

A fractional-order theory of phase transformation in presence of anomalous heat transfer

Gianmarco Nuzzo^{1, a*}, Fabiana Amiri¹, Salvatore Russotto¹, Emanuela Bologna¹,
and Massimiliano Zingales¹

¹Department of Engineering, University of Palermo, Viale delle Scienze ed. 8, 90128, Palermo, Italy

^agianmarco.nuzzo@unipa.it

Keywords: Fractional Calculus, Anomalous Heat Transfer, Stefan Problem

Abstract. In this paper the solution for the one-dimensional Stefan problem of fractional order was examined, considering a generalization of Fourier's law, in which flux is related to temperature through Caputo's fractional derivative.

Introduction

The term phase transformation denotes the transition of a thermodynamic system from one aggregate state to another. Dealing with phase transformations, it is necessary to refer to the so-called processes at the interface. They are characterized by two distinct phases and a moving interface advancing and consequently by the transformation of one phase and the gradual decrease of the other. Typical examples may be liquid-solid phase changes, chemical reactions, liquid-vapor transformations etc.

These phenomena were observed in the late 19th century by Slovenian physicist Joseph Stefan, especially the formation of ice in the polar seas, to whom we owe the so-called formulation of *Stefan's problem* [1].

Stefan problems are systems of partial derivative differential equations comprising two governing equations, for the two phases, with respective boundary conditions and another differential equation called *Stefan condition*, valid at the interface and binding the two phases [2]. Given the high nonlinearity of these problems, depending on the choice of boundary conditions and because, as time goes on, one domain widens and one shrinks, it is not always possible to derive analytical solutions, so it is often necessary to proceed numerically.

The pivotal equation governing the heat diffusion process of both phases is the *Fourier law*, which links the flux to the temperature gradient. In previous years, however, it has been observed that in multiphase conductors or in the presence of high-frequency phenomena, the Fourier equation, in its the steady state, cannot fully describe such processes [3]. For this reason, modifications and generalizations of Fourier's law have been proposed in the last half of the past century.

Cattaneo suggested a modification of Fourier's law, introducing a new term that considers the rate of heat flow [4], but Fourier/Cattaneo law-based models are not appropriate for capturing the behavior of recent applications such as high-efficiency exchangers, microprocessor cooling or additive manufacturing.

So, in [5] a fractional formulation of the Fourier equation was proposed, replacing the standard integer-order derivative and integral with real-order operators.

The aim of this paper is to exploit the fractional formulation of Fourier's law to reach the solutions found in [6], starting with physical considerations.



Derivation of fractional Fourier law

Considering an inhomogeneous medium (Fig. 1), consisting of several masses, m_i , with different heat capacities $C^{(V)}(z)$, separated by conductive material with different conductivities $\chi^{(V)}(z)$ and subjected to a flow of heat $\bar{q}(t)$:

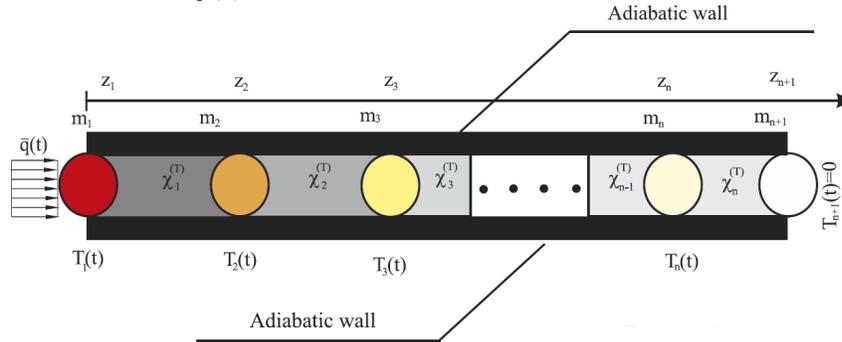


Fig. 1. Thermodynamical model of inhomogeneous medium [5].

Capacities and conductivities hold the following power laws: $C^{(V)}(z) = \frac{C_\beta^{(V)} z^{-\beta}}{\Gamma[1-\beta]}$, $\chi^{(V)}(z) = \frac{\chi_\beta^{(V)} z^{-\beta}}{\Gamma[1-\beta]}$ with dimensions $[C_\beta^{(V)}] = \frac{L^{2+\beta} T^2}{K}$, $[\chi_\beta^{(V)}] = \frac{ML^{1+\beta}}{KT^3}$. If we examine an infinitesimal part (Fig. 2) of the medium:

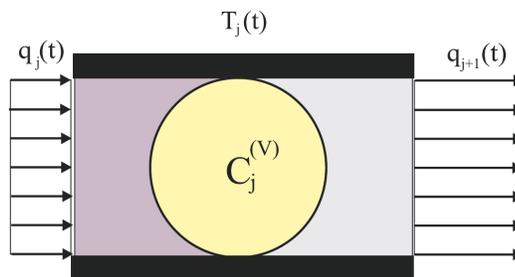


Fig. 2. Thermal energy balance of the j th-mass [5].

The energy balance for the generic mass m_j involves the rate of internal energy U_j of the mass and the incoming and outgoing energy fluxes:

$$\begin{aligned} \frac{dU_j(t)}{dt} &= m_j \frac{du_j(t)}{dt} = m_j C_j^{(V)} \frac{dT_j(t)}{dt} \\ &= A_j q_j(t) - A_{j+1} q_{j+1}(t). \end{aligned} \quad (1)$$

In which u_j is the internal density function of the mass m_j . The mass m_j occupies the volume of $A\Delta z$, so introducing the density ρ , we can express the mass as $m_j = \rho A\Delta z$. Simplifying the previous expression, we get (assuming $A_j = A_{j+1}$):

$$\rho C_j^{(V)} \frac{dT_j(t)}{dt} = - \frac{q_{j+1}(t) - q_j(t)}{\Delta z}. \quad (2)$$

Introducing the temperature field $T_j(t) \rightarrow T(z_j, t)$, the thermal energy flux field $q_j(t) \rightarrow q(z_j, t)$, $C_j^{(V)} \rightarrow C^{(V)}(z_j)$ and performing the limit $\Delta z \rightarrow 0$ in (2) we obtain the following balance equation:

$$\rho C^{(V)}(z) \frac{\partial T(z, t)}{\partial t} = - \frac{\partial q(z, t)}{\partial z}. \tag{3}$$

We can substitute to $q(z, t)$ the Fourier law: $q(z, t) = -\chi^{(V)}(z) \frac{\partial T(z, t)}{\partial z}$. Finally, we reach the diffusion temperature equation:

$$\rho C^{(V)}(z) \frac{\partial T(z, t)}{\partial t} = \frac{\partial}{\partial z} \left[\chi^{(V)}(z) \frac{\partial T(z, t)}{\partial z} \right]. \tag{4}$$

It remains only to associate the (4) with the corresponding boundary conditions: $\bar{q}(t) = \lim_{z \rightarrow 0} \left(-\chi^{(V)}(z) \frac{\partial T(z, t)}{\partial z} \right)$, $\lim_{z \rightarrow \infty} T(z, t) = 0$. The solution of (4) was found by applying the Laplace transform, applying boundary conditions, and then anti-transforming (refer to [5] for more details, R_β is the anomalous thermal conductivity coefficient):

$$\bar{q}(t) = R_\beta \left(D_{0+}^\beta T_0 \right)(t). \tag{5}$$

Formulation of Fractional Stefan Problem

Before writing the fractional system, we derive Stefan's condition by the fractional Fourier law. Consider two infinitesimal times (highlighted in the figure below) consider two infinitesimal times (accentuated in the figure below), in which we will obtain two different values of the interface, respectively $s(t_0)$ and $s(t_1)$:

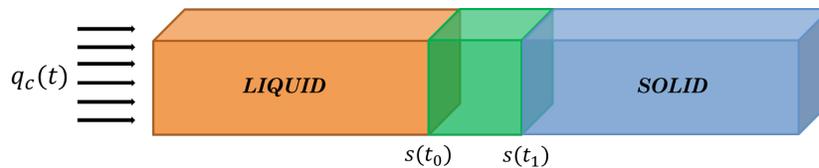


Fig. 3. Schematic representation of two generic heat diffusion times, at which we find two interface values.

We know from thermodynamics that to melt a piece of bar from $s(t_0)$ to $s(t_1)$ requires heat equal to:

$$Q_1 = V \rho \lambda = A (s(t_1) - s(t_0)) \rho \lambda. \tag{6}$$

Heat within both phases propagates through flux of fractional Fourier law, which takes this form:

$$q_{\beta,i} = -k_{\beta,i} \left({}_0^c D_t^\beta \frac{\partial T_i}{\partial x} \right) (x, t). \tag{7}$$

Where the dimensions of the anomalous diffusivity coefficient are $[k_{\beta,i}] = \frac{g \text{ cm}}{s^{3-\beta} K}$. To employ the principle of energy conservation and equalize the fluxes of liquid and solid to heat Q_1 , it is necessary to integrate them twice, first with respect to area and then with respect to time.

$$Q_2 = A \int_{t_0}^{t_1} \left(-k_{\beta,L} \left({}_0^c D_t^\beta \frac{\partial T_L}{\partial x} \right) (s(t), t) + k_{\beta,S} \left({}_0^c D_t^\beta \frac{\partial T_S}{\partial x} \right) (x, t) \right) dt. \quad (8)$$

Now we can equalize $Q_1 = Q_2$ and make some simplifications:

$$(s(t_1) - s(t_0))\rho\lambda = \int_{t_0}^{t_1} \left(-k_{\beta,L} \left({}_0^c D_t^\beta \frac{\partial T_L}{\partial x} \right) (s(t), t) + k_{\beta,S} \left({}_0^c D_t^\beta \frac{\partial T_S}{\partial x} \right) (s(t), t) \right) dt. \quad (9)$$

We divide both members by $(t_1 - t_0)$ and perform the limit for $t_1 \rightarrow t_0$. Then, since t_0 can be any instant, we substitute t :

$$\frac{ds}{dt}(t) = -\gamma_{\beta,L} \left({}_0^c D_t^\beta \frac{\partial T_L}{\partial x} \right) (s(t), t) + \gamma_{\beta,S} \left({}_0^c D_t^\beta \frac{\partial T_S}{\partial x} \right) (s(t), t). \quad (10)$$

Where $\gamma_{\beta,i} = \frac{k_{\beta,i}}{\rho\lambda}$ with these dimensions $[\gamma_{\beta,i}] = \frac{cm^2}{s^{1-\beta} K}$. It becomes interesting to note that for $\beta \rightarrow 0$ in (10) we again obtain the classic Stefan's condition. Then writing the complete system in term of Caputo derivative [7,8] with $0 < \beta < 1$:

Liquid side:

$$\left\{ \begin{aligned} \frac{\partial T_L}{\partial t}(r, t) &= \alpha_{\beta,L} \left({}_0^c D_t^\beta \frac{\partial^2 T_L}{\partial x^2} \right) (x, t) & 0 < x < s(t), t > 0. \end{aligned} \right. \quad (10.a)$$

$$\left\{ \begin{aligned} \frac{\partial T_L}{\partial x}(0, t) &= -\frac{q_c(t)}{k_L} = -\frac{q_0}{k_L \sqrt{t^{1-\beta}}}. \end{aligned} \right. \quad (10.b)$$

$$\left\{ \begin{aligned} T_L(s(t), t) &= T_{Melt}. \end{aligned} \right. \quad (10.c)$$

Solid side:

$$\left\{ \begin{aligned} \frac{\partial T_S}{\partial t}(r, t) &= \alpha_{\beta,S} \left({}_0^c D_t^\beta \frac{\partial^2 T_S}{\partial x^2} \right) (x, t) & s(t) < x < \infty, t > 0. \end{aligned} \right. \quad (11.a)$$

$$\left\{ \begin{aligned} T_S(s(t), t) &= T_{Melt}. \end{aligned} \right. \quad (11.b)$$

$$\left\{ \begin{aligned} T_S(\infty, t) &= T_{Cold}. \end{aligned} \right. \quad (11.c)$$

$$\left\{ \begin{aligned} T_S(x, 0) &= T_{Cold}. \end{aligned} \right. \quad (11.d)$$

Interface condition:

$$\begin{cases} \frac{ds}{dt}(t) = -\gamma_{\beta,L} \left({}_0^c D_t^\beta \frac{\partial T_L}{\partial x} \right) (s(t), t) + \gamma_{\beta,S} \left({}_0^c D_t^\beta \frac{\partial T_S}{\partial x} \right) (s(t), t). & (12.a) \\ s(0) = 0. & (12.b) \end{cases}$$

Where $\alpha_{\beta,i} = \frac{k_{\beta,i}}{\rho c_{p,i}}$ are the anomalous diffusivity coefficients: $[\alpha_{\beta,i}] = \frac{cm^2}{s^{1-\beta}}$. The solutions of (11. a – 12. b) were found in [6], not shown here for brevity.

Numerical Application

Now some comparisons between the classical and fractional solutions will follow. The numerical data that will be used, for example purposes only, are from a Titanium alloy. For simplicity, parameters such as thermal conductivity, which depend on the order of derivation in the fractional case, will be taken in equal number value with respect to their integer-order counterparts. So, for example, $k_{\beta,L} = k_L$. Here are data for the Titanium alloy used: $\rho = 2.67 \frac{g}{cm^3}$, $\lambda = 171.6 \frac{J}{g}$, $k_L = 0.3 \frac{W}{cm K}$, $c_{p,L} = 1.18 \frac{J}{g K}$, $k_S = 0.081 \frac{W}{cm K}$, $c_{p,S} = 0.43 \frac{J}{g K}$, $q_0 = 1000 \frac{W}{cm^2} \sqrt{s}$, $T_{Melt} = 1923 K$, $T_{Cold} = 298 K$. In the next graph it is possible to observe, for a certain fixed time, different interface curves as β changes:

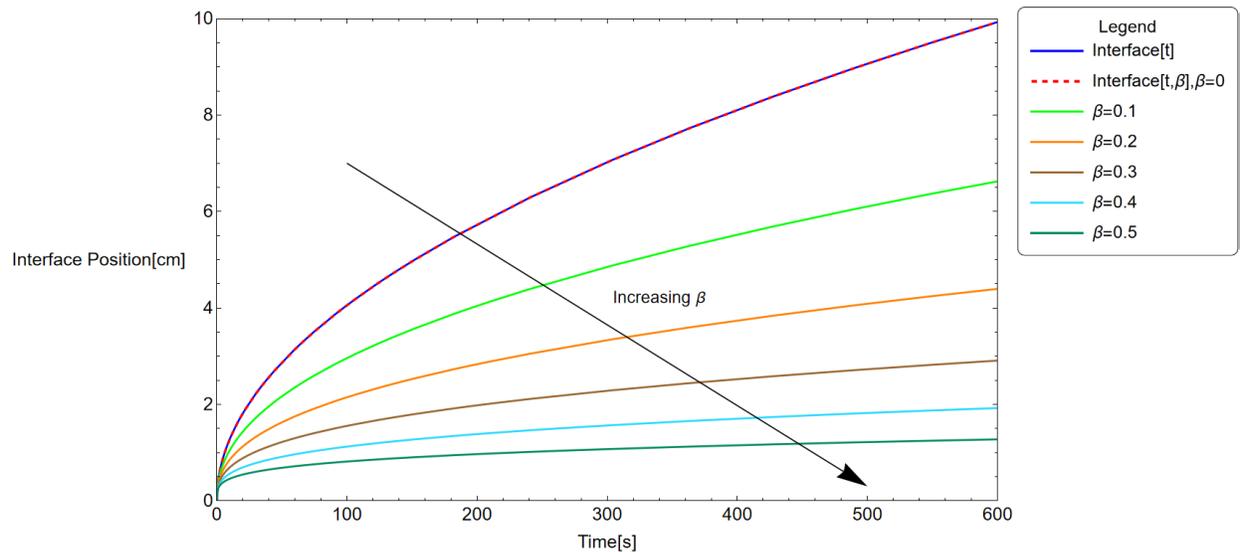


Fig. 4. Interface functions in β dependence, while in blue the classic solution.

For $\beta = 0$ the interface function derived from the problem in fractional form (dashed red curve) coincides with the classical solution (blue curve). Instead, as β increases there is a rapid decrease in the process, so fast that even just for a $\beta = 0.5$ the process reaches almost complete stationarity. Examples were not given for values above 0.5 because the curves were completely parallel to the x-axis, meaning that the interface remains in the same position for all time.

Lastly, in Fig. 4, the functions of temperature distributions at the same time fixed for the interface graph and at different values of β were plotted. Again, for $\beta = 0$, the fractional functions (black and grey) coincide with the classical functions (red and blue). The other liquid and solid curves have been plotted in the same colour for simplicity.

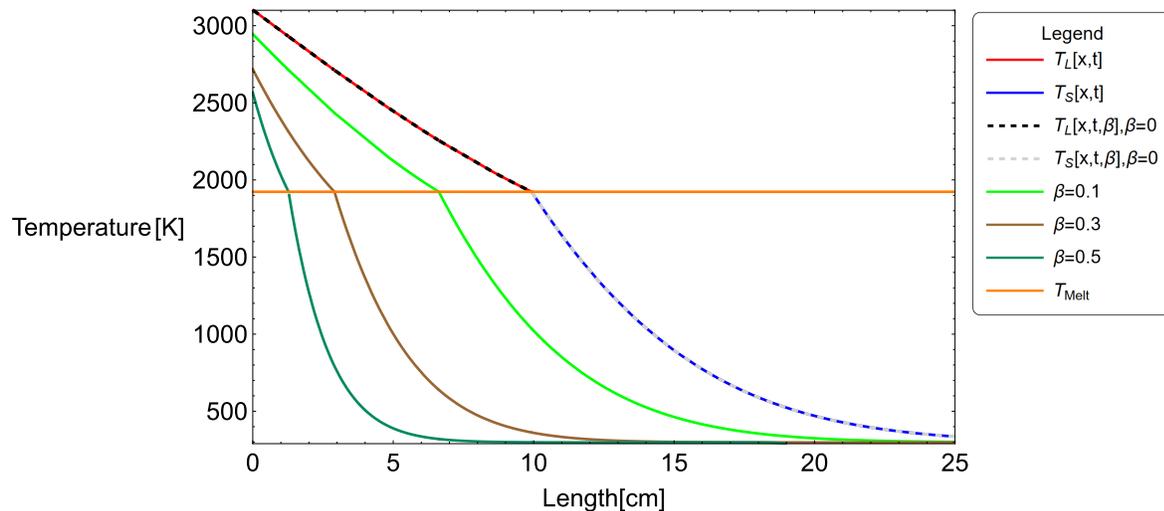


Fig. 5. Temperature distributions for liquid and solid in β dependence. In red and blue the solutions of the classical problem, in orange the melting temperature. The point where the curves meet on the melting line is the value of the interface.

Conclusions

In this paper, the solution for the one-dimensional stefan problem of fractional order was examined. It started from the fractional beta-order generalization of Fourier's law and then derived the formulation of the problem. By varying the order of the differintegral operator the process goes into *subdiffusion* and already for small values of beta slows down considerably, while for $\beta = 0$ we obtain to the solution of the classical problem.

References

- [1] C. Vuik (1993). Some historical notes about the Stefan problem.
- [2] S. C. Gupta (2017). *The classical Stefan problem: basic concepts, modelling and analysis with quasi-analytical solutions and methods* (Vol. 45). Elsevier. <https://doi.org/10.1016/B978-0-444-63581-5.00012-9>
- [3] G. Baffou, & R. Quidant (2013). Thermo-plasmonics: using metallic nanostructures as nano-sources of heat. *Laser & Photonics Reviews*, 7(2), 171-187. <https://doi.org/10.1002/lpor.201200003>
- [4] C. Cattaneo (1948). Sulla conduzione del calore. *Atti Sem. Mat. Fis. Univ. Modena*, 3, 83-101.
- [5] M. Zingales (2016). An exact thermodynamical model of power-law temperature time scaling. *Annals of Physics*, 365, 24-37. <https://doi.org/10.1016/j.aop.2015.08.014>
- [6] S. D. Roscani, & D. A. Tarzia (2018). Explicit solution for a two-phase fractional Stefan problem with a heat flux condition at the fixed face. *Computational and Applied Mathematics*, 37(4), 4757-4771. <https://doi.org/10.1007/s40314-018-0600-z>
- [7] I. Podlubny (1999). Fractional differential equations. *Mathematics in science and engineering*, 198, 41-119.
- [8] R. Gorenflo, A. A. Kilbas, F. Mainardi, & S. V. Rogosin (2020). *Mittag-Leffler functions, related topics and applications* (p. 540). New York, NY, USA: Springer. <https://doi.org/10.1007/978-3-662-61550-8>