Numerical Modelling of the Dynamical Evolution of Contact Lines in Fluid Flows

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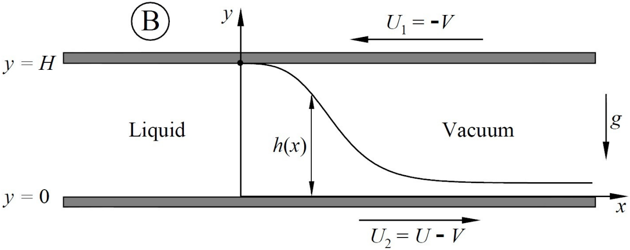
Introduction

- E.S. Benilov and M. Vynnycky, *Contact lines with a* 180° *contact angle*, J. Fluid Mech. (2013), vol. 718, pp. 481-506.



- Two-dimensional Couette flows with a free boundary, in the reference frame co-moving with the contact line.

The Reduced Model

The shape of the liquid-vacuum interface $h(x,t)$ is given by the solution of the linear advection-diffusion equation

$$\frac{\partial h}{\partial t} + \frac{\partial^4 h}{\partial x^4} = V(t)\frac{\partial h}{\partial x}, \quad x > 0, \quad t > 0, \tag{1}$$

subject to some suitable initial condition $h|_{x=0} = h_0(x)$ for $x \geq 0$, and the boundary conditions at $x = 0$:

$$h|_{x=0} = 1, \quad \left.\frac{\partial h}{\partial x}\right|_{x=0} = 0, \quad \left.\frac{\partial^3 h}{\partial x^3}\right|_{x=0} = -\frac{1}{2}, \quad t \geq 0. \tag{2}$$

The unknown velocity of the contact line $V(t)$ is to be determined dynamically from the system of overdetermined boundary conditions (2).

Properties of the Solution

- If the solution $h(x, t)$ is smooth at the boundary $x = 0$, then we have
$$\left.\frac{\partial^4 h}{\partial x^4}\right|_{x=0} = 0. \tag{3}$$
- h decays monotonically to some non-negative constant as $x \to \infty$, while all higher derivatives of h converge to zero;
- $x = 0$ is a non-degenerate maximum of h, that is, $h_{xx}|_{x=0} < 0$ for all $t \geq 0$.

Definition: If the solution $h(x, t)$ losses monotonicity during the dynamical evolution, then we say the reduced model *blows up*.

Claims

Claims by Benilov:

- for any suitable initial condition, there always exists a finite positive time t_0 such that $V(t) \to -\infty$ as $t \to t_0$;
- behavior of $V(t)$ near the blow-up time:

$$V(t) \sim C_1 \log(t_0 - t) + C_2, \quad \text{as} \quad t \to t_0, \tag{4}$$

  where C_1, C_2 are positive constants.

The first claim is confirmed by our numerical results, however, the power function

$$|V(t)| \sim \frac{c}{(t_0 - t)^p}, \quad \text{as} \quad t \to t_0, \tag{5}$$

with $c > 0$ and $p \approx 0.4$ is found to fit our numerical data better.

Reformulation of the Model

Let $u := \partial h/\partial x$, and differentiate (1) with respect to x:

$$\frac{\partial u}{\partial t} + \frac{\partial^4 u}{\partial x^4} = V(t)\frac{\partial u}{\partial x}, \quad x > 0, \quad t > 0. \tag{6}$$

Rewrite boundary conditions in (2) and (3):

$$u|_{x=0} = 0, \quad u_{xx}|_{x=0} = -\frac{1}{2}, \quad u_{xxx}|_{x=0} = 0, \quad t \geq 0. \tag{7}$$

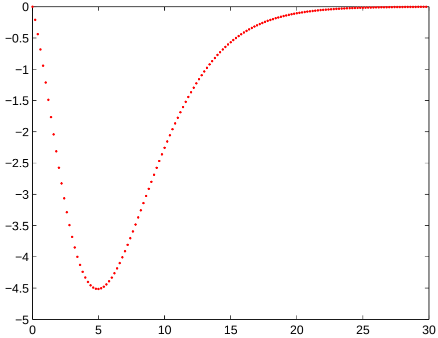
Then $V(t)$ can be determined by the pointwise equation

$$u_{xxxx}(0,t) = V(t)u_x(0,t), \quad t \geq 0, \tag{8}$$

provided that the solution is smooth at the boundary $x = 0$.

Initial Condition

The initial condition can be any function that satisfies all the boundary and decay conditions. All initial functions $u|_{t=0}(x)$ looks similar:



Numerical Solution: Finite Difference Method

The solution over x-axis will be approximated by the second order central difference method: at each $x = x_n$, we have

$$\frac{du_n}{dt} := V(t)\frac{u_{n+1} - u_{n-1}}{2(\Delta x)} - \frac{u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2}}{(\Delta x)^4} + O(\Delta x^2). \quad (9)$$

In matrix form, the above system of linear ODEs

$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{A}\boldsymbol{u}(t) + \boldsymbol{b} \quad (10)$$

can be evaluated by implicit Heun's method at $t = t_k$:

$$\boldsymbol{u}_{k+1} = \boldsymbol{u}_k + \frac{\Delta t}{2}[(\boldsymbol{A}_k\boldsymbol{u}_k + \boldsymbol{b}) + (\boldsymbol{A}_{k+1}\boldsymbol{u}_{k+1} + \boldsymbol{b})]. \quad (11)$$

Example: Negative Initial Velocity

Initial condition: $u_0(x) = -e^{-x/2}x(1 + \frac{3}{4}x + \frac{1}{4}x^2)$.

Initial velocity: $V(0) = -1.25$.

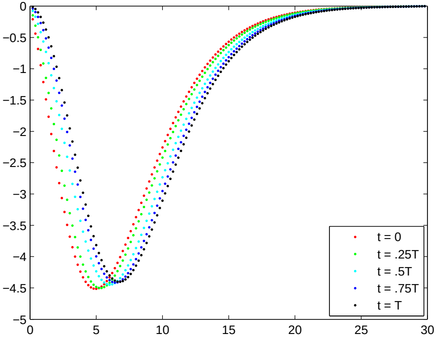


Figure: The dynamical evolution of u verses x at different time t.

Example: Negative Initial Velocity

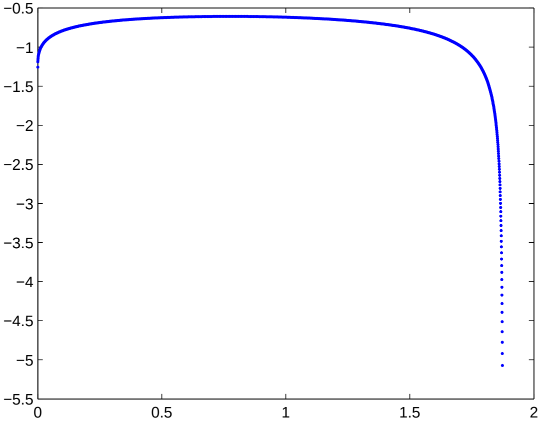


Figure: Change of velocity of the contact line V with respect to time t.

Example: Negative Initial Velocity

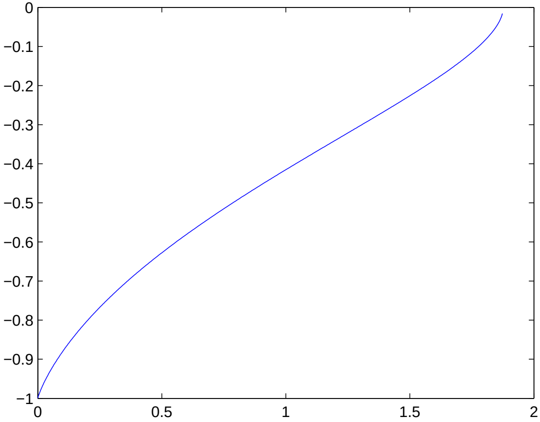


Figure: Change of $u_x|_{x=0}$ with respect to time t.

Example: Positive Initial Velocity

Initial condition: $u_0(x) = -\frac{1}{4}e^{-x/2}x(4 + 3x + x^2 + 0.6x^3)$.

Initial velocity: $V(0) = 2.35$.

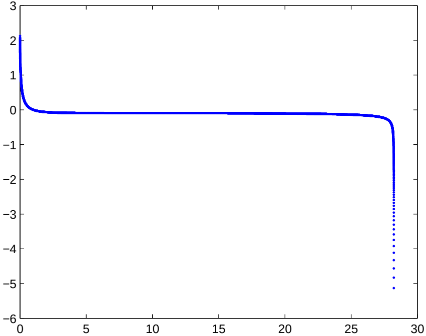


Figure: Change of velocity of the contact line V with respect to time t.

Example: Positive Initial Velocity

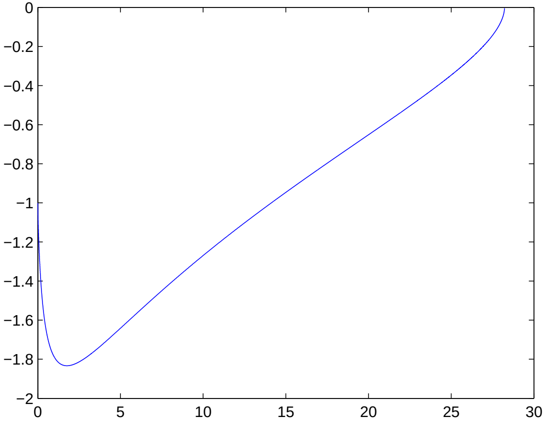
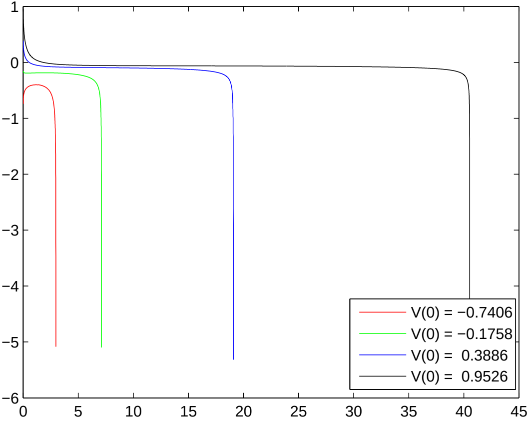


Figure: $u_x(0, t)$.

More Initial Velocities

Comparison of velocities $V(t)$ between different initial conditions:



Blow-up Rate

In order to analyse the behavior of V near the blow-up time t_0, we shall fit the numerical data with the logarithmic function claimed by Benilov:

$$V(t) \sim C_1 \log(t_0 - t) + C_2, \quad \text{as} \quad t \to t_0,$$

and compare the results with the power function:

$$V(t) \sim \frac{c}{(t_0 - t)^p}, \quad \text{as} \quad t \to t_0,$$

where p is the blow-up rate.

Data Fitting

Consider the initial condition:

$$u_0(x) = -e^{-x/2}x(1 + \frac{3}{4}x + \frac{1}{4}x^2), \quad V(0) = -1.25.$$

Tolerance level: 1e-006, number of iterations: 1448, terminal time = 1.8732

	Starting time	Blowup time t0	Blowup rate p or C1	Error
powerlaw:				
	1.8172	1.8753	0.3927	0.000033
	1.8360	1.8757	0.4009	0.000006
	1.8547	1.8760	0.4118	0.000000
loglaw:				
	1.8172	1.8688	0.5500	25.226547
	1.8360	1.8705	0.6343	33.937325
	1.8547	1.8724	0.7854	58.894321

Data Fitting

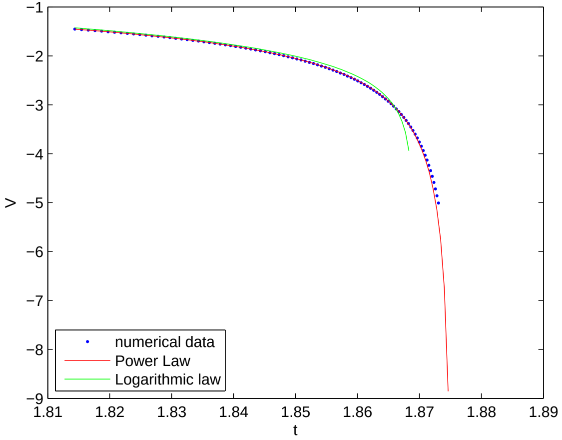


Figure: Comparison between data fitting with the logarithmic law and the power law.

More Examples

Initial condition:

$$u_0(x) = -\frac{1}{4}e^{-0.4x}x(4 + 2.6x + 0.72x^2), \quad V(0) = -0.736.$$

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Tolerance level: 1e-006, number of iterations: 1364, terminal time = 2.9654
  Starting time     Blowup time t0     Blowup rate p or C1       Error
powerlaw:
         2.8765           2.9662               0.4001             0.000164
         2.9063           2.9666               0.4085             0.000030
         2.9358           2.9671               0.4201             0.000002
loglaw:
         2.8765           2.9574               0.3959            12.052519
         2.9063           2.9599               0.4640            18.350765
         2.9358           2.9626               0.5945            32.196180
```

More Examples

Initial condition:

$$u_0(x) = -\frac{1}{4}e^{-0.4x}x(4 + 2.6x + 0.72x^2 + 0.2x^3), \quad V(0) = 0.464.$$

Tolerance level: 1e-006, number of iterations: 4233, terminal time = 19.0885

	Starting time	Blowup time t0	Blowup rate p or C1	Error
powerlaw:				
	18.5172	19.0815	0.3982	0.000715
	18.7069	19.0842	0.4073	0.000142
	18.8986	19.0867	0.4208	0.000009
loglaw:				
	18.5172	19.0382	0.1044	0.412399
	18.7069	19.0521	0.1241	0.660228
	18.8986	19.0670	0.1659	1.472944

Summary of Results

- For any suitable initial condition, there always exists a finite positive time t_0 such that $V(t) \to -\infty$ as $t \to t_0$.
- With a large positive initial velocity, the solution tends to have a longer equilibrium state before it eventually blows up, whereas a negative initial velocity yields a much faster blow-up.
- The behavior of $V(t)$ near the blow-up time satisfies the power law (5), with a blow-up rate $p \approx 0.4$.
- Because of the limited accuracy of finite difference method, the true value of p remains unknown at this time. More precise and computationally efficient numerical method, for instance, the collocation method involving discrete Fourier transform, is needed in further studies of this problem.