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FRACTIONAL BURGERS' MODEL: THERMODYNAMIC CONSTRAINTS AND COMPLETELY MONOTONIC RELAXATION FUNCTION

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Abstract

Fractional Burgers' constitutive equation for viscoelastic fluids is studied. Thermodynamic constraints on the parameters are discussed as well as conditions for complete monotonicity of the corresponding relaxation function. The relationship between thermodynamic compatibility of the model and complete monotonicity of the relaxation function is analyzed.

Key words: Riemann–Liouville fractional derivative, completely monotonic function, Mittag–Leffler function, viscoelastic fluid

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1. Introduction. Fractional calculus is extensively used in linear viscoelasticity [1–6]. Fractional derivatives provide a convenient way to describe the behaviour of realistic materials with a restricted number of parameters. One of the models of viscoelastic fluids which employs fractional derivatives is the so-called fractional Burgers' model. According to this model the relationship between stress $\sigma(t)$ and strain $\varepsilon(t)$ in a one-dimensional material is given by the following constitutive equation

$$\left(1 + a_1 D_t^{\alpha} + a_2 D_t^{2\alpha}\right) \sigma(t) = \left(1 + b_1 D_t^{\beta} + b_2 D_t^{2\beta}\right) \dot{\varepsilon}(t), \tag{1.1}$$

where $a_1, a_2, b_1, b_2 > 0$, $0 < \alpha, \beta \leq 1$, D_t^{γ} is the Riemann–Liouville fractional time derivative of order γ and the over-dot denotes the first time derivative. In the limiting case $\alpha = \beta = 1$ eq. (1.1) is the constitutive equation of the generalized Burgers model ([7], Ch 2).

The relaxation function $G(t)$ in a linear viscoelastic model is defined as the stress response to a unit step of strain. Specifically, for a quiescent system at $t = 0$ the following equation is satisfied [2, 4, 5]

$$\sigma(t) = \int_0^t G(t-\tau) \dot{\varepsilon}(\tau) \, \mathrm{d}\tau. \tag{1.2}$$

Recently, several initial-boundary value problems have been studied within the context of model (1.1), see e.g. [8] and the references cited there. However, the underlying constitutive equation, corresponding relaxation function and thermodynamic constraints have not been studied in detail.

In the present work we discuss thermodynamic restrictions on the parameters of the fractional Burgers' constitutive equation (1.1), formulate conditions under which the corresponding relaxation function is a completely monotonic function and analyze how this property is related to thermodynamic compatibility.

2. Preliminaries. Assume $\gamma > 0$ and $m - 1 < \gamma < m$, where m is a positive integer. The Riemann–Liouville fractional derivative of order γ is defined by

$$D_t^{\gamma} u(t) = \frac{1}{\Gamma(m-\gamma)} \frac{\mathrm{d}^m}{\mathrm{d}t^m} \int_0^t \frac{u(\tau)}{(t-\tau)^{\gamma+1-m}} \, \mathrm{d}\tau,$$

where $\Gamma(\cdot)$ is the Gamma function; $D_t^m = \mathrm{d}^m/\mathrm{d}t^m$.

The following notations for the Laplace transform of a function are used

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

If $u^{(k)}(0^+) = 0$ for $k = 0, 1, \ldots, m-1$, then

$$\mathcal{L}\{D_t^{\gamma} u\}(s) = s^{\gamma} \widehat{u}(s). \tag{2.1}$$

The two-parameter Mittag–Leffler function is defined by the series

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta, z \in \mathbb{C}, \ \Re\alpha > 0. \tag{2.2}$$

It is a generalization of the exponential function $E_{1,1}(z) = \exp(z)$. The asymptotic expansion of the Mittag–Leffler function for $t \to +\infty$ when $\alpha \in (0, 2), \beta > 0$, can be obtained from the identity:

$$E_{\alpha,\beta}(-t) = -\sum_{k=1}^{N-1} \frac{(-t)^{-k}}{\Gamma(\beta - \alpha k)} + O(t^{-N}), \quad t \to +\infty. \tag{2.3}$$

We make use of the Laplace transform pairs $(\alpha, \beta > 0)$

$$\mathcal{L}\left\{\frac{t^{\alpha-1}}{\Gamma(\alpha)}\right\}(s) = s^{-\alpha}; \quad \mathcal{L}\left\{t^{\beta-1} E_{\alpha,\beta}(-\lambda t^{\alpha})\right\}(s) = \frac{s^{\alpha-\beta}}{s^{\alpha} + \lambda}. \tag{2.4}$$

A function $u(t) \in C^{\infty}(0, +\infty)$ is said to be completely monotonic function (CMF) for $t > 0$ iff

$$(-1)^n u^{(n)}(t) \geq 0, \quad t > 0, n = 0, 1, 2, \ldots \tag{2.5}$$

It is well known that if $0 < \alpha \leq 1$ and $\lambda > 0$ the function $t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^{\alpha})$ is CMF for $t > 0$. This can be seen as an extension of the complete monotonicity property of the exponential function $\exp(-\lambda t)$.

For further details on fractional calculus operators and Mittag–Leffler functions we refer to [9].

3. Thermodynamic constraints. Applying Laplace transform to (1.1) and to (1.2) one obtains by the use of (2.1), respectively:

$$\begin{aligned} (1 + a_1 s^{\alpha} + a_2 s^{2\alpha})\widehat{\sigma}(s) &= (1 + b_1 s^{\beta} + b_2 s^{2\beta})\widehat{\varepsilon}(s), \\ \widehat{\sigma}(s) &= \widehat{G}(s)\widehat{\varepsilon}(s). \end{aligned}$$

Therefore, the relaxation function has the following representation in Laplace domain

$$\widehat{G}(s) = \frac{1 + b_1 s^{\beta} + b_2 s^{2\beta}}{1 + a_1 s^{\alpha} + a_2 s^{2\alpha}} \tag{3.1}$$

and our further study is based on this identity, where $\alpha, \beta \in (0, 1]$, $a_1, b_1, a_2, b_2 > 0$.

According to the procedure presented in [1] for consistency with the second law of thermodynamics the following two inequalities should be satisfied:

$$\Re\{\mathrm{i}\omega\widehat{G}(\mathrm{i}\omega)\} \geq 0, \quad \Im\{\mathrm{i}\omega\widehat{G}(\mathrm{i}\omega)\} \geq 0, \ \forall\omega > 0. \tag{3.2}$$

(Although the original conditions in [1] are in terms of Fourier transform, we have written them formally in terms of Laplace transform using the assumption that all functions vanish for $t < 0$.)

Restrictions on the parameters of model (1.1) following from inequalities (3.2) are given in the next theorem.

Theorem 3.1. *If the fractional Burgers' model is thermodynamically compatible, then*

$$\alpha = \beta,\ a_1 \geq b_1,\ a_2 \geq b_2,\ a_2 b_1 \geq a_1 b_2. \tag{3.3}$$

Proof. Constraints (3.3) will be derived from (3.2) using (3.1). The dominant terms in $\Re\{\mathrm{i}\omega\widehat{G}(\mathrm{i}\omega)\}$ are as follows: $a_2 b_2 \omega^{2\alpha+2\beta}\sin((\alpha-\beta)\pi)$ for large ω, and $a_1\omega^\alpha \sin(\alpha\pi/2) - b_1\omega^\beta \sin(\beta\pi/2)$ for small ω. The first is nonnegative only if $\alpha \geq \beta$, the nonnegativity of the second implies

$$\omega^{\alpha-\beta} \geq \frac{b_1 \sin(\beta\pi/2)}{a_1 \sin(\alpha\pi/2)},$$

which can be satisfied for $\omega \to 0$ only if $\alpha \leq \beta$. Therefore $\alpha = \beta$ and inequalities (3.2) imply

$$\begin{aligned} &(a_1 - b_1)\omega^\alpha \sin(\alpha\pi/2) + (a_2 - b_2)\omega^{2\alpha}\sin(\alpha\pi) \\ &+(a_2 b_1 - a_1 b_2)\omega^{3\alpha}\sin(\alpha\pi/2) \geq 0, \quad \forall \omega > 0. \end{aligned} \tag{3.4}$$

$$\begin{aligned} &1 + (a_1 + b_1)\omega^\alpha \cos(\alpha\pi/2) + (a_1 b_1 + (a_2 + b_2)\cos(\alpha\pi))\omega^{2\alpha} \\ &+((a_1 b_2 + a_2 b_1)\cos(\alpha\pi/2))\omega^{3\alpha} + a_2 b_2 \omega^{4\alpha} \geq 0, \quad \forall \omega > 0. \end{aligned} \tag{3.5}$$

Since $\sin(\alpha\pi/2) > 0$ for $\alpha \in (0,1]$, one deduces from (3.4) that $a_1 \geq b_1$ (considering small ω) and $a_2 b_1 - a_1 b_2 \geq 0$ (considering large ω). The last two inequalities together with the positivity of all parameters imply $a_2/b_2 \geq a_1/b_1 \geq 1$. Therefore $a_2 \geq b_2$ and the proof is completed. □

Let us note that the inequalities in (3.3) are necessary and sufficient for fulfilling of (3.4), while (3.5) is satisfied if in addition it is supposed that

$$a_1 b_1 + (a_2 + b_2)\cos(\alpha\pi) \geq 0. \tag{3.6}$$

In this way the following result is obtained:

Theorem 3.2. *Assume that conditions* (3.3) *and* (3.6) *are satisfied. Then the fractional Burgers' model is thermodynamically compatible.*

Corollary 3.3. *Assume* $\alpha \in (0, 1/2]$. *Then conditions* (3.3) *are necessary and sufficient for thermodynamic compatibility of the fractional Burgers' model.*

Proof. Since in this case $\cos(\alpha\pi) \geq 0$ condition (3.6) is automatically satisfied. □

We close this section with a discussion of the asymptotic behaviour of the relaxation function $G(t)$ when constraints (3.3) are fulfilled and $0 < \alpha < 1$. It follows from (3.1)

$$\widehat{G}(s) = \frac{1 + b_1 s^{\alpha} + b_2 s^{2\alpha}}{1 + a_1 s^{\alpha} + a_2 s^{2\alpha}} = \frac{b_2}{a_2} + \frac{c_1 + c_2 s^{\alpha}}{1 + a_1 s^{\alpha} + a_2 s^{2\alpha}}, \tag{3.7}$$

where

$$c_1 = 1 - \frac{b_2}{a_2} \geq 0, \quad c_2 = b_1 - \frac{a_1 b_2}{a_2} \geq 0. \tag{3.8}$$

Therefore, taking the inverse Laplace transform and using the identity $\mathcal{L}\{\delta(t)\} = 1$ for the Dirac delta function $\delta(t)$, it follows

$$G(t) = \frac{b_2}{a_2}\delta(t) + F(t), \quad t \geq 0, \tag{3.9}$$

where

$$\widehat{F}(s) = \frac{c_1 + c_2 s^{\alpha}}{1 + a_1 s^{\alpha} + a_2 s^{2\alpha}}. \tag{3.10}$$

Therefore, $\widehat{F}(s) \approx (c_2/a_2)s^{-\alpha}$ for large s and applying Tauberian theorem one obtains the following asymptotic expansion for small t:

$$F(t) \approx \frac{a_2 b_1 - a_1 b_2}{a_2^2} \frac{t^{\alpha-1}}{\Gamma(\alpha)}, \quad t \to 0. \tag{3.11}$$

On the other hand, for small s we can neglect the term $s^{2\alpha}$ in (3.10) and, taking the inverse Laplace transform, it follows using (2.4) and (2.3)

$$F(t) \approx \frac{1}{a_1}\left(1 - \frac{b_1}{a_1}\right) t^{\alpha-1} E_{\alpha,\alpha}\left(-\frac{1}{a_1}t^{\alpha}\right) \approx \frac{b_1 - a_1}{\Gamma(-\alpha)} t^{-\alpha-1}, \quad t \to +\infty. \tag{3.12}$$

Therefore

$$\lim_{t\to+\infty} G(t) = 0; \quad \int_0^{\infty} G(t)\,\mathrm{d}t < \infty. \tag{3.13}$$

(In fact, by taking $s \to 0$ in (3.1), it follows that the integral in (3.13) equals $\widehat{G}(0+) = 1$.) Properties (3.13) imply that the Burgers' constitutive equation models fluid-like behaviour (see for the general conditions [5], Section 2). Asymptotic expansion (3.12) implies that $tG(t)$ is not integrable for $t \to \infty$, therefore characteristic times can not be determined (see also [2]).

4. Completely monotonic relaxation function. The class of completely monotonic functions (CMF), often encountered in applications, consists of nonnegative nonincreasing function, see (4.7). Due to the physical phenomenon of stress relaxation the relaxation function in a viscoelastic model is nonnegative and nonincreasing [4,5]. Asymptotic expansions (3.11) and (3.12) show that the relaxation function of the fractional Burgers' model $G(t)$ is CMF both for small and for large times. In this section we discuss conditions for complete monotonicity of $G(t)$ on $(0, \infty)$.

First we show that constraints (3.3) are necessary for nonnegativity of $G(t)$.

Theorem 4.1. *If $G(t) \geq 0$ for $t > 0$, then conditions* (3.3) *are satisfied.*

Proof. By the Bernstein's theorem if $G(t)$ is nonnegative, then $\widehat{G}(s)$ is CMF for $s > 0$. From (3.1) we find the following asymptotic behaviour of $\widehat{G}(s)$ for large s:

$$\widehat{G}(s) \approx \frac{b_2}{a_2} s^{2(\beta-\alpha)}, \quad s \to +\infty.$$

Hence $\widehat{G}(s)$ is CMF only if $\alpha \geq \beta$. On the other hand, using the expansion

$$\frac{1}{1+z} = \sum_{n=0}^{\infty} (-1)^n z^n, \ |z| < 1,$$

we obtain from (3.1) for small s

$$\widehat{G}(s) \approx 1 + b_1 s^{\beta} - a_1 s^{\alpha}, \quad s \to 0. \tag{4.1}$$

If $\alpha > \beta$, then the term $b_1 s^{\beta}$ will dominate over the term $a_1 s^{\alpha}$ in (4.1) and the first derivative of $\widehat{G}(s)$ will be positive for small s. This contradicts the complete monotonicity of $\widehat{G}(s)$. Therefore $\alpha = \beta$. Then from (4.1)

$$\frac{\mathrm{d}}{\mathrm{d}s}\widehat{G}(s) \approx \alpha(b_1 - a_1)s^{\alpha-1}, \quad s \to 0,$$

and the complete monotonicity of $\widehat{G}(s)$ implies $a_1 \geq b_1$.

Knowing that $\alpha = \beta$ we examine again the behaviour of $\widehat{G}(s)$ as $s \to +\infty$. Neglecting the first terms in the numerator and the denominator of (3.1), we get

$$\widehat{G}(s) \approx \frac{b_1 + b_2 s^{\alpha}}{a_1 + a_2 s^{\alpha}} = \frac{b_2}{a_2} + \frac{a_2 b_1 - a_1 b_2}{a_2^2} \frac{1}{s^{\alpha} + a_1/a_2}, \quad s \to +\infty. \tag{4.2}$$

This function admits nonpositive first derivative iff $a_2 b_1 \geq a_1 b_2$. The proof can be completed as that of Theorem 3.1. □

We note first that conditions (3.3) are not sufficient for nonnegativity of $G(t)$. For example, the model with $\alpha = \beta = 0.8$, $a_1 = 2, a_2 = 10, b_1 = 1.5, b_2 = 0.5$, complies with constraints (3.3), however $\widehat{G}(s)$ is not CMF (its second derivative admits negative values: e.g. $\widehat{G}''(s) = -18.87$ at $s = 0.01$). Therefore $G(t)$ is not a nonnegative function for all $t > 0$.

If we complement conditions (3.3) with (3.6), then the model is thermodynamically consistent (Theorem 3.2). However, these conditions are still not sufficient for nonnegativity of $G(t)$ as we can see from the following example. Let

$$a_1 = 3\ a_2 = 2,\ b_1 = 2.75,\ b_2 = 1, \tag{4.3}$$

and $\alpha = \beta = 0.9$. Then (3.3) and (3.6) are satisfied. However, $\widehat{G}(s)$ is not CMF since its fourth derivative admits negative values: e.g. $\widehat{G}^{(4)}(s) = -1.77$ for $s = 0.2$.

Therefore, thermodynamic compatibility of model (1.1) does not ensure nonnegativity of the corresponding relaxation function. This is in contrast to the case of fractional Jeffreys fluid ($a_2 = b_2 = 0$). It is proven in [10] that in this case model (1.1) is thermodynamically consistent if and only if $\alpha = \beta$ and $a_1 \geq b_1$, which implies that the corresponding relaxation function is a completely monotonic function.

Sufficient conditions for complete monotonicity of $G(t)$ are formulated next. In particular they guarantee its nonnegativity on $(0, \infty)$.

Theorem 4.2. *Assume that constraints* (3.3) *are satisfied and*

$$a_1^2 - 4a_2 > 0. \tag{4.4}$$

Then the relaxation function $G(t)$ admits the representation (3.9) *where*

$$F(t) = \int_0^\infty e^{-rt} K(r)\, dr, \tag{4.5}$$

with

$$K(r) = \frac{r^\alpha \sin(\alpha\pi)}{\pi} \frac{P}{Q^2 + R^2}, \tag{4.6}$$

$$\begin{aligned}
P &= (b_1 a_2 - a_1 b_2) r^{2\alpha} + 2(a_2 - b_2) r^\alpha \cos(\alpha\pi) + (a_1 - b_1),\\
Q &= 1 + a_1 r^\alpha \cos(\alpha\pi) + a_2 r^{2\alpha} \cos(2\alpha\pi),\\
R &= a_1 r^\alpha \sin(\alpha\pi) + a_2 r^{2\alpha} \sin(2\alpha\pi).
\end{aligned}$$

If, in addition $\alpha \in (0, 1/2]$ or

$$(a_1 - b_1)(b_1 a_2 - a_1 b_2) \geq (a_2 - b_2)^2 \cos^2(\alpha\pi), \tag{4.7}$$

then $F(t)$ is CMF for $t > 0$.

Proof. Taking the inverse Laplace integral one obtains from (3.10)

$$F(t) = \frac{1}{2\pi \mathrm{i}} \int_{Br} e^{st} \frac{c_1 + c_2 s^\alpha}{1 + a_1 s^\alpha + a_2 s^{2\alpha}} \, \mathrm{d}s, \tag{4.8}$$

where $Br = \{s;\ \mathrm{Re}\, s = \sigma\}$, with $\sigma > 0$. Due to assumption (4.4) the quadratic polynomial $f(x) = 1 + a_1 x + a_2 x^2$ has two real negative zeros. Therefore the function under the integral sign in (4.8) has no poles and we can bend the contour Br into the Hankel path $Ha(\rho)$, which starts from $-\infty$ along the lower side of the negative real axis, encircles the disc $|s| = \rho$ counterclockwise and ends at $-\infty$ along the upper side of the negative real axis. Taking $\rho \to 0$, one obtains (4.5) with

$$\begin{aligned} K(r) &= -\frac{1}{\pi} \Im \left\{ \left. \frac{c_1 + c_2 s^\alpha}{1 + a_1 s^\alpha + a_2 s^{2\alpha}} \right|_{s = re^{\mathrm{i}\pi}} \right\} \\ &= \frac{r^\alpha \sin(\alpha\pi)}{\pi} \frac{a_2 c_2 r^{2\alpha} + 2a_2 c_1 r^\alpha \cos(\alpha\pi) + (a_1 c_1 - c_2)}{|1 + a_1 r^\alpha e^{\mathrm{i}\alpha\pi} + a_2 r^{2\alpha} e^{2\mathrm{i}\alpha\pi}|^2}. \end{aligned}$$

This together with (3.8) gives (4.6).

Next we prove that under the additional assumptions of the theorem $K(r) \geq 0$ for $r > 0$, which together with (4.11) implies that $F(t)$ is CMF. Since $\sin(\alpha\pi) \geq 0$ for $\alpha \in (0, 1]$, we have to check only if $P \geq 0$ for $r > 0$. Assumptions (3.3) ensure the nonnegativity of all terms in P except $\cos(\alpha\pi)$. If $\alpha \in (0, 1/2]$, then $\cos(\alpha\pi) \geq 0$ and thus $P \geq 0$. If $\alpha \in (1/2, 1]$, then inequality (4.7) implies that the quadratic polynomial $g(x) = (b_1 a_2 - a_1 b_2) x^2 + 2(a_2 - b_2) x \cos(\alpha\pi) + (a_1 - b_1)$ has no real zeros. Since $b_1 a_2 - a_1 b_2 \geq 0$, then $g(x) \geq 0$ and therefore $P = g(r^\alpha) \geq 0$. □

If (4.4) is satisfied, we can obtain explicit representation of the relaxation function $G(t)$ in terms of Mittag–Leffler functions.

Theorem 4.3. *Suppose* (3.3) *and* (4.4) *hold. Then*

$$F(t) = A_1 t^{\alpha - 1} E_{\alpha,\alpha} \left(-\frac{1}{\tau_1} t^\alpha \right) + A_2 t^{\alpha - 1} E_{\alpha,\alpha} \left(-\frac{1}{\tau_2} t^\alpha \right), \tag{4.9}$$

where $\tau_1, \tau_2 > 0$ *are such that* $\tau_1 + \tau_2 = a_1, \quad \tau_1 \tau_2 = a_2$ *and*

$$A_1 = \frac{c_2 - c_1 \tau_1}{\tau_1 (\tau_2 - \tau_1)}, \quad A_2 = \frac{c_1 \tau_2 - c_2}{\tau_2 (\tau_2 - \tau_1)}. \tag{4.10}$$

Proof. From (3.10) $\widehat{F}(s)$ can be represented in the form

$$\widehat{F}(s) = \frac{c_1 + c_2 s^\alpha}{(\tau_1 s^\alpha + 1)(\tau_2 s^\alpha + 1)} = \frac{\tau_1 A_1}{\tau_1 s^\alpha + 1} + \frac{\tau_2 A_2}{\tau_2 s^\alpha + 1}, \tag{4.11}$$

with A_1, A_2 defined in (4.10). Applying inverse Laplace transform to (4.11) we obtain (4.9) by the use of the second identity in (2.4). □

We finish with a comment on the signs of the coefficients A_1 and A_2. Since for any $\lambda > 0$ the function $t^{\alpha-1}E_{\alpha,\alpha}(-\lambda t^\alpha)$ is CMF for $t > 0$, it is clear from (4.9) that $F(t)$ is CMF if $A_1, A_2 \geq 0$. In fact, for complete monotonicity of $F(t)$ it is not necessary both coefficients A_1 and A_2 to be nonnegative. For example, consider a model satisfying (4.3). Then $\tau_1 = 1$, $\tau_2 = 2$ and $A_1 = 0.75$, $A_2 = -0.125$. Although $A_2 < 0$, for $\alpha \leq 0.5$ $F(t)$ is CMF according to Theorem 4.2. This is, however, not true for larger values of α. It is easy to see that if $\alpha = 1$ then (4.9) implies $F(t) = 0.75\exp(-t) - 0.125\exp(-0.5t)$ and $F(t) < 0$ for $t > 2\ln 6$.

5. Conclusions In this work, in the context of fractional Burgers' model, we study the relationship between two properties: thermodynamic compatibility (TDC) and complete monotonicity of the corresponding relaxation function (CMR). A set of restrictions on the parameters is proven to be necessary both for TDC and CMR. Sufficient conditions for TDC and CMR are also formulated. It is shown that for this model conditions (3.2) for TDC do not necessarily imply CMR, in fact they even do not ensure the nonnegativity of $G(t)$. Note that, in general, the inverse is always true: complete monotonicity of $G(t)$ implies (3.2). This will be proven in a more detailed future work.

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