

Nonnegative weak solutions for a degenerate system modelling the spreading of surfactant on thin films

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Pulmonary surfactant. Research motivation.

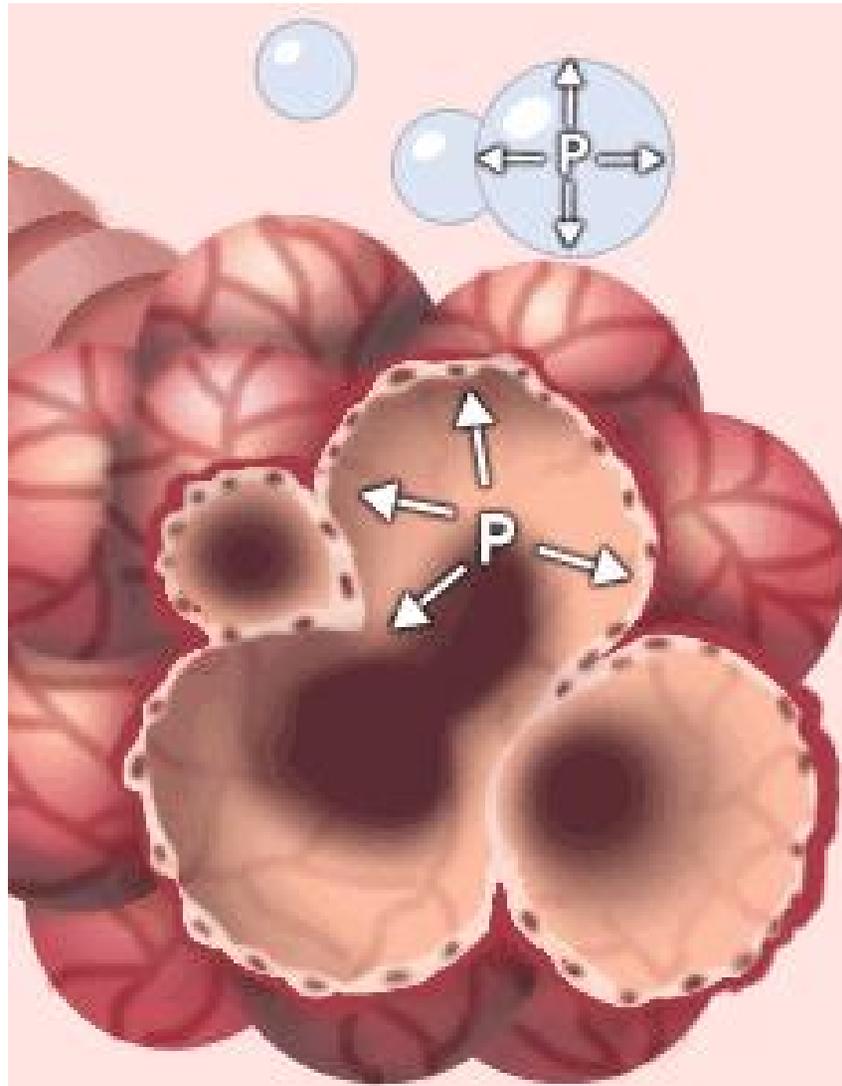
In late 1920s **von Neergaard**¹ identified the function of the pulmonary surfactant in increasing the compliance of the lungs by reducing surface tension. However the significance of his discovery was not understood by the scientific and medical community at that time. He also realized the importance of having low surface tension in lungs of newborn infants. Later, in the middle of the 1950s, **Pattle**² and **Clements**³ rediscovered the importance of surfactant and low surface tension in the lungs. At the end of that decade it was discovered that the lack of surfactant caused infant respiratory distress syndrome (IRDS).

¹Kurt von Neergaard. *Neue Auffassungen über einen Grundbegriff der Atemmechanik. Die Retraktionskraft der Lunge, abhängig von der Oberflächenspannung in den Alveolen.* Z. Gesant Exp Med (Germany) 66: 373-394 (1929)

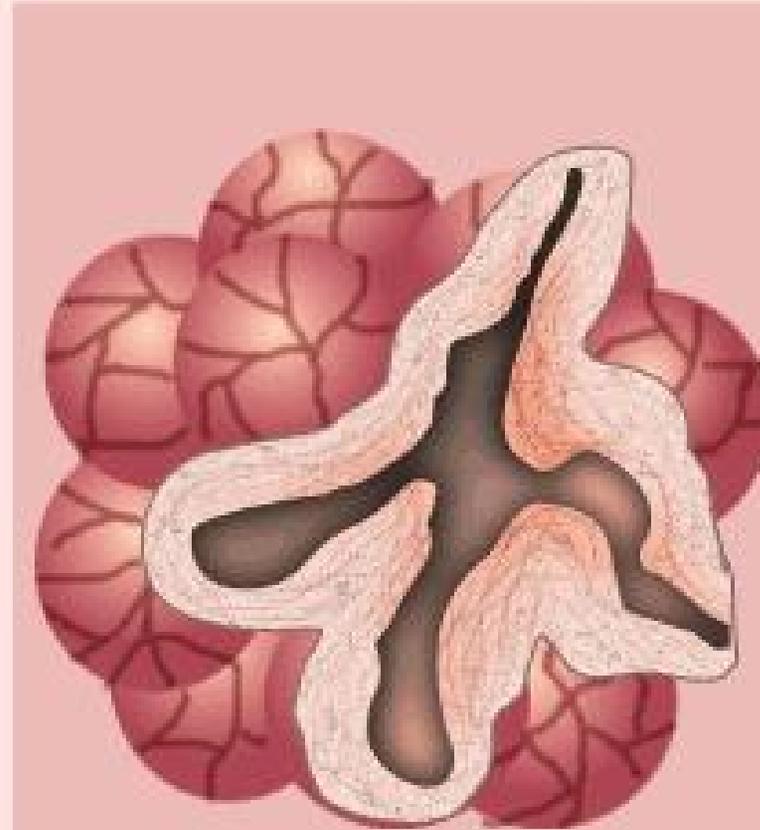
²R.E. Pattle. *Properties, function and origin of the alveolar lining layer.* Nature, 175: 1125-1126 (1955)

³J.A. Clements. *Surface tension of lung extracts.* Proc Soc Exp Biol Med, 95: 170-172 (1957)

Pulmonary surfactant. Research motivation.



Alveoli with surfactant



Alveoli without surfactant

Lubrication approximation model.

The lubrication approximation is widely used to study the dynamics of viscous thin films. The following model of a thin film of a viscous, incompressible, Newtonian fluid lying on a horizontal plane, with a monolayer of surfactant on its surface was derived by **Jensen and Grotberg**⁴ in 1992:

$$h_t + \frac{1}{3}(h^3(\mathcal{S}h_{xxx} - \mathcal{G}h_x + 3\mathcal{A}h^{-4}h_x))_x + \frac{1}{2}(h^2\sigma_x)_x = 0, \quad (1)$$

$$\Gamma_t + \frac{1}{2}(\Gamma h^2(\mathcal{S}h_{xxx} - \mathcal{G}h_x + 3\mathcal{A}h^{-4}h_x))_x + (\Gamma h\sigma_x)_x = (\mathcal{D}\Gamma_x)_x, \quad (2)$$

This model is the generalization of the original system derived by **Gaver and Grotberg**⁵ in 1990; the new model includes a nonlinear equation of state and van der Waals forces.

⁴O.E. Jensen, J.B. Grotberg. *Insoluble surfactant spreading on a thin viscous film: shock evolution and film rupture*. J. Fluid Mech., 240:259–288, 1992

⁵D.P. Gaver, J.B. Grotberg. *The dynamics of a localized surfactant on a thin film*. J. Fluid Mech., 213:127–148, 1990

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- h is the film height

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- Γ is the **surfactant concentration** in the monolayer normalized on the saturation surfactant concentration Γ_s

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- σ is the **surface tension**

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- \mathcal{S} is connected with **capillarity forces** (Marangoni effects)

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- \mathcal{G} is a parameter representing a **gravitational force** directed vertically downwards

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- \mathcal{A} is related to the Hamaker constant and connected with intermolecular **van der Waals forces**

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This model is the generalization of the original system derived by **Gaver and Grotberg**⁵ in 1990; the new model includes a nonlinear equation of state and van der Waals forces.

- \mathcal{D} is related to the **surface diffusion** and it is assumed constant

Lubrication approximation model: equations of state

Assume that the local surface tension and local surface diffusivity are functions of the local surface concentration. Accordingly we write

$$\sigma = \sigma(\Gamma), \quad \mathcal{D} = \mathcal{D}(\Gamma).$$

Borgas&Grotberg⁶ in 1988 proposed the following equations of state (**Sheludko** (1966) $\sigma \sim \Gamma^{-3}$)

$$\sigma(\Gamma) = (1 + \theta\Gamma)^{-3}, \quad \mathcal{D}(\Gamma) = (1 + \tau\Gamma)^{-k}, \quad (3)$$

where θ , τ and k are positive empirical parameters. In fact, the parameter θ depends on the material properties of the monolayer; and the alternative 'switch off' laws are

$$\sigma(\Gamma) \simeq (1 - \Gamma)_+^\ell, \quad \mathcal{D}(\Gamma) \simeq (1 - \Gamma)_+^q, \quad (4)$$

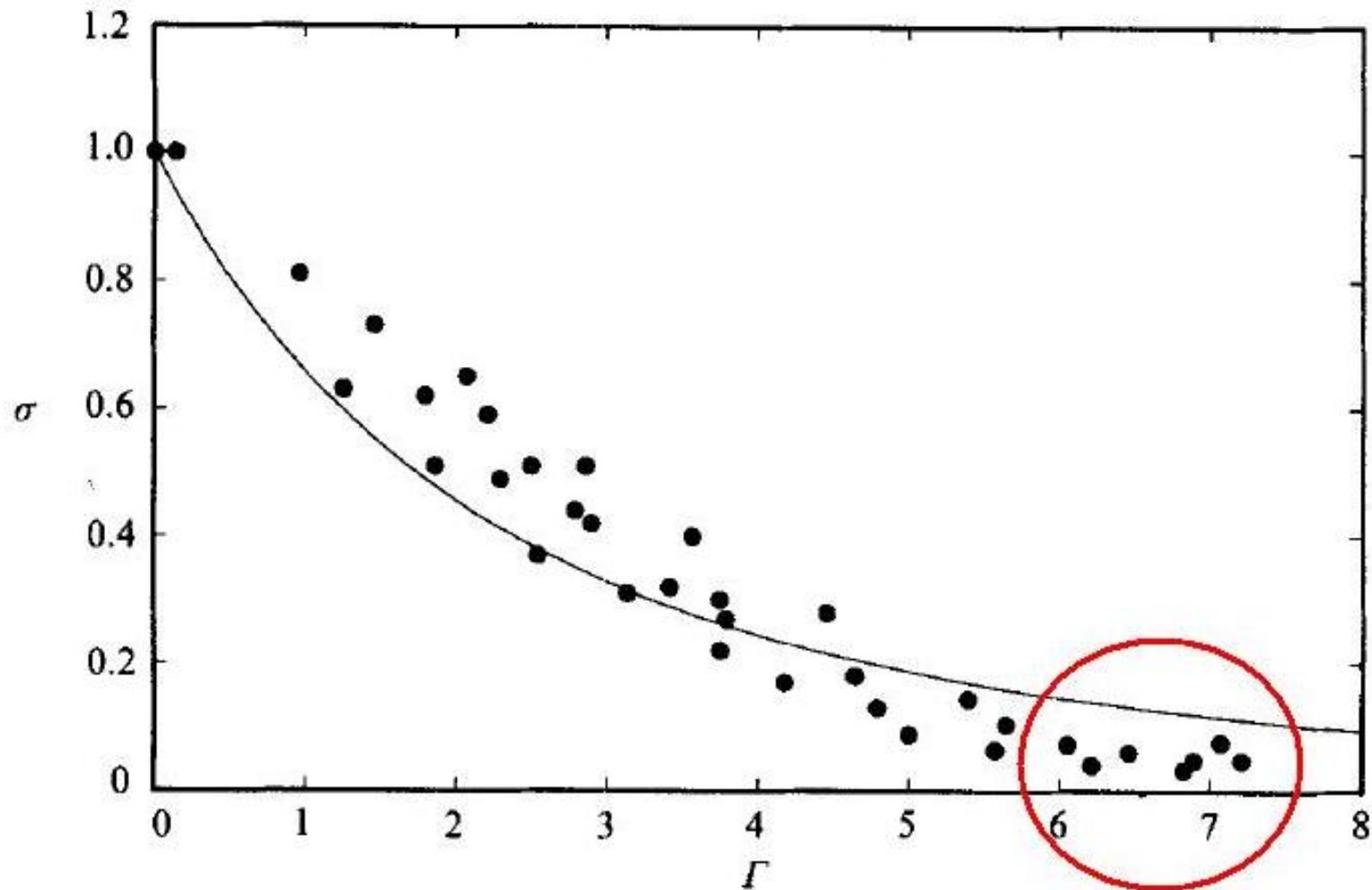
where $\ell > 0$ and $q > 0$. **Jensen&Grotberg**¹ in 1992 specified **(3)**:

$$\sigma(\Gamma) = \frac{\beta+1}{(1+\theta(\beta)\Gamma)^3} - \beta, \quad \theta(\beta) = \left(\frac{\beta+1}{\beta}\right)^{\frac{1}{3}} - 1, \quad \mathcal{D}(\Gamma) = \text{const} > 0, \quad (5)$$

where β relates to the "activity" of the surfactant.

⁶M.S. Borgas, J.B. Grotberg. *Monolayer flow on a thin film*. J. Fluid Mech., 193:151–170, 1988

Lubrication approximation model: equations of state



Foda&Cox's results⁷ for an oil layer on water (experimental data points (•)) and a curve from the model equation of state (3) with $\theta = 0.15$.

⁷M. Foda, R.G. Cox, J. Fluid Mech. 101, 33-57 (1980).

Lubrication approximation model: equations of state

Also in many physical applications the dependence $\sigma(\Gamma)$ is taken from **Frumkin**⁸ surface equation of state (by **Lucassen& Hansen**⁹ in 1967):

$$\sigma(\Gamma) = \sigma_0 + 2.303RT\Gamma_s \left(b \left(\frac{\Gamma}{\Gamma_s} \right)^2 + \ln \left(1 - \frac{\Gamma}{\Gamma_s} \right) \right), \quad (6)$$

where σ_0 is the surface tension of pure solvent and b is the Frumkin constant (for example, $b = 0$ for pentanoic acid). This equation, first formulated as an empirical relation, can be obtained from a general surface equation of state if one assumes ideal surface behaviour. This assumption has been found to be generally valid for **ionic surfactants** at the aqueous solution-air and aqueous solution-hydrocarbon interfaces, with the exception of C_{18} or longer compounds at the aqueous solution-air interface.

⁸Alexander Naumovich Frumkin, Electrocapillary curve of higher aliphatic acids and the state equation of the surface layer, *Zeitschrift für Physikalische Chemie*. (Leipzig) 116, 466–484 (1925)

⁹J. Lucassen, Robert S. Hansen. *Damping of Waves on Monolayer-Covered Surfaces II. Influence of Bulk-to-Surface Diffusional Interchange on Ripple Characteristics*. *Journal of Colloid and Interface Science*, 23: 319–328 (1967)

Mathematical overview: existence

Observe that the coupled system of interest (1)–(2) is degenerate parabolic in the sense that uniform parabolicity is lost if h vanishes. While modeling issues related to surfactant spreading on thin liquid films have attracted considerable interest since the early 1970th, the analytical research has started only recently.

- **Renardy**¹⁰ in 1996:

$$\mathcal{S} = \mathcal{G} = \mathcal{A} = 0, \text{ and } \sigma(\Gamma) > 0, \sigma'(\Gamma) < 0, \mathcal{D}(\Gamma) > 0$$

local existence of weak solutions;

- **Barrett, Garcke, Nürnberg**¹¹ in 2003:

$$\mathcal{G} = 0, \text{ and } \sigma(\Gamma) = 1 - \Gamma, \mathcal{D}(\Gamma) = D_0 > 0, h_0 \geq \nu > 0$$

local existence of weak solutions **under conjecture** $\Gamma \leq 1$.

¹⁰M. Renardy. *On an equation describing the spreading of surfactants on thin films*. *Nonlinear Anal.*, 26:1207–1219, 1996

¹¹J.W. Barrett, H. Garcke, R. Nürnberg. *Finite Element Approximation of Surfactant Spreading on a Thin Film*. *SIAM J. Numer. Anal.*, 41(4):1427–1464, 2003

Mathematical overview: existence

- **Garcke, Wieland**¹² in 2006:

$\mathcal{G} = \mathcal{A} = 0$, and $-C_1\Gamma(1 + |\Gamma|^r) \leq \sigma'(\Gamma) \leq -C_2\Gamma$ ($r \in (0, 2)$),
 $\mathcal{D}(\Gamma) = D_0 > 0$, $h_0 \geq 0$ **global existence** of weak solutions;

- **Escher, Hillairet, Ph. Laurencot, Walker**^{13,14} in 2011:

$\mathcal{S} = \mathcal{A} = 0$, and $\sigma \in C^3([0, \infty))$, $\sigma(0) > 0$, $0 < \sigma_0 \leq -\sigma' \leq \sigma_\infty$ or
 $\mathcal{G} = \mathcal{A} = 0$, and $\sigma \in C^1((0, \infty)) \cap C([0, \infty))$, $\sigma(1) = 0$,
 $0 < -\sigma'(z) < \sigma_0 \forall z \in (0, 1)$, $\frac{\sigma_1}{1+z^\theta} \leq -\sigma'(z) < \sigma_0 \forall z \geq 1$ ($\theta \in [0, 1)$);
 $\mathcal{D}(\Gamma) = D_0 > 0$, $h_0 \geq 0$, $\Gamma_0 \geq 0$ **global existence** of weak solutions.

¹²H. Garcke, S. Wieland. *Surfactant spreading on thin viscous films: nonnegative solutions of a coupled degenerate system*. SIAM J. Math. Anal., 37(6):20252048, 2006

¹³J. Escher, M. Hillairet, Ph. Laurencot, Ch. Walker. *Global weak solutions for a degenerate parabolic system modeling the spreading of insoluble surfactant*, to appear in Indiana Math. Journal, preprint 2011

¹⁴J. Escher, M. Hillairet, Ph. Laurencot, Ch. Walker. *Weak solutions to a thin film model with capillary effects and insoluble surfactant*. arXiv:1109.6762v1, 2011

Summary of unsolved problems to existence:

- the case of degenerate diffusion $\mathcal{D}(\Gamma) \geq 0$, $\mathcal{D}(1) = 0$ has not been studied;
- the case of presence of van der Waals forces ($\mathcal{A} \neq 0$) and nonnegative initial data $h_0 \geq 0$ has not been studied;
- the boundedness of $\Gamma \geq 0$, i. e. $\Gamma \leq 1$, has not been proven.

Generalization and assumptions

We will consider natural generalization of (1)–(2) in a dimensionless form, namely, the following problem:

$$h_t + (f_n(h)(h_{xxx} - h_x + F''_{n,m}(h)h_x))_x + (f_{n-1}(h)\sigma_x)_x = 0, \quad (7)$$

$$\Gamma_t + (\Gamma f_{n-1}(h)(h_{xxx} - h_x + F''_{n,m}(h)h_x))_x + (\Gamma f_{n-2}(h)\sigma_x)_x = (D(\Gamma)\Gamma_x)_x, \quad (8)$$

$$h_x(\pm a, t) = h_{xxx}(\pm a, t) = \Gamma_x(\pm a, t) = 0 \quad (9)$$

$$h(x, 0) = h_0(x), \quad \Gamma(x, 0) = \Gamma_0(x), \quad (10)$$

in $Q_T = (0, T) \times \Omega$, where $\Omega = (-a, a)$, $n \geq 2$.

$$f_n(z) = \frac{|z|^n}{n}, \quad f_0(z) = 1, \quad F''_{n,m}(z) = \frac{|z|^m}{f_n(z)} \geq 0.$$

For example,

$$F_{3,-1}(z) = \frac{1}{2}z^{-2} + z - \frac{3}{2} \text{ for } n = 3, \quad m = -1.$$

Generalization and assumptions

Assume that the initial data satisfy the conditions:

$$\begin{aligned} 0 \leq h_0 \in H^1(\Omega), F_{n,m}(h_0) \in L^1(\Omega), \\ \Gamma_0 \in L^2(\Omega), 0 \leq \Gamma_0 \leq 1, \Phi(\Gamma_0) \in L^1(\Omega). \end{aligned} \quad (11)$$

$\sigma(z) = \Phi(z) - z\Phi'(z)$, where $\Phi(z)$ is the free energy

(A1) the function $\Phi : [0, 1] \rightarrow \mathbb{R}_0^+$ is convex, $\Phi'(z) \leq 0$, and

$$\lim_{z \rightarrow 0^+} z \Phi''(z) = C_0 \quad (\Leftrightarrow \lim_{z \rightarrow 0^+} \sigma'(z) = -C_0), \quad 0 < C_0 < +\infty;$$

(A2) the function $D : [0, 1] \rightarrow \mathbb{R}_0^+$, $D'(z) \leq 0$, and

$$\lim_{z \rightarrow 1^-} D(z)\Phi''(z) = C_1 \quad (\Leftrightarrow \lim_{z \rightarrow 1^-} D(z)\sigma'(z) = -C_1), \quad (12)$$

where $0 < C_1 \leq \infty$ if $D(1) = 0$, and $C_1 = \infty$ if $D(1) > 0$.

Generalization and assumptions

For $C_1 = \infty$ the condition (12) is in the agreement with the Frumkin surface equation.

For $D(z) = D_0(1 - z)_+^q$, $q \in (0, 1)$ and $C_1 < \infty$ we have

$$\sigma \sim 1 - C_0 z \text{ as } z \rightarrow 0^+, \quad \sigma \sim \frac{C_1}{D_0(1-q)}(1 - z)_+^{1-q} \text{ as } z \rightarrow 1^-.$$

Conjecture: we believe that the boundedness of Γ , i. e. $\Gamma \leq 1$, is the result of the local concavity $\sigma(\Gamma)$ as $\Gamma \rightarrow 1^-$.

Main results: existence

Theorem 1 . *Let $m > n - 2$ for $n \in [2, 4)$, $m \geq \frac{n}{2}$ for $n \in [4, \infty)$, and (A1)–(A2) hold. Assume that the initial data (h_0, Γ_0) satisfy (11). Then for some time $T_{loc} > 0$ there exists a weak generalized solution (h, Γ) of the problem (7)–(10), in addition, $h \geq 0$ and $0 \leq \Gamma \leq 1$ almost everywhere in $Q_{T_{loc}}$. If $m \leq n + 2$ (and $M < M_c$ for $m = n + 2$) then T_{loc} can be taken arbitrarily large.*

Note that the Theorem 1 holds true in **the absence of van der Waals forces**. In this special case the solution exists globally in time for all $n \geq 2$.

If $D(z) = D_0(1-z)^q$, where $q \geq 0$ and $D_0 > 0$, then $\Gamma \in C_{loc}^{\alpha, \frac{\alpha}{2}}(Q_T)$ for some $\alpha = \alpha(q) \in (0, 1)$.

Main results: rupture

For the case $m \leq -1$ under an additional assumption

$$h_0 \in H^1(\Omega) \cap C^{4+\alpha}(\bar{\Omega}), \quad h_0 \geq \nu > 0,$$

using the method described in [Kai-Seng Chou, Ying-Chuen Kwong. Finite time rupture for thin films under van der Waals forces. *Nonlinearity*, 20(2): 299-317, 2007], one can show that there exists a time $\tau = \tau(\nu)$ such that

$$\lim_{t \rightarrow \tau} \|h(\cdot, t)\|_{H^1(\Omega)} = \infty \quad \mathbf{and} \quad \liminf_{t \rightarrow \tau} h(x, t) = 0$$

In the general situation, finite time rupture for the case

$$-1 < m < \min\left\{\frac{n}{2}, n - 2\right\}$$

is still an **open question**.

Now we have some progress in obtaining 'exact' sufficient conditions

- for **finite speed of support propagation** when

$$2 \leq n < 3 \text{ and } \frac{n}{2} < m \leq n + 2$$

- for **waiting time phenomenon** when

$$2 \leq n < 3 \text{ and } \frac{2n}{3} < m \leq n + 2$$

Summary of main results:

- we proved **existence** of weak generalized solutions with nonnegative initial data in the case of degenerate diffusion $\mathcal{D}(\Gamma) \geq 0$ under presence of van der Waals forces;
- we proved **boundedness** of Γ , i. e. $0 \leq \Gamma \leq 1$;
- we proved $\Gamma \in C_{loc}^{\alpha, \frac{\alpha}{2}}(\bar{Q}_T)$ when $D(z) = D_0(1 - z)^q$, where $\alpha \in (0, 1)$, $q \geq 0$ and $D_0 > 0$;

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Thank you !

THANK YOU FOR YOUR ATTENTION

THE END.