used:

$$\frac{\partial^2 C}{\partial x^2} \approx a_1^i \cdot C_{i-2}^j + a_2^i \cdot C_{i-1}^j + a_3^i \cdot C_i^j + a_4^i \cdot C_{i+1}^j + a_5^i \cdot C_{i+2}^j.$$

The definition of the coefficients  $a_k^i$  can be found e.g. in [18].



**FIGURE 2.** Comparison between the two numerical methods in the case of air/liquid surface: Fractional Adams method for the Ward-Tordai equation (marks) and FDM for the diffusion-adsorption equation (lines).

Numerical computations for some test problems are performed and the results are given in Figs. 2 and 3. Since in experiments the amount of surfactant  $\Gamma(t)$  adsorbed at an interface can not be measured directly and is usually calculated indirectly from interfacial tension measurements [19, 20], in the figures we present plots for the interfacial tension  $\gamma(t)$ . The results have been obtained with the help of the Frumkin adsorption isotherm

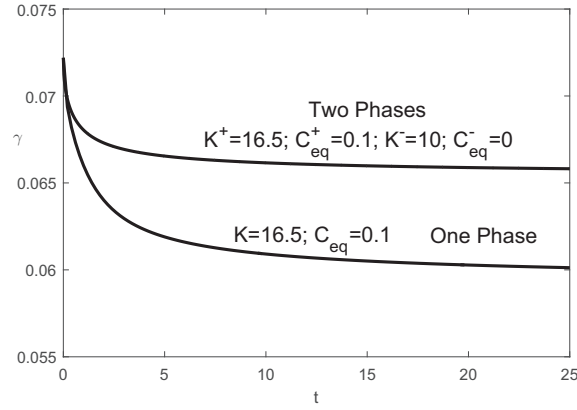
$$KC_s = \frac{\theta}{1 - \theta} \exp(-\beta\theta)$$

and the corresponding equation of state

$$\frac{\gamma_0 - \gamma}{E_B \Gamma_\infty} = -\ln(1 - \theta) - \frac{\beta}{2} \theta^2,$$

where  $\theta(t) \equiv \Gamma(t)/\Gamma_\infty$  is the surface coverage, with  $\Gamma_\infty$  being the maximum surfactant concentration, and  $\beta$  is an interaction parameter. In all computations initially the interface is clean of surfactants,  $\Gamma_0 = 0$ , with initial interfacial tension  $\gamma_0 = 0.0722 \text{ N/m}$ , and the other parameters in the equation of state are:  $\beta = 1.62$ ,  $E_B = 2479 \text{ N.m/mol}$ .

Fig. 2 corresponds to the case of air/liquid surface and classical diffusion. Two sets of parameters are considered. A very good agreement between the results obtained by the different numerical methods is seen, which indicates the high accuracy of both methods. It is worth mentioning that further mesh refinement (in space or time) in both methods does not affect the results. The fractional Adams method has the advantage to give directly the surfactant concentration  $\Gamma(t)$  on the interface, without computation of the surfactant concentration in the bulk phases. However, due to the presence of convolutional integral in the Ward-Tordai equation the CPU time and the computer memory required for a single step of calculation increase with time. On the other hand, the FDM simulates the whole process of surfactant diffusion in the bulk phases and its adsorption on the interface. In the classical case ( $\mu = \nu = 1$ ) the CPU time and computer memory required for a single time step do not increase with time. The latter is, however, not valid when anomalous diffusion is considered in one or both phases.



**FIGURE 3.** Comparison between adsorption on air/liquid surface with that on liquid/liquid interface.

In Fig. 3 the change with time of the interfacial tension  $\gamma(t)$  is given in the cases of adsorption at air/liquid surface and at liquid/liquid interface. The main difference between the two cases is that in the first one the surfactant is soluble only in one of the phases (liquid), while in the second one they are soluble in both phases. Classical diffusion in all liquid phases ( $\mu = \nu = 1$ ) is considered. The numerical computations are performed employing the finite difference method. The parameters in the liquid/liquid case for one of the phases ( $x > 0$ ) are chosen to be the same as those in the case of one liquid phase (liquid/air interface). The other phase ( $x < 0$ ) is initially clean of surfactants,  $C_{eq}^- = 0$ . Thus, part of the surfactants that are adsorbed on the interface from the liquid phase in the half-space  $x > 0$  desorb to the other liquid phase (in the half-space  $x < 0$ ). This results in a smaller concentration of surfactants  $\Gamma(t)$  in the case of two phases (liquid/liquid case) compared to the case of one phase (air/liquid case), and respectively, higher interfacial tension  $\gamma(t)$  as it is seen in Fig. 3.

## CONCLUDING REMARKS

The Ward-Tordai integral equation governing the diffusion-controlled adsorption of surfactant at air/liquid interface is generalized in two directions: the adsorption is considered at an interface between two liquids and memory effects in the diffusion in both bulk phases are introduced. The generalized Ward-Tordai equation is a nonlinear integral equation containing two Riemann-Liouville integral operators of orders between 0 and 1. For the numerical computation of the change of adsorption with time two numerical techniques are proposed: Fractional Adams method for numerical

solution of the generalized Ward-Tordai equation and Finite difference method for the original diffusion-adsorption problem.

In this paper only the case of classical diffusion in both phases is treated in the numerical experiments. The general problem will be solved numerically in a future work.

In the light of Fractional Calculus another generalization of the problem is feasible: to introduce memory effects not only in the diffusion components of the model, but also in the adsorption part. This is done in [13] for the case of air/liquid surface. Replacing the first derivative of  $\Gamma(t)$  in (18) by a fractional derivative of order  $\delta \in (0, 1)$  will lead to operators in the corresponding generalized Ward-Tordai equation, which are either integral or differential operators of fractional order, depending on the relations between the fractional parameters  $\mu$ ,  $\nu$  and  $\delta$ . This will lead to different regimes in the diffusion-adsorption process.

## ACKNOWLEDGMENT

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## APPENDIX

### Fractional order operators

Next we give definitions and some basic properties of the operators of fractional integration and differentiation [21].

The Riemann-Liouville fractional integral  $\mathbf{J}_t^\alpha$  is defined as follows

$$\mathbf{J}_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) d\tau, \quad \alpha > 0; \quad \mathbf{J}_t^0 f(t) = f(t); \quad (23)$$

where  $\Gamma(\cdot)$  is the Euler Gamma function. To avoid confusion, let us note that in this paper the symbol  $\Gamma(\cdot)$  denotes Gamma function only in the Appendix In the main body of the paper it always denotes the surfactant concentration on the interface.

The Caputo fractional derivatives,  $\mathbf{D}_t^\alpha$  is defined for  $\alpha \in (0, 1]$  by the identity

$$\mathbf{D}_t^\alpha = \mathbf{J}_t^{1-\alpha} \frac{d}{dt}, \quad \alpha \in (0, 1]. \quad (24)$$

Some basic properties of the fractional order operators are listed next:

$$\mathbf{J}_t^\alpha \mathbf{J}_t^\beta = \mathbf{J}_t^{\alpha+\beta}, \quad \alpha, \beta > 0; \quad \mathbf{D}_t^\alpha \mathbf{J}_t^\alpha f(t) = f(t), \quad \mathbf{J}_t^\alpha \mathbf{D}_t^\alpha f(t) = f(t) - f(0), \quad \alpha \in (0, 1]. \quad (25)$$

Application of Laplace transform to the fractional order operators obeys the following identities

$$\mathcal{L}\{\mathbf{J}_t^\alpha f\}(s) = s^{-\alpha} \widehat{f}(s), \quad \alpha > 0; \quad \mathcal{L}\{\mathbf{D}_t^\alpha f\}(s) = s^\alpha \widehat{f}(s) - s^{\alpha-1} f(0), \quad \alpha \in (0, 1]. \quad (26)$$

They can be derived from the Laplace transform pair

$$\mathcal{L}\left\{\frac{t^{\alpha-1}}{\Gamma(\alpha)}\right\} = s^{-\alpha}, \quad \alpha > 0, \quad (27)$$

and the identity for the first order derivative  $\mathcal{L}\{f'\}(s) = s\widehat{f}(s) - f(0)$ .

### Fractional Adams method

The fractional Adams method, proposed and analyzed in [22, 23], is a predictor-corrector numerical method for solution of nonlinear integral equations in the form

$$y(t) = y_0 + \mathbf{J}_t^\alpha F(y(t)), \quad 0 \leq t \leq T. \quad (28)$$



To find a numerical solution of Eq. (28) a uniform grid  $\{t_j = jh, j = 0, 1, \dots, N\}$  is considered with some integer  $N$  and  $h = T/N$ . Denote by  $y_j$  the approximation for  $y(t_j)$ ,  $j = 0, 1, \dots, N$ . The predictor  $y_{k+1}^P$  is determined by the formula

$$y_{k+1}^P = y_0 + \sum_{j=0}^k b_{\alpha,j,k+1} F(y_j), \quad b_{\alpha,j,k+1} = \frac{h^\alpha}{\Gamma(\alpha+1)} ((k+1-j)^\alpha - (k-j)^\alpha). \quad (29)$$

The corrector scheme is:

$$y_{k+1} = y_0 + \sum_{j=0}^k a_{\alpha,j,k+1} F(y_j) + a_{\alpha,k+1,k+1} F(y_{k+1}^P), \quad a_{\alpha,j,k+1} = \frac{h^\alpha}{\Gamma(\alpha+2)} A_{\alpha,j,k+1} \quad (30)$$

where

$$A_{\alpha,j,k+1} = \begin{cases} k^{\alpha+1} - (k-\alpha)(k+1)^\alpha & \text{if } j = 0, \\ (k-j+2)^{\alpha+1} + (k-j)^{\alpha+1} - 2(k-j+1)^{\alpha+1} & \text{if } 1 \leq j \leq k, \\ 1 & \text{if } j = k+1. \end{cases}$$

## REFERENCES

- [1] J. Machado and V. Kiryakova, *Fract. Calc. Appl. Anal.* **20**, 307–336 (2017).
- [2] R. Hilfer, *Applications of Fractional Calculus in Physics* (World Scientific, 2000).
- [3] F. Mainardi, *Fractional Calculus and Waves in Linear Viscoelasticity* (Imp. College Press, London, 2010).
- [4] T. M. Atanacković, S. Pilipović, B. Stanković, and D. Zorica, *Fractional Calculus with Applications in Mechanics: Vibrations and Diffusion Processes* (John Wiley & Sons, London, 2014).
- [5] A. Ward and L. Tordai, *J. Chem. Phys.* **14**, 453–461 (1946).
- [6] R. Miller, E. Aksenenko, and V. Fainerman, *Adv. Colloid Interface Sci.* **247**, 115–129 (2017).
- [7] J. Liu and U. Messow, *Colloid Polym. Sci.* **278**, 124–129 (2000).
- [8] J. Liu, C. Yang, C. Zhang, and U. Messow, *Colloid Polym. Sci.* **284**, 92–96 (2005).
- [9] D. A. Edwards, H. Brenner, and D. T. Wasan, *Interfacial Transport Processes and Rheology* (Butterworth-Heinemann, 1991).
- [10] C. Chang and E. Frances, *Colloids Surf. A* **100**, 1–45 (1995).
- [11] I. Bazhlekova, S. Dimova, P. Hjørrth, T. Ivanov, A. Slavova, and R. Yordanova, in *104-th European Study Group with Industry, Sept. 23-27, 2014, Sofia, Bulgaria. Problems & Final Reports.* (2014), pp. 48–59.
- [12] J. Hristov, *Journal of King Saud University - Science* **28**, 7–13 (2016).
- [13] G. Baumann and F. Stenger, *Fract. Calc. Appl. Anal.* **16**, 737–764 (2013).
- [14] R. Metzler and J. Klafter, *Phys. Rep.* **339**, 1–77 (2000).
- [15] L. Vlahos, H. Isliker, Y. Kominis, and K. Hizonidis, in *Order and chaos*, Vol. 10, edited by T. Bountis (Patras University Press, 2008).
- [16] T. Sandev, R. Metzler, and A. Chechkin, *Fract. Calc. Appl. Anal.* **21**, 10–28 (2018).
- [17] X. Li, R. Shaw, G. Evans, and P. Stevenson, *Comput. Chem. Eng.* **34**, 146–153 (2010).
- [18] I. Bazhlekova and D. Vasileva, *J. Comput. Appl. Math.* **293**, 7–19 (2016).
- [19] K. Danov, V. Kolev, P. Kralchevsky, G. Broze, and A. Mehreteab, *Langmuir* **16**, 2942–2956 (2000).
- [20] V. Dudnik and K. Lunkenheimer, *Langmuir* **16**, 2802–2807 (2000).
- [21] R. Gorenflo and F. Mainardi, in *Fractals and Fractional Calculus in Continuum Mechanics*, edited by A. Carpinteri and F. Mainardi (Springer-Verlag, Wien/New York, 1997), pp. 223–276.
- [22] K. Diethelm, N. Ford, and A. Freed, *Nonlinear Dynam.* **29**, 3–22 (2002).
- [23] K. Diethelm, N. Ford, and A. Freed, *Numer. Algorithms* **36**, 31–52 (2004).