The Impact of Liquid Drops on Solid Surfaces

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Abstract

We build a model for the deformation of a liquid drop as it approaches a solid surface in the presence of an ambient gas which is trapped below the drop. This model can be augmented to include Knudsen slip, which becomes relevant when the layer is very thin and may provide a mechanism for the viscous air layer to be punctured in a finite time.

1 Introduction

In 3D printing, structures are built up from microdrops. It is often desirable in these applications to ensure that the drops do not splash when they impact the solid, and this topic has been an area of intense research. Currently, it is unclear how the bubble formed underneath a falling drop affects the splash phenomena.

It is known from experiments (e.g. [9]) that the behaviour of liquid drops hitting a hard surface, for example whether they splash, depends on the pressure of the ambient gas. It is observed that a drop deforms because the pressure is greater under its centre, and first touchdown is along a circle around the centre, possibly trapping an air bubble. There is no accepted theoretical model for this behaviour for fast falling drops. More recently, the skating of the drop across the gas film (as the bubble expands) has been observed in detail from below using a technique based on Total Internal Reflection Microscopy [5].

The surface tension, inertia and viscous forces of the drop as a whole are relevant to how it deforms. The drop diameter is a much larger scale (e.g. 1 mm or 1 cm) than the width of the thin gas film beneath the drop by the time the pressure in the gas film is enough to deform the drop (e.g. 1 µm or less). This makes it hard to perform a complete computational fluid mechanics simulation of the situation, because the high resolution would be needed everywhere.

Asymptotic approaches have been introduced to make progress with simulation while avoiding these difficulties. In [8], a two dimensional formulation is introduced, with incompressible flow, inviscid in the drop and highly viscous in the gas. A fast numerical method is available. The paper shows that a corner forms which pierces the thin film of gas, trapping a bubble. However this mechanism is known to be unphysical, as surface tension will act to prevent such a corner from forming [7, 6],

An alternative method with similar assumptions but with full 3D geometry uses a boundary integral method to solve the Laplace equation in the liquid [4, 1]. Because this method does not take height of the drop to be a single-valued function of horizontal position, it does not break down as the free surface ‘overturns’ when a corona begins to be ejected from the bottom surface of the drop.

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As noted in [1] and [2], the thin film of gas is typically at the scales where rarefied gas effects may be relevant and in [2] it is shown, using scaling arguments, how this *could* allow touchdown. This is what will be considered in more detail in this work.

In this project, we added first order effects from rarefied gas dynamics to the two dimensional method developed in [8]. In §2 the original setup is presented; it is expanded to include surface tension in §3 and slip in §4, with the whole setup presented in §5. Sample results are shown in §6. §7 concludes.

2 Governing equations

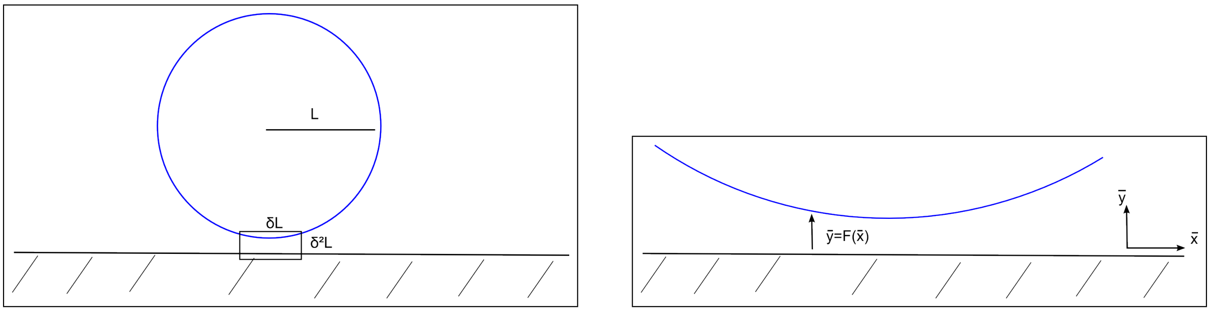

Figure 1: A schematic diagram of the whole drop (left) approaching the surface, and (right) the region of interest

In this section, we summarise the formulation in [8], which is to be adapted later. The setting is 2-dimensional. The liquid and the gas are taken to be incompressible and Newtonian. The liquid has density ρ_ℓ and viscosity μ_ℓ and the gas has density ρ_g and viscosity μ_g.

Consider a circular drop of radius L falling towards a surface at a constant velocity V. To consider the dynamics in the impact zone, take a small thin horizontal region of characteristic width δL and height from the wall about $\delta^2 L$ where δ is small. We scale, in the horizontal direction $x = \bar{x}\delta L$ and in the vertical direction $y = \bar{y}\delta^2 L$. Time is scaled as $t = \bar{t}\frac{\delta^2 L}{V}$, and pressure as $p = \bar{p}\frac{\rho_\ell V^2}{\delta}$. We make the assumptions that $\mu_\ell \gg \mu_g$ and $\rho_\ell \gg \rho_g$ so much that $\frac{\rho_g}{\rho_\ell} \ll \delta \ll \frac{\rho_\ell}{\rho_g}$, and take δ to be defined by assuming that the constant $\Gamma = \frac{\mu_\ell}{V L \rho_\ell \delta^3}$ is 1. The interface will be denoted by $\bar{y} = F(\bar{x})$.

When scaled in this way, the pressure in the gas is a function of $\bar{x}$ and not $\bar{y}$. Under these assumptions, the lubrication-type equations that govern the evolution of F and $\bar{p}$ are:

$$12\Gamma F_{\bar{t}} = (F^3\bar{p}_{\bar{x}})_{\bar{x}} = 3F^2 F_{\bar{x}}\bar{p}_{\bar{x}} + F^3\bar{p}_{\bar{x}\bar{x}} \tag{1}$$

$$F_{\bar{t}\bar{t}} = \frac{1}{\pi}\,\mathrm{PV}\int_{-\infty}^{\infty} \frac{\bar{p}_{\bar{x}'}}{\bar{x} - \bar{x}'} d\bar{x}'. \tag{2}$$

The first equation is the Reynolds lubrication equation ([3]), which relates to the dynamics in the gas layer, and it is generalised in §4 to account for rarefied gas effects. The second equation is a consequence of the fact that the pressure in the drop is harmonic.

3 Surface tension

The surface is at $\bar{y} = F$ or $y = \delta^2 LF$, so that its curvature is

$$\frac{\frac{\partial^2(\delta^2 LF)}{\partial x^2}}{\left(1 + \left(\frac{\partial(\delta^2 LF)}{\partial x}\right)^2\right)^{\frac{3}{2}}} = \frac{\frac{1}{L}\frac{\partial^2 F}{\partial \bar{x}^2}}{\left(1 + \delta^2\left(\frac{\partial F}{\partial \bar{x}}\right)^2\right)^{\frac{3}{2}}} \tag{3}$$

which can be taken to be $\frac{1}{L}\frac{\partial^2 F}{\partial \bar{x}^2}$ as the δ^2 term is small.

To model surface tension with magnitude σ, we use the Young-Laplace equation, which says that the pressure in the liquid will exceed that in the gas by a factor of σ times the curvature. Using p and $\bar{p}$ specifically for the pressure in the liquid, the pressure in the gas will be $p - \sigma \frac{1}{L}\frac{\partial^2 F}{\partial \bar{x}^2}$. In scaled units, the pressure in the gas is $\bar{p} - \bar{\sigma} F_{\bar{x}\bar{x}}$ where $\bar{\sigma} = \frac{\delta \sigma}{\rho_\ell V^2 L}$ is a dimensionless surface tension.

4 Derivation of the gas equation

In this section we derive a version of the Reynolds lubrication equation ([3]) for the current setup including a Maxwell boundary condition.

Let the horizontal component of velocity be $u = \bar{u}\frac{\delta L}{\delta^2 L/V} = \bar{u}\frac{V}{\delta}$ and the vertical $w = \bar{w}V$.

4.1 PDEs in the body

The continuity equation for an incompressible fluid is $\frac{\partial u}{\partial x} + \frac{\partial w}{\partial y} = 0$ which scales to $\frac{\partial \bar{u}}{\partial \bar{x}} + \frac{\partial \bar{w}}{\partial \bar{y}} = 0$.

The Navier-Stokes equations in our scaled variables are

$$\frac{\rho_g V^2}{\delta^3 L}\left(\frac{\partial \bar{u}}{\partial \bar{t}} + \bar{u}\frac{\partial \bar{u}}{\partial \bar{x}} + \bar{w}\frac{\partial \bar{u}}{\partial \bar{y}}\right) = -\frac{\rho_\ell V^2}{\delta^2 L}\frac{\partial \bar{p}}{\partial \bar{x}} + \mu_g\left(\frac{V}{\delta^3 L^2}\frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \frac{V}{\delta^5 L^2}\frac{\partial^2 \bar{u}}{\partial \bar{y}^2}\right) \tag{4}$$

$$\frac{\rho_g V^2}{\delta^2 L}\left(\frac{\partial \bar{w}}{\partial \bar{t}} + \bar{u}\frac{\partial \bar{w}}{\partial \bar{x}} + \bar{w}\frac{\partial \bar{w}}{\partial \bar{y}}\right) = -\frac{\rho_\ell V^2}{\delta^3 L}\frac{\partial \bar{p}}{\partial \bar{y}} + \mu_g\left(\frac{V}{\delta^2 L^2}\frac{\partial^2 \bar{w}}{\partial \bar{x}^2} + \frac{V}{\delta^4 L^2}\frac{\partial^2 \bar{w}}{\partial \bar{y}^2}\right) \tag{5}$$

The assumption that $\delta \ll \frac{\rho_\ell}{\rho_g}$ implies that the left hand side of each equation is less than the pressure term, and small δ makes the first term in each of the parentheses of the right much less than the second. The final term on the right hand side of the second equation is negligible as well because δ/Γ is assumed to be small.

This leaves the well-known lubrication equations for the gas layer dynamics:

$$\frac{\partial \bar{p}}{\partial \bar{x}} = \Gamma \frac{\partial^2 \bar{u}}{\partial \bar{y}^2}$$

$$\frac{\partial \bar{p}}{\partial \bar{y}} = 0$$

These, together with the continuity equation, are three PDEs for the three unknowns $\bar{p}$, $\bar{u}$ and $\bar{w}$.

4.2 Boundary conditions

The velocity of the gas perpendicular to the wall is zero at the wall and the velocity of the gas perpendicular to the interface at the interface is equal to the velocity of the interface.

The most common way to incorporate gas slip at these surfaces is using the Maxwell boundary condition which says that, at a surface, $A\ell\frac{\partial u}{\partial y} = u$, where A is a constant on the order of one which depends on the nature of the surface, ℓ is the mean free path of the gas, u is the velocity along the surface, and y is the distance along the surface. Rescaling, for our surface, the condition is $A\,\mathrm{Kn}\frac{\partial \bar{u}}{\partial \bar{y}} = \bar{u}$ where the Knudsen number $\mathrm{Kn} = \frac{\ell}{\delta^2 L}$. For simplicity, we assume that the same constant A can be used at the solid and liquid surfaces.

The boundary condition at the gas/solid interface is

$$A\,\mathrm{Kn}\frac{\partial \bar{u}}{\partial \bar{y}} = \bar{u}. \tag{6}$$

The boundary condition at the gas/liquid interface, which, to leading order, is considered flat, is

$$-A\,\mathrm{Kn}\frac{\partial \bar{u}}{\partial \bar{y}} = \bar{u}. \tag{7}$$

4.3 A new lubrication equation

The equation $\frac{\partial \bar{p}}{\partial \bar{x}} = \Gamma \frac{\partial^2 \bar{u}}{\partial \bar{y}^2}$ can be solved for $\bar{u}$ with the boundary conditions. The solution will have the form, for some a_1 and a_2,

$$\bar{u} = \frac{1}{\Gamma}\frac{\partial \bar{p}}{\partial \bar{x}}\left(\frac{1}{2}\bar{y}^2 + a_1\bar{y} + a_2\right)$$
$$\frac{\partial \bar{u}}{\partial \bar{y}} = \frac{1}{\Gamma}\frac{\partial \bar{p}}{\partial \bar{x}}\left(\bar{y} + a_1\right)$$

The boundary conditions determine a_1 and a_2 as satisfying $A\,\mathrm{Kn}\,a_1 = a_2$ and $-A\,\mathrm{Kn}\,(F + a_1) = \frac{1}{2}F^2 + a_1 F + a_2$. Thus $a_1 = -\frac{F}{2}$ and $a_2 = -A\,\mathrm{Kn}\frac{F}{2}$. Denote the value of $\bar{u}$ at the boundary by $u_F = \frac{1}{\Gamma}\frac{\partial \bar{p}}{\partial \bar{x}}\left(-A\,\mathrm{Kn}\frac{F}{2}\right)$. Hence

$$\bar{u} = \frac{1}{\Gamma}\frac{\partial \bar{p}}{\partial \bar{x}}\left(\frac{1}{2}\bar{y}^2 - \frac{F}{2}\bar{y} - A\,\mathrm{Kn}\frac{F}{2}\right)$$
$$\int_0^F \bar{u}\,d\bar{y} = \frac{1}{\Gamma}\frac{\partial \bar{p}}{\partial \bar{x}}\left(-\frac{1}{12}F^3 - A\,\mathrm{Kn}\frac{F^2}{2}\right)$$

By Leibnitz' rule and then the continuity equation and then the boundary conditions for $\bar{w}$

$$\frac{\partial}{\partial \bar{x}}\int_0^F \bar{u}\,d\bar{y} = \bar{u}_F\frac{\partial F}{\partial \bar{x}} + \int_0^F \frac{\partial \bar{u}}{\partial \bar{x}}\,d\bar{y} = \bar{u}_F\frac{\partial F}{\partial \bar{x}} - \int_0^F \frac{\partial \bar{w}}{\partial \bar{y}}\,d\bar{y} = \bar{u}_F\frac{\partial F}{\partial \bar{x}} - \frac{\partial F}{\partial \bar{t}}$$

Hence

$$\frac{\partial F}{\partial \bar{t}} = \frac{1}{\Gamma}\frac{\partial F}{\partial \bar{x}}\frac{\partial \bar{p}}{\partial \bar{x}}\left(-A\,\mathrm{Kn}\frac{F}{2}\right) + \frac{1}{\Gamma}\frac{\partial F}{\partial \bar{x}}\frac{\partial \bar{p}}{\partial \bar{x}}\left(\frac{1}{4}F^2 + A\,\mathrm{Kn}\,F\right) + \frac{1}{\Gamma}\frac{\partial^2 \bar{p}}{\partial \bar{x}^2}\left(\frac{1}{12}F^3 + \frac{A\,\mathrm{Kn}\,F^2}{2}\right)$$

Or, letting $A' = 6A\,\mathrm{Kn}$,

$$12\Gamma\frac{\partial F}{\partial \bar{t}} = \frac{\partial F}{\partial \bar{x}}\frac{\partial \bar{p}}{\partial \bar{x}}\left(3F^2 + A'F\right) + \frac{\partial^2 \bar{p}}{\partial \bar{x}^2}\left(F^3 + A'F^2\right) \tag{8}$$

5 The full system

Incorporating both surface tension and slip, the governing equations become

$$12\Gamma F_{\bar{t}} = (3F^2 + A'F)F_{\bar{x}}(\bar{p}_{\bar{x}} - \bar{\sigma}F_{\bar{x}\bar{x}\bar{x}}) + (F^3 + A'F^2)(\bar{p}_{\bar{x}\bar{x}} - \bar{\sigma}F_{\bar{x}\bar{x}\bar{x}\bar{x}}) \tag{9}$$
$$F_{\bar{t}\bar{t}} = \frac{1}{\pi}\,\mathrm{PV}\int_{-\infty}^{\infty}\frac{\bar{p}_{\bar{x}'}}{\bar{x} - \bar{x}'}d\bar{x}' \tag{10}$$

The method suggested in [8] for solving the system forward in time sets up an equal space and time grid. At each time step, it goes through the space steps enforcing these two equations and fourth-order-accurate relations on the space derivatives (F, $F_{\bar{t}}$, $F_{\bar{x}}$, $\bar{p}$, $\bar{p}_{\bar{x}}$, and $\bar{p}_{\bar{x}\bar{x}}$ are all maintained separately). We developed C++ code to run the method, augmented to this new system with $F_{\bar{x}\bar{x}\bar{x}}$ and $F_{\bar{x}\bar{x}\bar{x}\bar{x}}$ added to the calculation.

Without loss of generality, because the liquid and gas are incompressible, the far field pressure and the initial pressure are 0. The initial conditions are that the drop is far from the surface, so that the relevant part of the interface is a parabola. F is initially taken to be $10 + m\bar{x}^2$ with $F_{\bar{t}} = v = -1$ and the grid extends to the range $[-8, 8]$. This corresponds to a radius of curvature $\frac{1}{2m}$ in the vertical scaled units, which is $\frac{1}{\delta^2}$. The boundary conditions used are 'soft'.

5.1 Parameter regime considered

Consider a 1 mm-radius drop of water falling in air at room temperature and pressure at a speed of $10\,\mathrm{m\,s^{-1}}$. If $\Gamma = 1$, then (giving all quantities in SI units)

$$\delta^3 = \frac{1.8 \times 10^{-5}}{10 \times 10^{-3} \times 10^3} = 1.8 \times 10^{-6}$$

So $\delta \approx 0.01$, which is small. The inequalities described in §2 are easily satisfied. Our typical vertical length scale is $\delta^2 L$ which is about 100 nm. The mean free path of a particle of air is approximately $\ell = 7 \times 10^{-8}$m. If $A = 1$, then

$$A' = \frac{6A\ell}{\delta^2 L} = 6 \times \frac{7 \times 10^{-8}}{0.01^2 \times 10^{-3}} \approx 4$$

The surface tension of water-air is about $0.07\,\mathrm{N\,m^{-1}}$ so

$$\bar{\sigma} = \frac{\delta\sigma}{\rho_\ell V^2 L} = \frac{0.01 \times 0.07}{10^3 \times 10^2 \times 10^{-3}} = 7 \times 10^{-6}$$

The actual parameters which were chosen as instructive are $m = 2$, $A' = 5$ and $\bar{\sigma} = 0.03$.

5.2 Rescaling the system

The full system is unchanged under the following rescaling, for any fixed positive b and d.

$$\begin{aligned} \bar{x} &\to b\bar{x} \\ F &\to dF \\ \bar{t} &\to \frac{d^3}{b}\bar{t} \\ \bar{p} &\to \frac{b^3}{d^5}\bar{p} \\ A' &\to dA' \\ \bar{\sigma} &\to \frac{b^5}{d^6}\bar{\sigma} \end{aligned}$$

The corresponding change in the initial conditions is $m \to \frac{d}{b^2}m$ and $v \to \frac{b}{d^2}v$.

From the physical reality described above, v should be -1 and m should be $\frac{1}{2}\delta^2 = 0.0002$. In our calculations, $v = -1$ and $m = 2$, so the transformation with approximately $b = 460$ and $d = 22$ has been made. Thus the calculation corresponds to a real $\bar{\sigma}$ of 1.4×10^{-7} and a real A' of 0.25.

6 Results

We do reproduce the result that surface tension slows down the drop, preventing touchdown, and slip makes the slowing down less significant. This is shown in Figure 2.

Profiles of F and $\bar{p}$ are shown in Figure 3 at the end. The presence of surface tension clearly reduces the extreme pressure peak and slows the drop down. The presence of slip further reduces the maximum of the pressure and allows a faster approach to the surface.

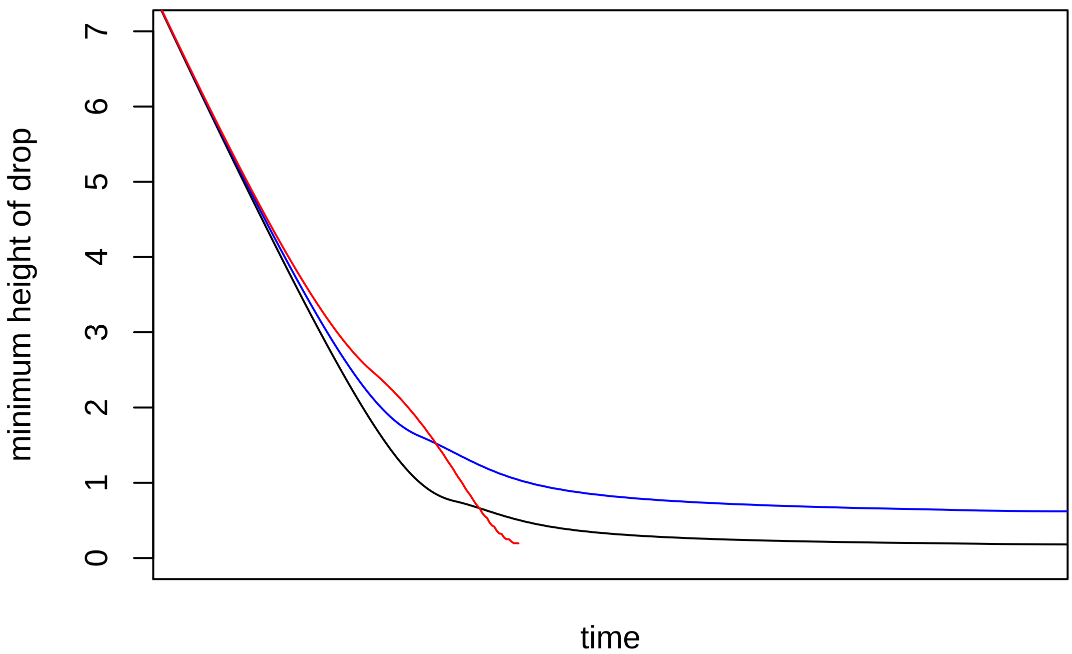

Figure 2: Drop height as a function of time. Red is without surface tension or slip. Blue is with surface tension but no slip. Black is with both surface tension and slip.

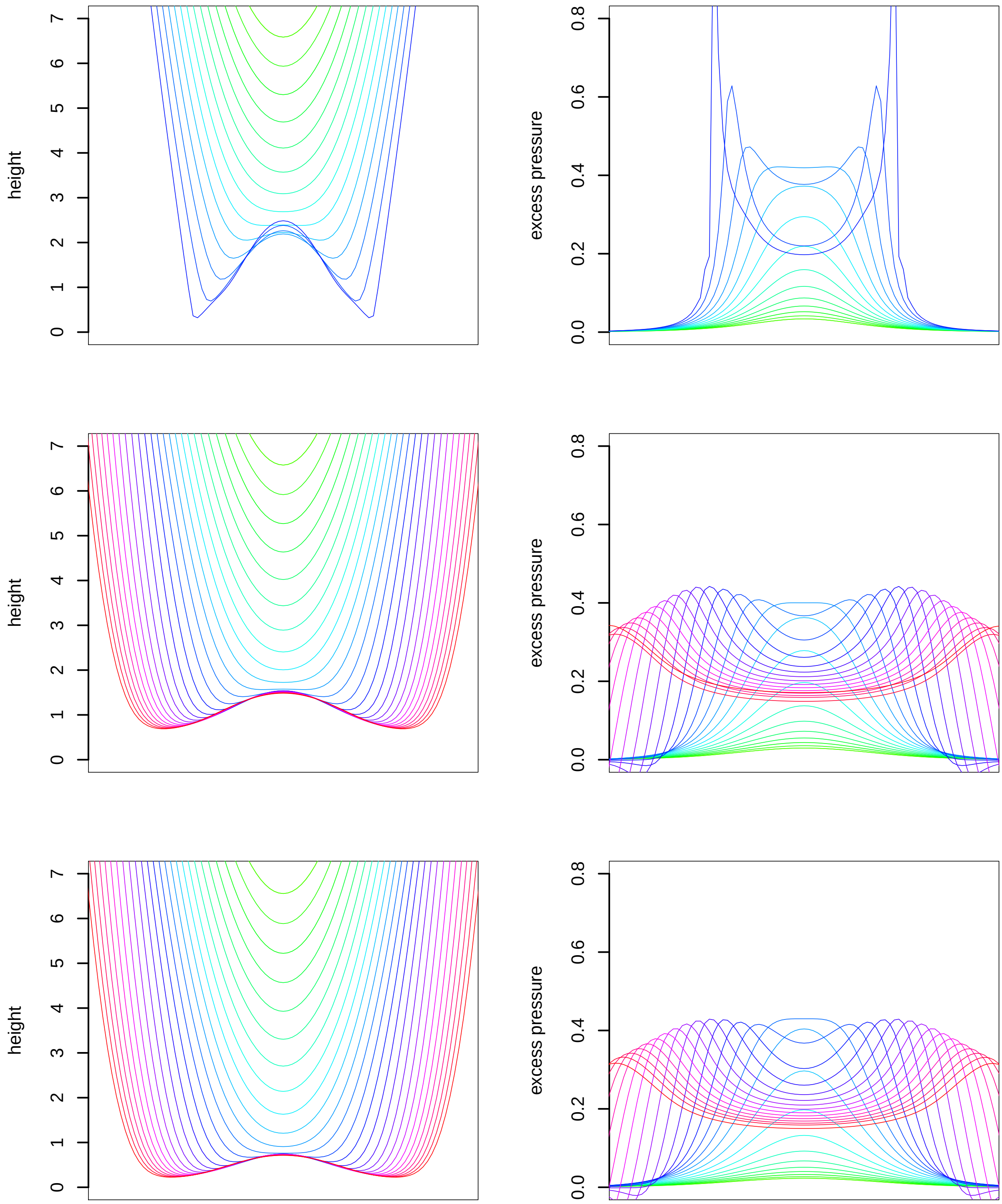

Figure 3: Drop height and pressure profiles at regular time intervals. A more red colour indicates a later time. The times and the x-axis (position) are the same in all cases, zoomed in to the contact area. The first row is without surface tension or slip, the second with surface tension but no slip and the third is with both surface tension and slip

7 Conclusions

There are some simple direct extensions of this work using the same method:

- It would be interesting to pay close attention to the numerical scheme used. For evaluating the integral (which is unchanged between this work and [8]), a slightly different expression was obtained, and looking into this discrepancy may be of interest.
- Very small timesteps were sometimes required to get stable results. The relationship between the time and space steps should be checked in detail. Even though the problem is nonlinear, an approach like von-Neumann stability analysis may help understand this effect.
- The code relies on a fixed time step and a fixed space step. It should be easy to make the grid adapt to have smaller space steps in areas of high curvature and smaller time steps when the surface is approached, which would be much more efficient.
- In Section 3 of [7], self-similar solutions to the governing equations are found and it is deduced that, with surface tension, there is no touchdown. This line of reasoning could possibly be extended to our situation with slip.
- It would be instructive to look at the results for other realistic parameter values.

More accurate models of rarefied gas dynamics are available and are relevant here, because the gas layer is so thin. A full finite-element simulation would be a much more flexible way to approach this problem. The results of our method could be useful in validating such work.

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