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Phase Transition in Compressible Media and Nonlocal Capillarity Terms

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Abstract. Nonlocal integral operators can be used to substitute the usually chosen high order differential operators to model the effect of capillarity close to phase boundaries in compressible media. We establish the existence of nonlocal viscosity-capillarity profiles for phase boundaries connecting states close to the Maxwell line. Furthermore numerical experiments in one space dimension comparing the local and the nonlocal approach are presented.

1. Introduction

One of the crucial issues in phase transition problems is the correct modelling of capillarity effects. In this context diffusive-dispersive models have been analyzed intensively in recent years. Typically the resulting evolution equations are nonlinear dissipative conservation laws with spatial differential operators of at least third order (see e.g. [5, 6, 8, 10, 11, 12, 13, 18]).

As an alternative to the local high order terms one can also use low-order but nonlocal terms that involve convolution integrals. For some analytical issues (e.g. local existence [15]) nonlocal models are more easy to treat. From the numerical point of view explicit schemes get along with much less restrictive time steps restrictions. More important is that the physical derivation usually leads to nonlocal models and the local models appear then by a Taylor approximation argument. In this sense the nonlocal approach is more fundamental [2]. It is our general goal to develop a theory for this kind of models and compare them with the local models. Results in this direction can be found in [15, 16, 17].

In the HYP2004-contribution we report on some recent analytical and numerical results for phase transitions in compressible media in the one-dimensional case. In Sect. 2 we consider the dynamics of phase transitions for liquid-vapour flow in a pipe. We introduce the nonlocal model and prove the existence of a traveling wave solution for phase boundaries (Theorem 2.1). In a certain sense this is an analogue of a result due to Slemrod in the local case [18].

The final Sect. 3 is devoted to a numerical experiment to compare the behaviour of the local and the global approach. The experiment is for the one-dimensional elasticity system but the results should directly transfer to the liquid-vapour case.

2. Traveling-wave Solutions for a Nonlocal Navier-Stokes-Korteweg Model

In Lagrangian coordinates the dissipation-free dynamics of an isothermal fluid is described by the system

$$\tau_t^0 - v_\xi^0 = 0, \qquad v_t^0 + p(\tau^0)_\xi = 0 \text{ in } \mathbb{R} \times (0,\infty). \tag{1}$$

Unknowns are the specific volume $\tau^0 = \tau^0(\xi,t) > 0$ and the velocity $v^0 = v^0(\xi,t) \in \mathbb{R}$. The given positive pressure function $p \in C^2((0,\infty))$ is supposed to have Van-der-Waals shape (see Fig. 1).

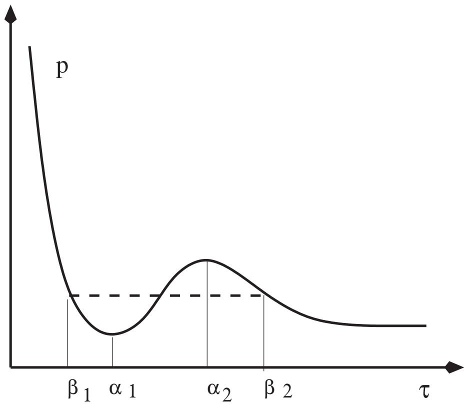


FIGURE 1. Graph of the pressure p. The horizontal dashed line connecting $(\beta_1, p(\beta_1))$ and $(\beta_2, p(\beta_2))$ is the Maxwell line.

The non-monotone shape of the pressure allows to define different phases. A state with specific volume $\tau \in (0,\alpha_1)$ is called a *liquid* state while a state with $\tau \in (\alpha_2,\infty)$ is called a *vapour* state. The *Maxwell states* β_1, β_2 are chosen such that $\int_{\beta_1}^{\beta_2} p(\tau)\,d\tau = p(\beta_1)(\beta_2-\beta_1)$ and $p(\beta_1) = p(\beta_2)$ holds.
If we take into account the small-scale effects of viscosity and capillarity the dynamics can be described for some regularization parameter $\varepsilon > 0$ by the system

$$\tau_t^\varepsilon - v_\xi^\varepsilon = 0, \qquad v_t^\varepsilon + p(\tau^\varepsilon)_\xi = \varepsilon\alpha v_{\xi\xi}^\varepsilon - D^\varepsilon[\tau_\xi^\varepsilon]. \tag{2}$$

Here $\alpha > 0$ is a positive number. For the capillarity term D^ε possible choices are

$$D_{local}^\varepsilon[\tau] = \varepsilon^2 \tau_{\xi\xi} \text{ or } D_{global}^\varepsilon[\tau] = \phi_\varepsilon * \tau - \tau. \tag{3}$$

In the latter case $*$ denotes convolution and the kernel ϕ_ε is given by $\phi_\varepsilon(\xi) = \phi(\xi/\varepsilon)/\varepsilon$. The function $\phi \in C^1(\mathbb{R}) \times W^{1,1}(\mathbb{R})$ is supposed to be nonnegative and even. For the derivation of both regularizations and its motivation we refer to [3, 7, 14]. The local version is called a Navier-Stokes-Korteweg system.

We consider now traveling waves for (1) and (2) with $D^\varepsilon \equiv D^\varepsilon_{global}$ (for the local choice see [5, 18] and [9] for a related model).
Let $(\tau_\pm, v_\pm) \in \mathcal{U} := (0,\infty)\times\mathbb{R}$, and $s \in \mathbb{R}$ be given. A function

$$\begin{pmatrix}\tau^0\\ v^0\end{pmatrix} = \begin{pmatrix}\tau^0(\xi,t)\\ v^0(\xi,t)\end{pmatrix} = \begin{cases}(\tau_-, v_-)^T\ :\xi - st < 0,\\ (\tau_+, v_+)^T\ :\xi - st > 0\end{cases} \tag{4}$$

is called a *phase boundary* if the Rankine-Hugoniot conditions

$$\begin{aligned} s(\tau_+ - \tau_-) &= -(v_+ - v_-),\\ s(v_+ - v_-) &= p(\tau_+) - p(\tau_-)\end{aligned} \tag{5}$$

hold and if τ_- and τ_+ lie in different phases. In particular we then get a weak solution of (1).

Let $(\tau_\pm, v_\pm) \in \mathcal{U}$ and $s \in \mathbb{R}$ be given such that (τ^0, v^0) from (4) is a phase boundary. A function $(\tau, v)^T : \mathbb{R} \to \mathcal{U}$ with $\tau \in C^1(\mathbb{R})$, $\ v \in C^2(\mathbb{R})$ is a *non-local viscosity-capillarity profile for* $(\tau^0, v^0)^T$ if it solves in $\mathbb{R}$ the differential-integro boundary value problem

$$\begin{gathered} -s\tau - v = -s\tau_- - v_-,\\ \alpha\dot{v} - (\phi * \tau - \tau) = p(\tau) - sv - (p(\tau_-) - sv_-),\\ \tau(\pm\infty) = \tau_\pm, \quad v(\pm\infty) = v_\pm.\end{gathered} \tag{6}$$

If problem (6) has a solution a traveling wave solution for (2) can be constructed: Taking into account $\phi_\varepsilon(\xi) = \phi(\xi/\varepsilon)/\varepsilon$ for each $\varepsilon > 0$ and $\xi \in \mathbb{R}$ the functions $\tau^\varepsilon \in C^1(\mathbb{R}\times(0,\infty))$ and $v^\varepsilon \in C^2(\mathbb{R}\times(0,\infty))$ defined by

$$\tau^\varepsilon(\xi,t) = \tau\left((\xi - st)/\varepsilon\right), \quad v^\varepsilon(\xi,t) = v\left((\xi - st)/\varepsilon\right) \quad ((\xi,t)\in\mathbb{R}\times(0,\infty))$$

are classical solutions of (2). Moreover we have for almost all $(\xi,t)\in\mathbb{R}\times(0,\infty)$

$$\tau^\varepsilon(\xi,t) \to \tau^0(\xi,t), \quad v^\varepsilon(\xi,t) \to v^0(\xi,t).$$

This observation and the fact that (6) does not depend on ε indicate that we have chosen the correct scaling with respect to ε. The main result is now

Theorem 2.1. *Assume that p satisfies $2p' < 1$ and that p'' vanishes only at a finite number of points.*
Then there exists a $\delta_0 > 0$ such that for all states

$$(\tau_-, v_-) \in \left\{(\tau, v) \in (\alpha_2, \infty)\times\mathbb{R}\,\middle|\, \left|p(\tau) - p(\beta_1)\right| < \delta_0\right\} \tag{7}$$

there is a number $\alpha > 0$, a speed $s \in \mathbb{R}\setminus\{0\}$ and a state $(\tau_+, v_+) \in (0,\alpha_1)\times\mathbb{R}$ with the properties

(a) *$\tau_\pm, v_\pm, s$ satisfy the Rankine-Hugoniot condition (5),*

(b) *the phase boundary* $(\tau^0, v^0)^T$ *from (4) has a non-local viscosity-capillarity profile* $(\tau, v)^T \in C^2(\mathbb{R}) \times C^2(\mathbb{R})$.

Proof. We can reduce the problem (6) to a first-order differential-integro problem for τ alone:

$$(8)\qquad \begin{aligned} s\alpha\dot{\tau} + \phi * \tau - \tau = h(\tau, \tau_-, s^2) &:= -(s^2(\tau - \tau_-) + p(\tau) - p(\tau_-)),\\ \tau(\pm\infty) &= \tau_\pm. \end{aligned}$$

The proof now relies essentially on a result from [4] for general boundary value problems of type (8) which is cited below (Theorem 2.2). For $\delta > 0$ we define

$$\mathcal{S}_\delta := \left\{\tau \in (0, \alpha_1) \cup (\alpha_2, \infty) \;\middle|\; \left|p(\tau) - p\big(\beta_2\big)\right| < \delta\right\}.$$

Furthermore we introduce for $\tau_1, \tau_2 > 0$ with $\tau_1 \neq \tau_2$ the quantity

$$q[\tau_1, \tau_2] = \frac{p(\tau_1) - p(\tau_2)}{\tau_1 - \tau_2}.$$

Now we choose $\delta_0 > 0$ so small such that we have for all $\tau_1 \in \mathcal{S}_{\delta_0} \cap (\alpha_2, \infty)$ and $\tau_2 \in \mathcal{S}_{\delta_0} \cap (0, \alpha_1)$ the properties

$$(9)\qquad \max\{p'(\tau_1), p'(\tau_2)\} < -q[\tau_1, \tau_2],$$

$$(10)\qquad 2q[\tau_1, \tau_2] < 1,$$

(11) the chord between $(\tau_2, p(\tau_2))$ and $(\tau_1, p(\tau_1))$ intersects p in (α_1, α_2).

Note that we always find a $\delta_0 > 0$ since we have $q[\beta_1, \beta_2] = 0$ (cf. Fig. 1).
Now according to the assumptions of the theorem we choose an arbitrary state $(\tau_-, v_-) \in (\mathcal{S}_{\delta_0} \cap (\alpha_2, \infty)) \times \mathbb{R}$. Furthermore we take a number $\tilde{\tau}_+$ with $\tilde{\tau}_+ \in \mathcal{S}_{\delta_0} \cap (0, \alpha_1)$ and

$$(12)\qquad p(\tilde{\tau}_+) > p(\tau_-).$$

Consider the auxiliary problem to find $\tilde{\alpha} \in \mathbb{R}$ and $\tau \in C^1(\mathbb{R})$ such that

$$(13)\qquad \phi * \tau - \tau + \tilde{\alpha}\dot{\tau} \;=\; h(\tau, \tau_-, q[\tau_-, \tilde{\tau}_+]),\ \tau(-\infty) = \tau_-,\ \tau(\infty) = \tilde{\tau}_+$$

holds. Note that $q[\tau_-, \tilde{\tau}_+]$ is positive due to (12).
We apply Theorem 2.2 with $F(\tau) = h(\tau, \tau_-, q[\tau_-, \tilde{\tau}_+])$ to solve (13).
Condition (i) is clear since $\tau_- > \tilde{\tau}_+$ by construction. The Rankine-Hugoniot relations (5) imply $F(\tau_-) = F(\tilde{\tau}_+) = 0$. We have for $\tau > 0$

$$\frac{\partial}{\partial \tau} h(\tau, \tau_-, q[\tau_-, \tilde{\tau}_+]) = -p'(\tau) - q[\tau_-, \tilde{\tau}_+].$$

The latter quantity is positive for $\tau = \tau_-, \tilde{\tau}_+$ due to (9). Thus (ii) holds.
Condition (iii) is a direct consequence of the definition of h (cf. (8)), (11) and the fact that $p' > 0$ in (α_1, α_2).
Using (10) we compute for $\tau \in (\tilde{\tau}_+, \tau_-)$

$$\frac{\partial}{\partial \tau} h(\tau, \tau_-, q[\tau_-, \tau_+]) + 1 = -p'(\tau) - q[\tau_-, \tilde{\tau}_+] + 1 > -p'(\tau) + 1/2.$$

The assumption $p' < 1/2$ on the pressure function assures condition (iv).
We can apply Theorem 2.2 which tells us that there is a unique (up to translation) function $\tau \in C^1(\mathbb{R})$ and a unique number $\tilde{\alpha} \in \mathbb{R}$ that solves (13).
In the next step we want to show that $\tilde{\tau}_+$ can be chosen such that $\tilde{\alpha} \neq 0$. To determine the sign of $\tilde{\alpha}$ it suffices to compute the sign of

$$H := \int_{\tau_-}^{\tilde{\tau}_+} h(\tau, \tau_-, q[\tau_-, \tilde{\tau}_+])\, d\tau.$$

We obtain for some function W with $W' = p$ after straightforward calculations

$$\begin{aligned} H &= \frac{\tilde{\tau}_+ - \tau_-}{2}\left(p(\tilde{\tau}_+) + p(\tau_-) - 2\frac{W(\tilde{\tau}_+) - W(\tau_-)}{\tilde{\tau}_+ - \tau_-}\right) \\ &=: \frac{\tilde{\tau}_+ - \tau_-}{2} G(\tilde{\tau}_+, \tau_-). \end{aligned}$$

To analyze the function $G(., \tau_-)$ we compute

$$\frac{d}{d\tau} G(\tau, \tau_-) = \frac{(\tau - \tau_-)}{3} p''(\xi_{\tau_-}(\tau)).$$

Here $\xi_{\tau_-}(\tau)$ denotes the third-order Taylor point in the Taylor expansion of $\tilde{W}$.
The preceding computation and the assumption that p'' vanishes only in finitely many points implies the following. Assume that $G(., \tau_-)$ vanishes in $\tilde{\tau}_+$ and thus we have $\tilde{\alpha} = 0$ in (13). Then there is a specific volume $\tau_+ \in \mathcal{S}_{\delta_0} \cap (0, \alpha_1)$ close to $\tilde{\tau}_+$ with $p(\tau_+) > p(\tau_-)$such that $G(., \tau_-)$ does not vanish. In this degenerate case we take the new specific volume τ_+ (and let it as it was if $G(., \tau_-)$ does not vanish in $\tilde{\tau}_+$) as a new end state in (13).
By repeating all arguments above with the new end state and applying Theorem 2.2 we obtain a solution $(\tilde{\alpha}, \tau) \in \mathbb{R} \setminus \{0\} \times C^2(\mathbb{R})$ of (13).
In the final step we construct a solution of the original problem (8) by

$$s := \operatorname{sgn}(\tilde{\alpha}) \sqrt{\frac{p(\tau_+) - p(\tau_-)}{\tau_- - \tau_+}}, \quad \alpha := \frac{|\tilde{\alpha}|}{|s|}.$$

To fulfill the Rankine-Hugoniot conditions for the velocity components we set $v_+ = v_- - s(\tau_+ - \tau_-)$. Note that v_- was given. We have proven (b). By construction it is clear that also (a) holds.

□

The following theorem can be deduced from the results in [4].

Theorem 2.2 ([4]). *Let $u_-, u_+ \in \mathbb{R}$ and $F \in C^1(\mathbb{R})$ be given. For the unknowns $u : \mathbb{R} \to \mathbb{R}$ and $\beta \in \mathbb{R}$ consider the problem*

$$\beta \dot{u} + \phi * u - u = F(u), \qquad u(\pm\infty) = u_\pm. \tag{14}$$

We suppose that the states $u_\pm \in \mathbb{R}$ and the function F satisfy

(i) $u_- > u_+$, (ii) $F(u_\pm) = 0$, $F'(u_\pm) > 0$,

(iii) $\exists!\, u_0 \in (u_+, u_-) : F(u_0) = 0$, (iv) $u \in [u_+, u_-] \Rightarrow F'(u) + 1 > 0$.

Then exactly one of the following statements holds true.

(a) *There is a monotonely decreasing function $u \in C^2(\mathbb{R})$ and a unique $\beta \in \mathbb{R} \setminus \{0\}$ such that (14) holds. In this case we have*

$$\beta = H(u_-, u_+) \left(\int_{-\infty}^{\infty} (\dot{u}(\xi))^2 \, d\xi \right)^{-1}, \quad H(u_-, u_+) := \int_{u_-}^{u_+} F(u) \, du.$$

(b) *There is a monotonely decreasing function $u \in C^1(\mathbb{R})$ such that (14) holds for $\beta = 0$. In this case we have $H(u_-, u_+) = 0$.*

In both cases the function u is unique up to translation.

3. A Numerical Experiment

Finally we present a numerical experiment for the 1D-elasticity model with the unknowns strain $w^\varepsilon : \mathbb{R} \times [0, \infty) \to \mathbb{R}$ and velocity $v^\varepsilon : \mathbb{R} \times [0, \infty) \to \mathbb{R}$ that is given by

$$w_t^\varepsilon - v_\xi^\varepsilon = 0, \quad v_t^\varepsilon - \sigma(w^\varepsilon)_\xi = \varepsilon v_{\xi\xi}^\varepsilon - D^\varepsilon[w^\varepsilon]_\xi \text{ in } (0,1) \times (0, \infty). \tag{15}$$

Here the stress strain relation σ is given by the non-monotone function

$$\sigma(w) = w^3 - w \quad (w \in \mathbb{R}).$$

and for D^ε we consider choices as in (3). With the definition for σ the model (15) allows to define a high- and a low-strain phase according to the w-intervals that correspond to the monotone-increasing branches of the graph of σ. The model (15) obviously has the same kind of structure as the model (2) and we expect also that a theorem like Theorem 2.1 holds for (15). On the other hand the subsequent numerical experiment should also provide information on the liquid-vapour case (2).

We choose the initial datum

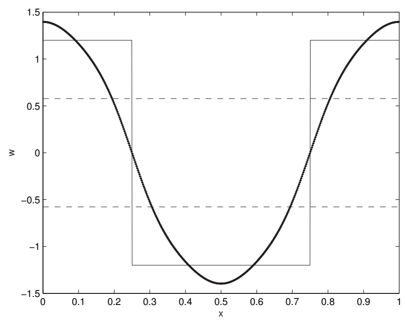
$$w_0(\xi) = \begin{cases} 1.2 : \xi \in (0, 1/4) \cup [3/4, 1), \\ -1.2 : \xi \in [1/4, 3/4), \end{cases} \qquad v_0 \equiv 0 \text{ in } (0,1).$$

As boundary conditions we take periodic conditions, i.e., $w(0,t) = w(1,t)$ and $v(.,t) = v(.,t)$ for $t \geq 0$.

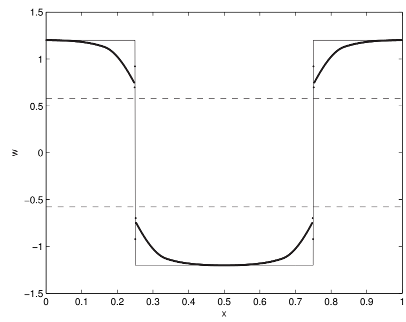
For the numerical discretization we have chosen explicit (centered) finite difference approximations. For $D^\varepsilon = D^\varepsilon_{global}$ from (3) the kernel function ϕ is chosen to be

$$\phi(\xi) = \begin{cases} \exp\left(\frac{1}{\xi^2 - 1}\right) \left(\int_{-1}^{1} \exp\left(\frac{1}{\tilde{\xi}^2 - 1}\right) d\tilde{\xi} \right)^{-1} : \xi \in (-1, 1), \\ 0 : \text{otherwise}. \end{cases}$$

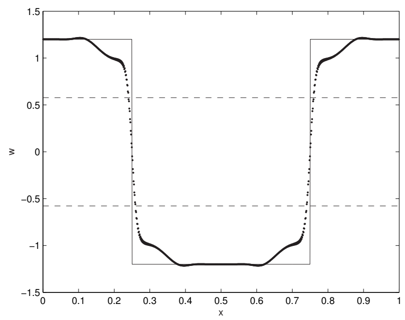
We present the results for two choices of ε with numerical discretization parameter $\Delta x = 10^{-3}$ in Fig. 2. One observes for $t = 0.06$ that a (smeared) Riemann pattern evolves. It is remarkable that the width of the transition layer for the phase boundary in the global model is much smaller as in the local counterpart. We note that it has been observed that the transition layer in local models is much wider than predicted by large-scale Monte Carlo simulations [1]. The phase boundaries that evolve are static phase boundaries, that is, they connect the Maxwell states ($w = \pm 1$ in this case). In particular from the upper right figure in Fig. 2 one may conclude that the static profile is not continuous. In this context note that the profile equation (6) for $v \equiv 0$ becomes a pure integral equation which might lead naturally to discontinuous solutions.



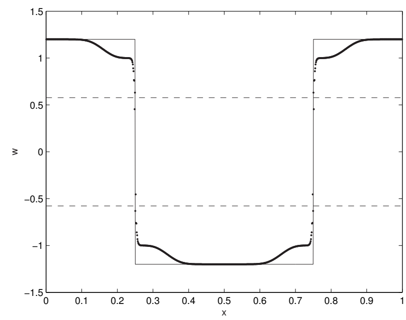
(a) $D^\varepsilon = D^\varepsilon_{local}$, $t = 0.06$.



(b) $D^\varepsilon = D^\varepsilon_{global}$, $t = 0.06$.



(c) $D^\varepsilon = D^\varepsilon_{local}$, $t = 0.06$.



(d) $D^\varepsilon = D^\varepsilon_{global}$, $t = 0.06$.

FIGURE 2. Graphs of the w-component for different choices of the capillarity operator and $\varepsilon = 0.1$ (upper row) and $\varepsilon = 0.01$ (lower row). The graphs contain also the initial datum. The dashed lines in the graphs indicate the position of the phases.

References

[1] F.F. Abraham, *On the thermodynamics, structure and phase stability of the nonuniform fluid state*, Phys. Rep., **53** (1979), 93–156.

[2] G. Alberti, G. Bellettini, M. Cassandro, and E. Presutti, *Surface tension in Ising systems with Kac potentials*, J. Stat.Phys., **82** (1996), no. 3/4, 743–793.

[3] D.M. Anderson, G.B. McFadden, and A.A. Wheeler, *Diffuse interface methods in fluid mechanics*, Ann. Rev. Fluid Mech. **30** (1998), 139–165.

[4] P.W. Bates, P.C. Fife, X. Ren, and X. Wang, *Traveling waves in a convolution model for phase transitions*, Arch. Ration. Mech. Anal. **138** (1997), 105–136.

[5] S. Benzoni-Gavage, *Nonuniqueness of phase transitions near the Maxwell line*, Proc. AMS **127** (1999), 1183–1190.

[6] D. Bresch, B. Desjardins, and C.-K. Lin, *On some compressible fluid models: Korteweg, lubrication, and shallow water systems*, Commun. Partial Differ. Equations **28** (2003), no. 3-4, 843–868.

[7] J.E. Dunn and J. Serrin, *On the thermomechanics of interstitial working*, Arch. Ration. Mech. Anal. **88** (1985), 95–133.

[8] H. Fan, *A vanishing viscosity approach on the dynamics of phase transitions in van der Waals fluids*, J. Differ. Equations **103** (1993), no. 1, 179–204.

[9] H. Garcke, *Travelling wave solutions as dynamic phase transitions in shape memory alloys*, J. Diff. Equations **121** (1995), 203–231.

[10] B.T. Hayes and P.G. LeFloch, *Non-classical shocks and kinetic relations: Scalar conservation laws*, Arch. Ration. Mech. Anal. **139** (1997), no. 1, 1–56.

[11] D. Jacobs, W. McKinney, and M. Shearer, *Travelling wave solutions of the modified Korteweg-deVries-Burgers equation*, J. Differ. Equations **116** (1995), no. 2, 448–467.

[12] D. Jamet, O. Lebaigue, N. Coutris, and J.M. Delhaye, *The second gradient method for the direct numerical simulation of liquid-vapor flows with phase change*, J. Comput. Phys. **169** (2001), no. 2, 624–651.

[13] P.G. LeFloch, *Hyperbolic systems of conservation laws. The theory of classical and nonclassical shock waves*, Lectures in Mathematics, ETH Zürich. Basel, 2002.

[14] C. Rohde, *On local and non-local Navier-Stokes-Korteweg systems for liquid-vapour phase transitions*, Z. Angew. Math. Mech. **85** (2005), no. 12, 839–857.

[15] ———, *Phase transitions and sharp-interface limits for the 1D-elasticity system with non-local energy.*, Interfaces Free Bound. **7** (2005).

[16] ———, *Scalar conservation laws with mixed local and non-local diffusion-dispersion terms*, SIAM J. Math. Anal., **37** (2005), no. 1, 103–129.

[17] C. Rohde and M.D. Thanh, *Global existence for phase transition problems via a variational scheme*, J. Hyperbolic Equations **1** (2004), no. 4, 747–768.

[18] M. Slemrod, *Admissibility criteria for propagating phase boundaries in a van der Waals fluid*, Arch. Ration. Mech. Anal. **81** (1983), 301–315.

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