Structure evolution in the evaporation of complex fluids

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2 Abstract

The effect of thixotropy on a two-dimensional evaporating, particle laden sessile droplet has been modelled using Lubrication Theory. We use lubrication theory to derive a coupled system of equations that govern the drop thickness and the concentration of particles. These equations account for capillarity, viscous stress, van Der Waals forces, evaporation, and thixotropy. An ultra thin film is considered at the precursor to account for the no slip boundary condition. The effect of thixotropy is incorporated by the inclusion of a structure parameter, λ, measuring structure build-up governed by an evolution equation linked to the droplet micromechanics. The rheological properties of the material are assumed to evolve over time due purely to changes in its internal structure. Numerical solution of the governing equations show that thixotropy has a profound effect on the spreading and evaporating characteristics. Pure evaporating and mixed cases for spreading and evaporation have been considered and the results have been plotted.

3 Introduction

Thixotropy is of central importance in a variety of applications, due to its presence in a wide range of fluids, which include natural muds, slurries, clay suspensions, greases, paints, gels and adhesives. The mechanism underlying thixotropy is normally attributed to the interactions of polymers, particles and colloids within the fluid capable of forming a microstructure. The evolving microstructure modifies the internal stress of the fluid and consequently alters the rheological response. Here we will model thixotropy by the direct inclusion of a structure parameter λ. On the initiation of the flow, if microstructure breaks, such a state can only persist if the shear rate is maintained above another critical value. If the fluid flows in such a way that shear rates decline below the threshold value, the microstructure swiftly recovers and jams, abruptly increasing the viscosity and blocking flow.

Numerical studies show that thixotropy can have a dramatic effect on the regimes observed. We have studied the effect of thixotropy on the two-dimensional spreading and evaporation of a sessile drop without particle. Also the effect of thixotropy on a two-dimensional evaporating, particle laden droplet has been studied. For this we adapted structure evolution to be concentration dependent.

Lubrication theory has been used to reduce the full navier-stokes equations to 1-dimensional equation for the interfacial position. This theory uses that fact of naturally occurring small aspect ratio. It helps to find the solution for the depth dependence of the velocity field, and the derivation of an evolution equation for the interface. It is not possible, however, to remove the depth dependence completely in the presence of thixotropy using lubrication theory. Typically, a "1.5D model" is obtained characterised by a one-dimensional (1D) equation for the interface coupled to a two-dimensional equation for the structure parameter, that must be integrated over the depth.

4 Problem Formulation

Considering a droplet of density ρ and viscosity μ and using cartesian cordinate system(x, z) oriented parallel and normal to the substrate, re- spectively and with origin at the centreline of the droplet. The interface of the droplet with atmosphere is given by $z = h(x,t)$. Velocity is (u, w).
Starting with most basic equations, continuity equation and the navies stokes equation, we get
$u_x + w_z = 0$
$\nabla p = \nabla.\tau$ Non dimensionalising these equations along with the boundary conditions we get:
$u_x + w_z = 0$, $(\mu(\lambda)u_z)_z = p_x$, $p_z = 0$
The kinematic condition is given by:
$h_t + uh_x - w = 0$ at $z = h$
The stress boundary conditions are given by: $p = p_0 - h_{xx} - \pi$ and $u_z = 0$ at $z = h$
where $\pi = A/h^3$
where A is the Hamaker constant and π is the disjoining pressure
Evaporative flux is given by:
$J = (\theta + \Delta p)/(K + h)$
Depth averaging the continuity equation to generate evolution equation for interface at $z = h$ gives
$h_t + (h\bar{u})_x + J = 0$
Also,
$\lambda_t = (1 - \lambda)/D_b - B\lambda|\dot{\gamma}|$
Finally substituting we get:
$h_t - (h^3 p_x/(3\mu))_x + J = 0$
$\lambda_t = (1 - \lambda)f(1, 2, 3)/D_b - B\lambda h|h_{xxx}|/\mu(\lambda)$
Also the concentration condition is given by:
$c_t - (h^2 p_x/(3\mu) = (hc_x)_x/(hP_e) + cJ/h$
The initial condition are taken as:
$h(x, 0) = 2(1 - x^2) + h_{base}$ when $|x| < 1$
$h(x, 0) = h_{base}$ when $|x| > 1$ $\lambda(x, 0) = 0$
$C(x, 0) = 0$
We get 3 sets of simultaneous equations to solve.
Where f(1, 2 and 3) is a concentration dependent term and can be one of the following:
$f1 = (1 + c)^2$
$f2 = (1 + c)$
$f3 = c/(1 + c)$
The viscosity is taken to be a function of structure evolution and hence thixotropy given by:
$\mu(\lambda) = 1 + \delta\lambda$

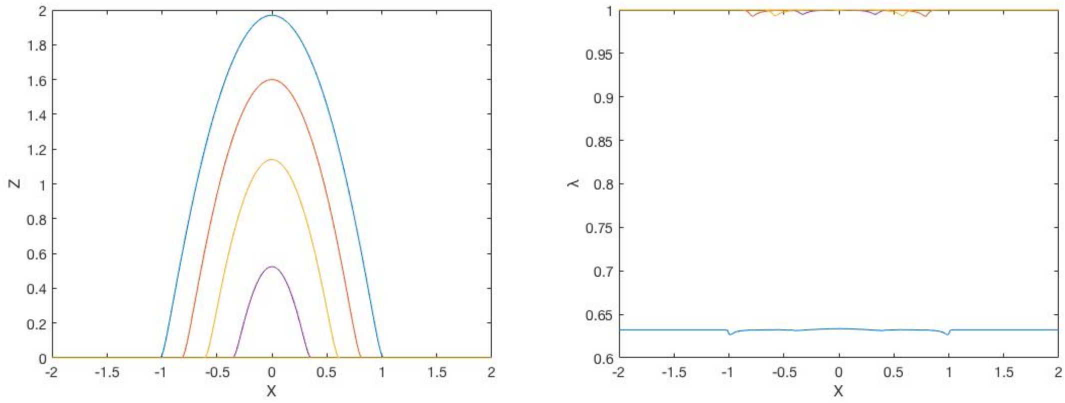
5 Results and Discussion

Figure 1 and 2 shows evolution of a thixotropic droplet without particles. When considering pure evaporating droplet, spreading must be decreased. Spreading would decrease if viscosity increases resulting from the increase in structuration. Hence, decreasing B, Db and K and increasing δ, θ and Δ will result in pure evaporation. Here no peaks in thixotropic profiles are observed due to the absence on particles. Also, the drop completely evaporated after t=4. Mixed case is shown in figure 2. Initially spreading dominates in the drop. But with time, as the drop spreads, viscosity increases near the precursor and thus evaporation dominates after t=2.

When the evolution of particle laden drops are considered, structuration term is taken to be concentration dependent. Three cases are considered for this dependency. Adjusting parameters give us the condition for pure evaporation i.e. evaporation»>spreading. First two cases give almost similar results for all the cases. f3 is more physically relevant as the structuration term goes to zero when the concentration of the particles become zero which is not true for the case of f1 and f2.

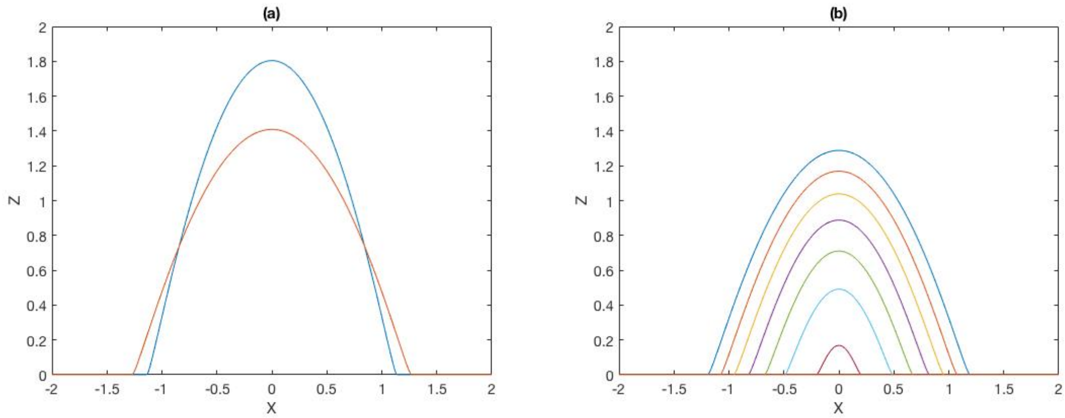
Figure 7 and 8 gives the account of the loglog plots for fluid mass, leading edge position and maximum height comparing these 3 cases. If evaporation wasn't to be considered in this model then these curves would have been straight lines with a slope of 1/7. As the fluid mass curve shows, the drop completely evaporates at about t=4.

Mixed case for particle laden drop is shown in figure 9, 10 and 11. Initially spreading dominates



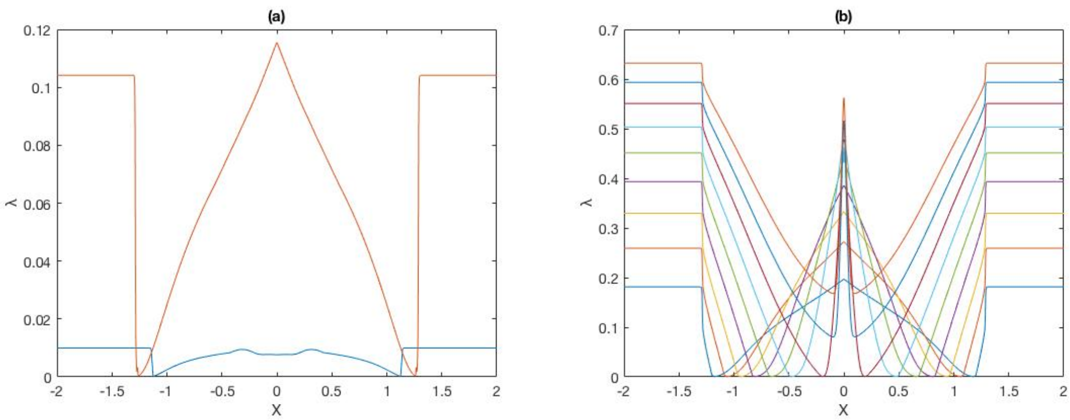
(a) (b)

Figure 1: Pure Evaporation: h and λ field at t=1(green), 5(yellow) and 10(red). We fix Db =0.1 and δ=100, B=0.1, A=10E-7, θ=1, k=1 and Δ=0.01



(a) (b)

Figure 2: Mixed Case: h field: a and c (spreading dominates for t= 1 to 2) and b and d(evaporation dominates for t = 3 to 10). We fix Db =10 and δ=49, B=5, A=10E-7, θ=0.1, k=0.1 and Δ=0.001



(a) (b)

Figure 3: Mixed Case: λ field: a and c (spreading dominates for t= 1 to 2) and b and d(evaporation dominates for t = 3 to 10). We fix Db =10 and δ=49, B=5, A=10E-7, θ=0.1, k=0.1 and Δ=0.001

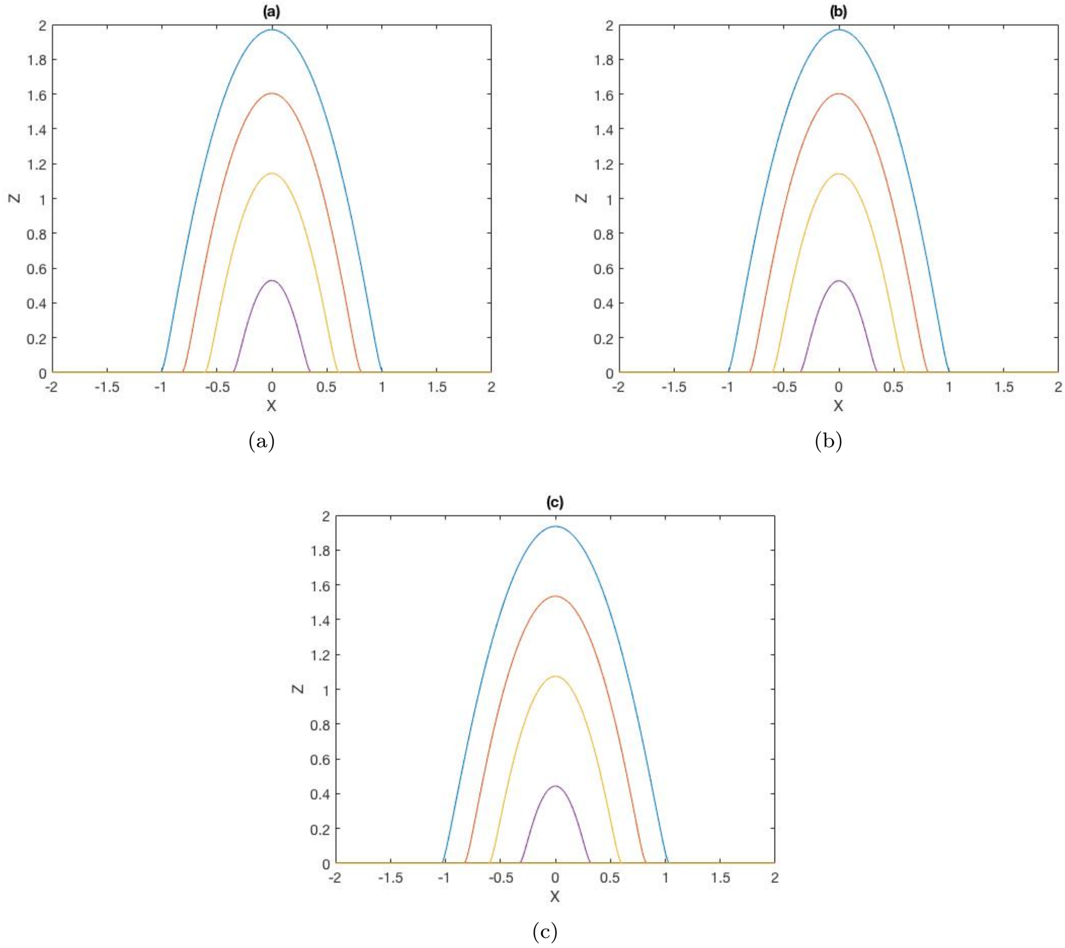


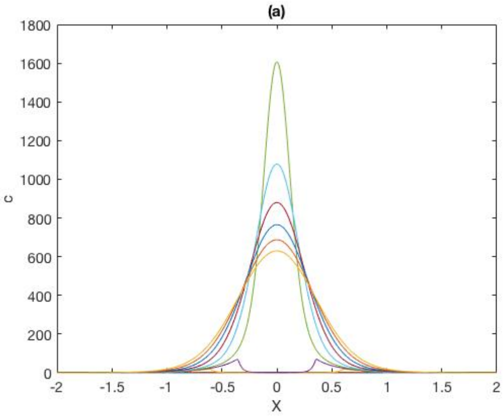
Figure 4: Pure Evaporation(h, c and λ: h curves for pure evaporation: a (f1 = $(1+c)^2$), b (f2 = (1+c)) and c ($f3 = c/(1+c)$). We fix Db =0.1 and δ=100, B=0.1, A=10E-7, θ=1, k=1 and Δ=0.01

in the drop. But with time, as the fluid mass decreases due to evaporation, particle concentration would increase. This would result in increasing viscosity and thus evaporation dominates after t=2. We observed that the evaporative flux is largest near the contact line of a drop. Hence, evaporation increases the particle concentration in this region, resulting in peaks in concentration curves near the contact line. This also lead to an increase in viscosity in that region retarding spreading. Thus these two phenomenon compete with each other at the precursor.

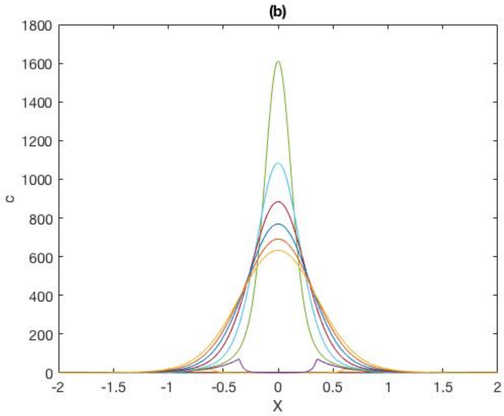
Again, loglog plots for fluid mass, leading edge position and maximum height have been plotted comparing all the three cases.

6 Conclusion

Two dimensional spreading and evaporating dynamics of a particle laden droplet has been considered. We used Lubrication Approximation to reduce the full navier-stokes equations to 1D equation for the interfacial position. Also the evolution equation is considered to be structure dependent. Three cases for dependency of structuration on concentration has been considered and all of them are compared to find the best model.
Dassl in Fortran has been used to solve these 3 interdependent equation and profiles for depth, concentration and thixotropy have been obtained. For the mixed cases shown, spreading dominates initially over evaporation and after some time evaporation start dominating over spreading.
We observed that the evaporative flux is largest near the contact line of a drop. Hence, evaporation increases the particle concentration in this region, resulting in peaks in concentration curves near the contact line. This also lead to an increase in viscosity in that region retarding spreading. Thus



(a)



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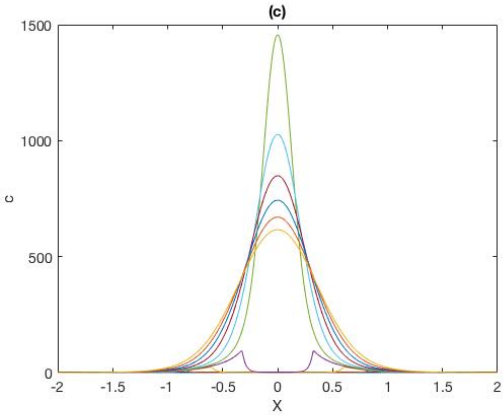

(c)

Figure 5: Pure Evaporation(h, c and λ: Concentration curves for pure evaporation: a (f1 $=(1+c)^2$), b (f2 = (1+c)) and c ($f3 = c/(1+c)$). We fix Db =0.1 and δ=100, B=0.1, A=10E-7, θ=1, k=1 and Δ=0.01

these two phenomenon compete with each other at the precursor.

7 References

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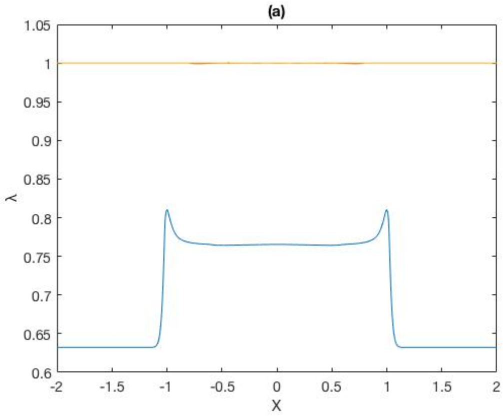

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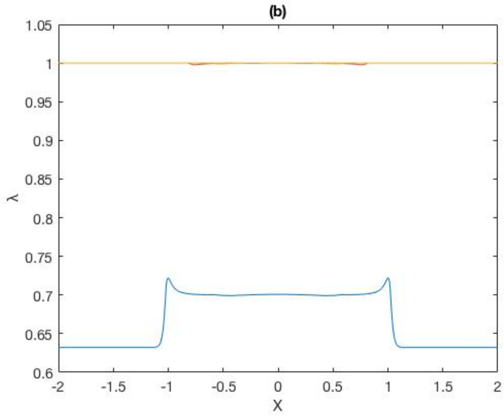

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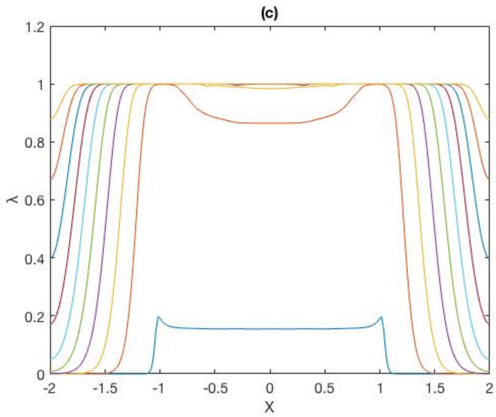
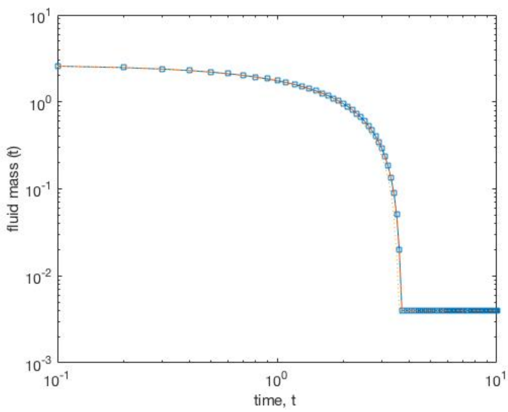


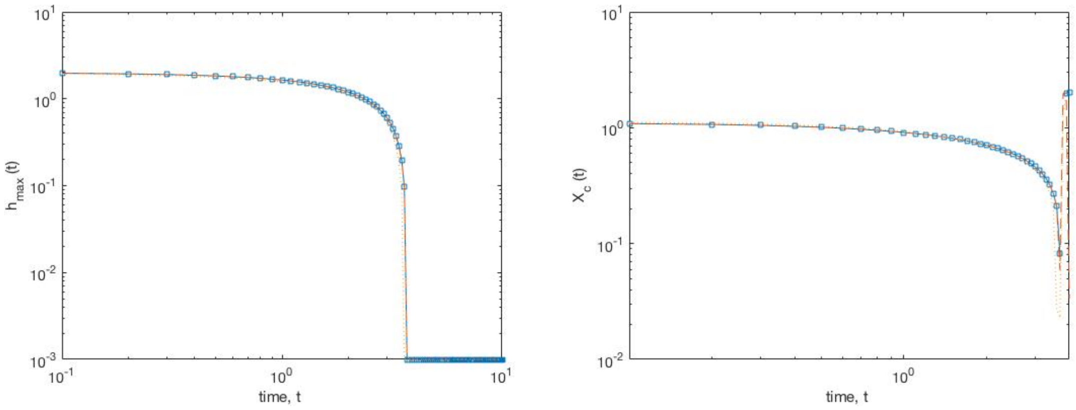
(c)

Figure 6: Pure Evaporation(h, c and λ: λ curves for pure evaporation: a (f1 $= (1+c)^2$), b (f2 = (1+c)) and c ($f3 = c/(1+c)$). We fix Db =0.1 and δ=100, B=0.1, A=10E-7, θ=1, k=1 and Δ=0.01



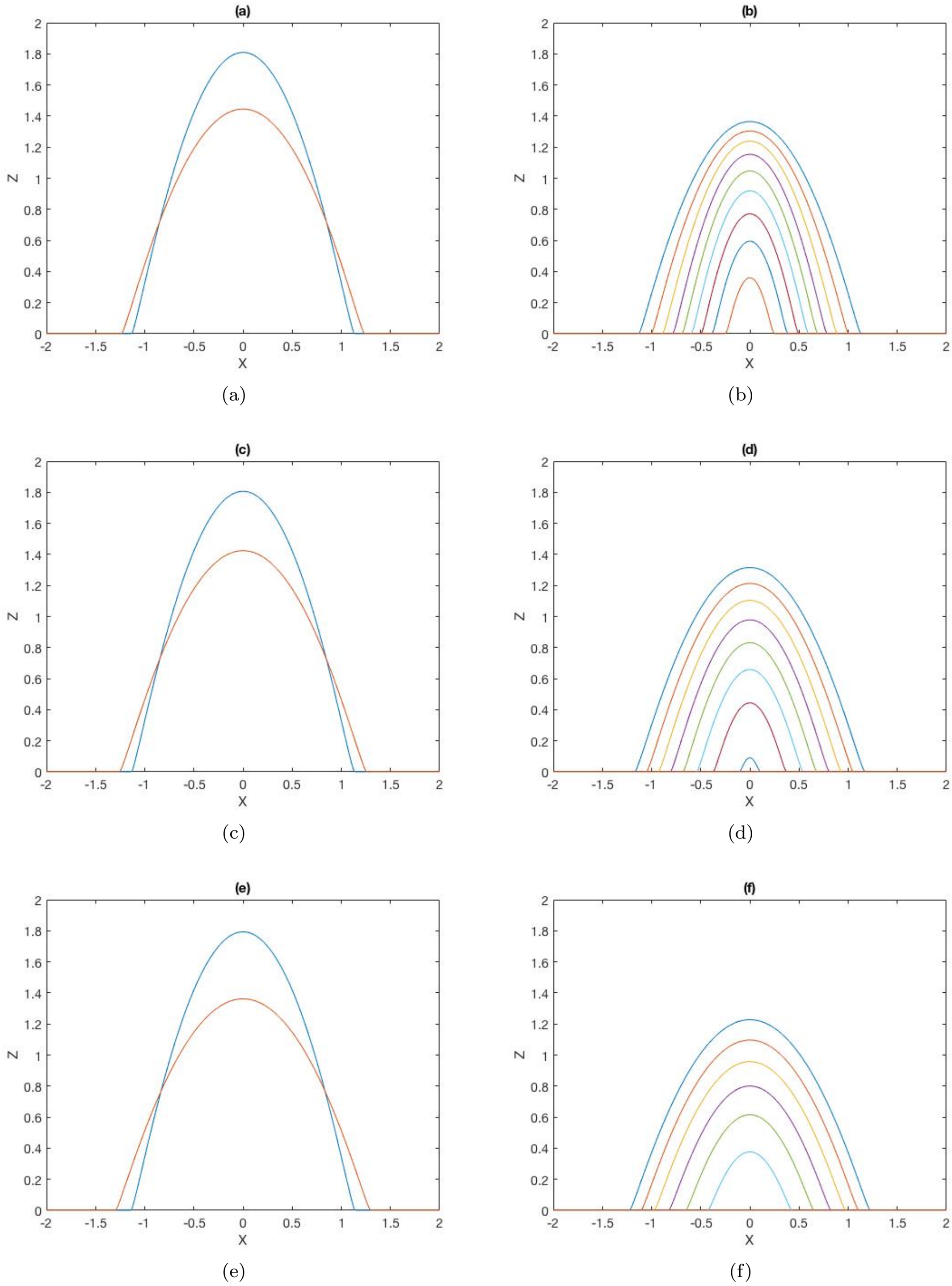
(a)

Figure 7: Loglog plots of the Fluid Mass(t) versus time, t showing comparisons between 3 model f1, f2 and f3. The prediction of the f1 model are shown by squares, while those of the f2 and f3 models are shown by the dashed and dotted lines respectively.



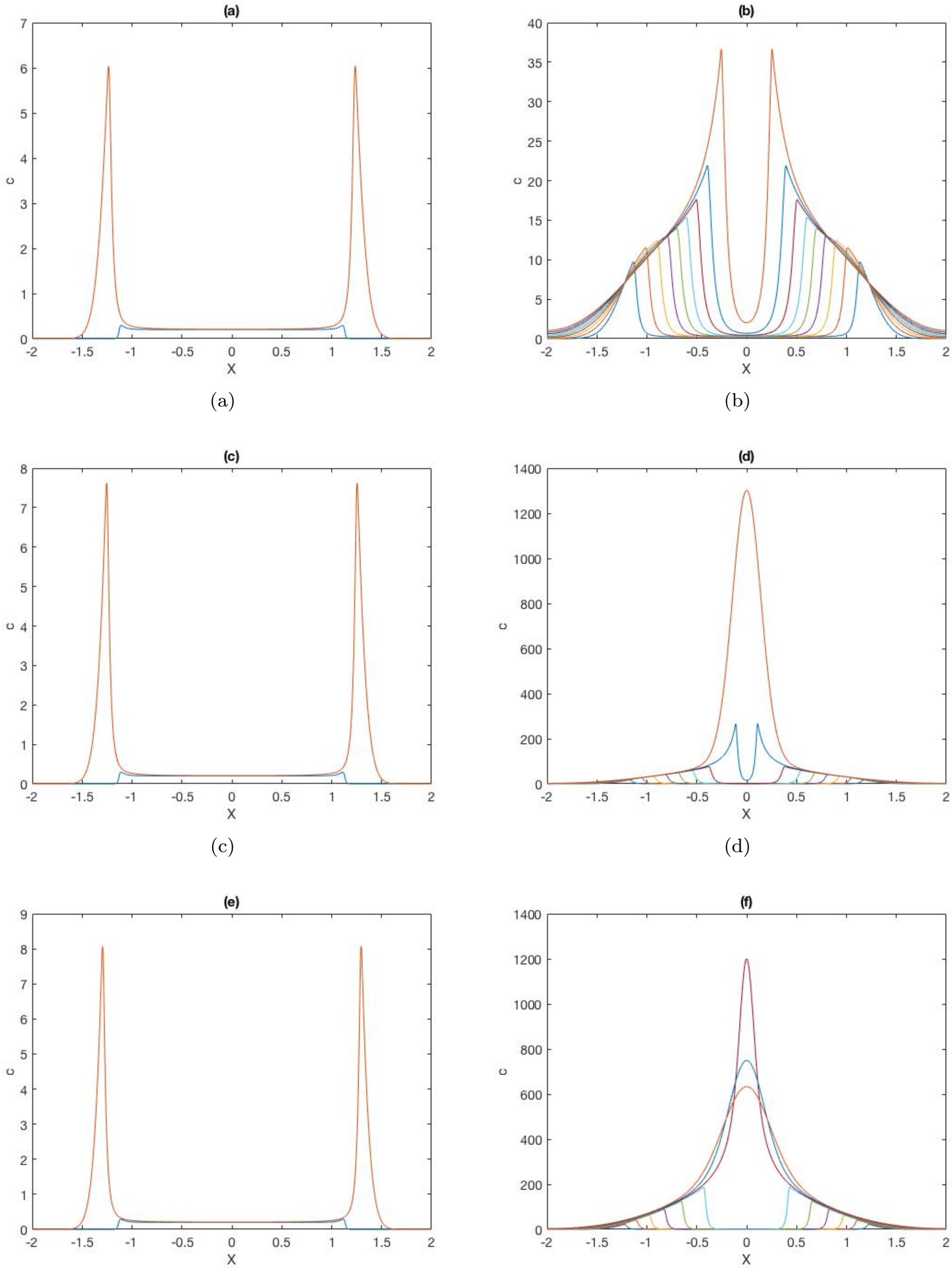
(a) (b)

Figure 8: Loglog plots of the leading edge position, xc(t) and maximum height, h_max showing comparisons between 3 model f1, f2 and f3. The prediction of the f1 model are shown by squares, while those of the f2 and f3 models are shown by the dashed and dotted lines respectively.



(a) (b) (c) (d) (e) (f)

Figure 9: Mixed Case(h, c and λ): h field: a, c and e(spreading dominates for t= 1 to 2) and b, d and f(evaporation dominates for t = 3 to 10). We fix Db =10 and δ=49, B=5, A=10E-7, θ=0.1, k=0.1 and Δ=0.001 for a and b (f1 = $(1+c)^2$), c and d(f2 = (1+c)) and e and f($f3 = c/(1+c)$)

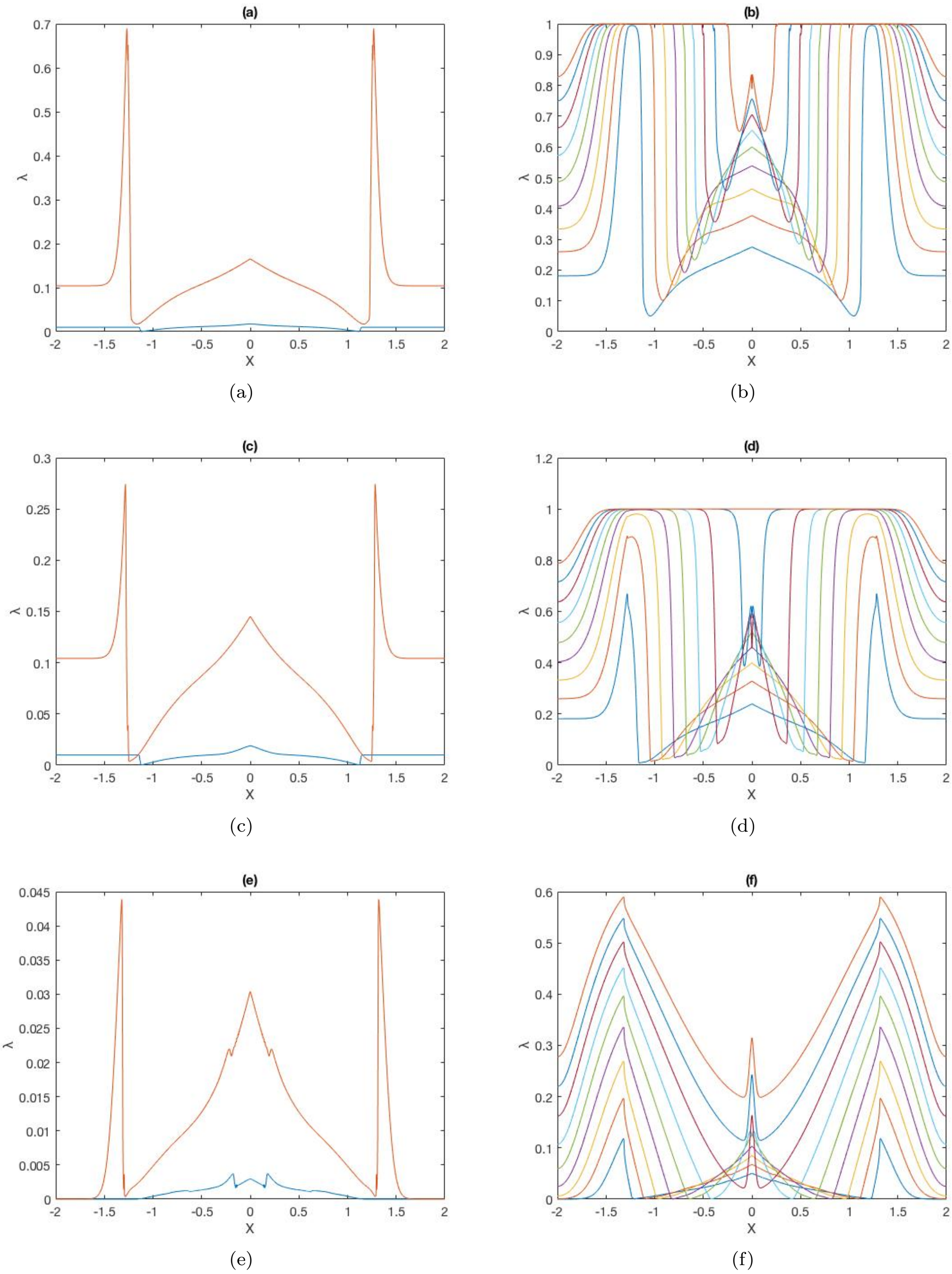


(a) (b)

(c) (d)

(e) (f)

Figure 10: Mixed Case(h, c and λ): Concentration field: a, c and e(spreading dominates for t= 1 to 2) and b, d and f(evaporation dominates for t = 3 to 10). We fix Db =10 and δ=49, B=5, A=10E-7, θ=0.1, k=0.1 and Δ=0.001 for a and b (f1 = $(1+c)^2$), c and d(f2 = (1+c)) and e and f($f3 = c/(1+c)$)

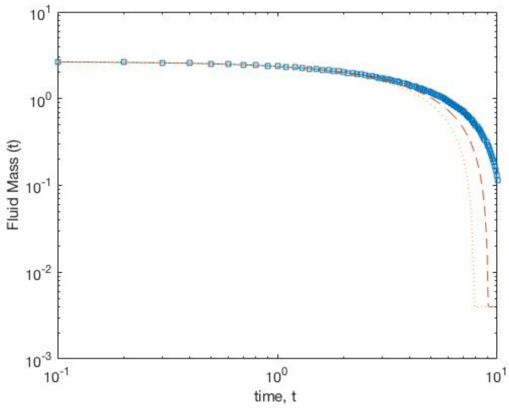


(a) (b)

(c) (d)

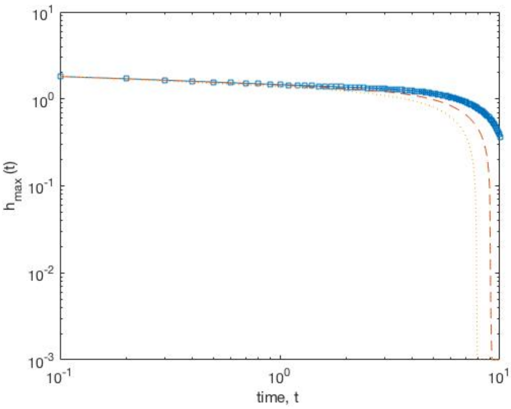
(e) (f)

Figure 11: Mixed Case(h, c and λ): Thixotropic field: a, c and e(spreading dominates for t= 1 to 2) and b, d and f(evaporation dominates for t = 3 to 10). We fix Db =10 and δ=49, B=5, A=10E-7, θ=0.1, k=0.1 and Δ=0.001 for a and b (f1 = $(1+c)^2$), c and d(f2 = (1+c)) and e and f($f3 = c/(1+c)$)



(a)

Figure 12: Mixed Case(h, c and λ): Loglog plots of the Fluid Mass(t) versus time, t showing comparisons between 3 model f1, f2 and f3. The prediction of the f1 model are shown by squares, while those of the f2 and f3 models are shown by the dashed and dotted lines respectively.



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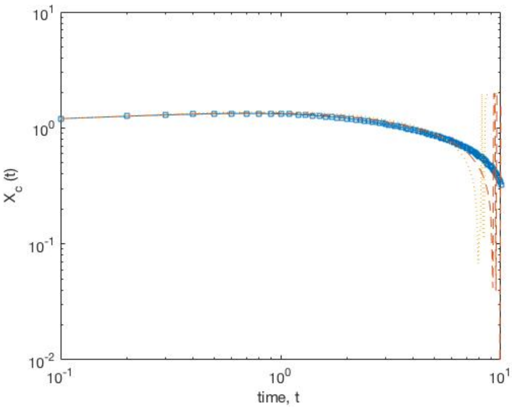

(b)

Figure 13: Mixed Case(h, c and λ): Loglog plots of the leading edge position, xc(t) and maximum height, hmax showing comparisons between 3 model f1, f2 and f3. The prediction of the f1 model are shown by squares, while those of the f2 and f3 models are shown by the dashed and dotted lines respectively.