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Computing inertial two- and three-dimensional thin film flow on planar surfaces featuring topography

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Abstract

A range of problems is investigated, involving the gravity-driven inertial flow of a thin viscous liquid film over a planar surface containing topographical features, modelled via a depth-averaged form of the governing unsteady Navier-Stokes equations. The discrete analogue of the resulting coupled equation set, employing a staggered mesh arrangement for the dependent variables, is solved accurately using an efficient Full Approximation Storage (FAS) algorithm and Full Multigrid (FMG) technique together with adaptive time-stepping and proper treatment of the nonlinear convective terms. A unique, comprehensive set of results is presented for both one- and two-dimensional topographical features, and errors quantified via detailed comparisons drawn with complementary experimental data and predictions from finite element analyses where they exist. It is found in the case of one-dimensional (spanwise) topography that for small Reynolds number and shallow/short features the depth-averaged form produces results that are in close agreement with corresponding finite element solutions of the full free-surface problem. For the case of flow over two-dimensional (localised) topography the free-surface disturbance observed is influenced significantly by the presence of inertia. It leads, as in the case of spanwise topography, to an increase in the magnitude and severity of the capillary ridge/trough patterns which form.

1 Introduction

Numerous manufacturing processes require the deposition of thin liquid films, involving a balance between viscous and surface tension forces, on a variety of surfaces. In the coating industries for example, several devices exist which have been optimised specifically for the continuous production and fast throughput of uniform, defect free, films on flat homogeneous substrates, made from plastic, metal, paper, etc. These encompass a wide range of applications and about which much of the underpinning basic science is now reasonably well documented [1]. In contrast the problem of thin film flow on surfaces containing man-made, micro-scale topographical features, with a predetermined functionality, such as displays, printed circuits and sensors, is less well understood. Indeed, the areas in which such flow is encountered is endless, encompassing latterly the rapidly evolving area of microfluidics, see for example [2], and the need to manipulate flow on an ever decreasing scale in the context of lab-on-chip devices. In addition, one should not forget the consequence(s) associated with the presence of unwanted surface topography, contaminates such as dust specks or irregularities resulting from a particular stage in a manufacturing process.

From a traditional standpoint the overall goal might arguably be one of identifying the parameters that influence the planarity of such films and thus guide its effective control, which represents a considerable challenge in itself given the diversity and nature of the topography encountered in practice. On the other hand, the realisation that naturally occurring surface patterns, regular and randomly distributed, is a key feature of numerous biological systems provides a different impetous; thin liquid films being important in areas as diverse as the redistribution of the liquid lining of the lung [3], plant disease control [4], biofilms [5] and water snail locomotion [6], plus the strong driver associated with ultimately mimicking the behaviour of nature's surfaces [7], has brought the subject of film flow over topography into even sharper focus.

Accurate prediction of the associated three-dimensional free-surface flow by solving the governing unsteady Navier-Stokes equations remains elusive; not from the point of view of being unable to develop suitable discrete analogues, simply that the computational resource required to solve them is currently prohibitive. Accordingly, the bulk of the theoretical work that has appeared to date has relied on the assumption that creeping flow conditions prevail allied to the fact that for many thin film flows the ratio of the undisturbed asymptotic film thickness to that of the characteristic in-plane length-scale of the flow is small. If the velocity and pressure fields are expanded in terms of this small parameter and substituted into the Stokes equations [8] then, retaining leading order terms, a fourth-order nonlinear degenerate partial differential equation for the film thickness, referred to as the lubrication approximation, results.

It is no surprise that the above long wavelength approximation has proved popular, and the equations involved solved using a variety of numerical methods, with semi-implicit, alternating direction, time-splitting schemes [9, 10] enjoying wide usage. The argument for employing such schemes is that they combine some of the stability properties of implicit schemes with the cost efficiency of explicit ones. However, when fine meshes are required to ensure grid independent solutions the choice of time-step is severely restricted. With this in mind an investigation concerning droplet motion [11] showed that the alternative approach of adopting a fully implicit multigrid formulation to: (i) be more robust; (ii) return an order of magnitude improvement in the rate of convergence for the levels of grid refinement required for accuracy; (iii) utilise far less memory. The point was reinforced still further by [12] who combined a multigrid approach with error-controlled adaptive time-stepping. This same algorithm was used in a detailed study of the flow of gravity-driven thin liquid films on non-porous substrates with topography, showing that the long wavelength approximation leads to very good solutions, even in regions of parameter space where it is not strictly valid [13]. The methodology has subsequently been refined to embody error-controlled automatic mesh adaption [14, 15] leading to significant further improvement in solution times without loss of accuracy, and to include additional physics [16] - in this case evaporation.

In addition and from the point of view of completeness it is important to mention that for Stokes flow the boundary element method has proven effective as a means of investigating three-dimensional continuous thin film flow over a small particle adjacent to a flat surface [17, 18]. A Stokes flow perturbation analysis has also been used to study the particular case of gravity-driven flow over doubly-periodic surface corrugations, and extended to consider cases with finite Reynolds number [19, 20].

Unfortunately, few complementary purely experimental investigations involving thin film flow over topography have appeared in the literature affording direct comparison with theory, due to the formidable practical challenges involved. Early examples, featuring complementary long wavelength analysis, include [21, 22, 23] and [24] who considered radial outflow during spin coating and gravity-driven flow down an inclined plane, respectively. A key finding by both sets of authors was that lubrication theory proved surprisingly accurate for their modelling purposes; in addition [23] are credited as being the first to obtain a one-dimensional analytic expression for the standing capillary wave which forms at the leading edge of a trench topography and its associated downstream exponential decay. This problem was subsequently revisited by [25]; their Green's function formulation showed good agreement, with the second order term contained therein having the effect of locating the capillary ridge further upstream of the topography the deeper the trench becomes. In a similar vein [26, 27] have reported both experimental and numerical results for spin coating that are in qualitative agreement; the absolute accuracy of their experimental data is, however, questionable for the case of shallow topography. Considerable time then lapsed before a more useful batch of experimental data materialised [28, 29, 30]; culminating ultimately in the results presented by [31] and which form the experimental benchmark against which predictions may be compared.

As an alternative to employing lubrication theory, the influence of inertia, for the particular case of gravity driven film flow over a plane containing steep spanwise topography only, has begun to be explored recently in terms of the so-called integral-boundary-layer approximation. The mathematical formulation of the latter, in which the resulting equations are expressed in terms of the film thickness and mean flow rate, can be traced back to Shkadov 1967/1968 [32, 33], who used it to predict solitary waves in thin films on flat substrates. Recently, Saprykin, Koopmans and Kalliadasis 2007 [34] extended Shkadov's idea to explore the influence of inertia and viscoelasticity on thin film flow over step-down topography taken to be in vertical alignment. A key feature of the integral-boundary-layer approximation is the assumption that the velocity profile across the film has a self-similar parabolic form. Ruyer-Quil and Manneville 1998 [35, 36, 37] show how to generalise the IBL model in two ways. Firstly by approximating the velocity profile using high-order polynomials instead of quadratic polynomials only in IBL, the coefficients of the polynomials are derived by gradient expansion of the solution. Obtained approximation is called first-order model in their work. Secondly by keeping terms of second-order-accuracy of the long-wave expansion of the N-S equations and free surface stress balance boundary condition. This approximation is called second-order model in their work and leads to a more sophisticated system of the equations for three unknowns - film thickness, mean flow rate and shear stress at the substrate. A more general approach than second-order model of Ruyer-Quil and Manneville is developed in Amaouche, Mehidi and Amatousse 2005 [38] third-order-accuracy terms of the of the long-wave expansion of the N-S equations are kept and the velocity profile is approximated using polynomials up to eighth-order, which coefficients are obtained by Galerkin projection. Another approach worth mentioning is the depth averaged kinetic energy balance or energy integral method based on a velocity weighted average of the N-S equations was offered by Usha 2004 [39]. It is shown to be a reasonable alternative to a standard IBL avaraging of the N-S equations. Last but not least, Bontozoglou and Serifi (2008) [40] carried out a numerical investigation of the flow of a thin film down a vertically aligned wall containing steep isolated step topograpy. They solved the full Navier-Stokes equations using a finite element method showing that, for large capillary numbers, increasing inertia first amplifies and then diminishes the capillary features - an effect that is not observed with the integral-boundary-layer approach which is valid for small capillary numbers only.

Although not considered here, it is essential not to lose sight of the fact that inertial effects cause the free surface flows of interest to become unstable when the Reynolds number exceeds a critical value; several analyses of the instability mechanism for the case of flat substrates have emerged, see for example [xxx] but few have considered the influence of topography. Recent experiments have demonstrated, however, that there is a strong coupling between inertia and topographic effects in gravity-driven flow over substrates containing rectangular (Vlachogiannis and Bontozoglou 2002 [41]) or wavy (Wierschem, Lepski and Aksel 2005 [42]) corrugations. The significant rise in critical Reynolds number that occurs due to the presence of topography, as observed experimentally, has also been predicted theoretically (Wierscem and Aksel 2003 [43]). Recently, Trifonov 2007 [44], examined the stability of a viscous film flowing over a vertically aligned wavy surface, showing that there is a region of corrugation geometry (amplitude and period) where disturbances decay resulting in a stabalising effect, outside this region the flow is unstable. The reader is also directed to the recent work by Aksel et al in relation linear and nonlinear resonance of thin films (2008,2009 [45, 46]) and to the work of Kayat, Kim and Delosquer 2004 [47] who provide a detailed expose on the influence of inertia, topography and gravity on transient axisymmetric thin film flow.

The approach adopted in the present work involves the efficient solution of a depth-averaged form, akin to the integral-boundary-layer approximation, of the governing unsteady Navier-Stokes equations; in particular in the case of the three-dimensional flow associated with thin films encountering steep two-dimensional, localised topography. The associated mathematical formulation and method of solution required to guarantee accurate mesh-independent solutions are provided in Sections 2 and 3, respectively. A comprehensive set of results is presented in Section 4, including comparison of computed free-surface profiles with experimental data, where it exists. The case of flow over spanwise topography serves to illustrate the depth-averaged form's ability to cater for inertia effects since direct comparison can be made with finite element solutions of the full free-surface problem. Conclusions are drawn in Section 5.

2 Mathematical Formulation

Consider, as illustrated in Figure 1, the case of time-dependent gravity-driven thin film flow down a planar substrate containing topography, that is inclined at an angle θ ($\neq 0$) to the horizontal. The liquid is assumed to be incompressible and to have constant density, ρ, viscosity, μ, and surface tension, σ. The chosen Cartesian streamwise, X, spanwise, Y, and normal, Z, coordinates are as indicated and the solution domain bounded from below by the substrate, $Z = S(X,Y)$, from above at time T by the free-surface, $Z = F(X,Y,T)$, upstream and downstream by the inflow, $X = 0$, and outflow, $X = L_p$, planes, respectively, and to the left and right by the side planes at $Y = 0$ and $Y = W_p$. The film thickness at any point in the (X,Y) plane is given by $H = F - S$. The resulting laminar flow is described by the Navier-Stokes and continuity equations, namely:

$$\rho\left(\frac{\partial \boldsymbol{U}}{\partial T} + \boldsymbol{U}\cdot\nabla\boldsymbol{U}\right) = -\nabla P + \nabla\cdot\boldsymbol{T} + \rho\boldsymbol{G}, \tag{1}$$

$$\nabla\cdot\boldsymbol{U} = 0, \tag{2}$$

where $\boldsymbol{U} = (U,V,W)$ and P are the fluid velocity and pressure, respectively; $\boldsymbol{T} = \mu\left(\nabla\boldsymbol{U} + (\nabla\boldsymbol{U})^T\right)$ is the viscous stress tensor, $\boldsymbol{G} = g_0(\sin\theta, 0, -\cos\theta)$ is the acceleration due to gravity where g_0 is the standard gravity constant.

Taking the reference length-scale in all directions to be the asymptotic, or fully developed, film thickness, H_0, and scaling the velocities and pressure (stress tensor) by the free-surface (maximum) velocity, $U_0 = \rho g_0 H_0^2 \sin\theta/2\mu$, and average pressure, $P_0 = \mu U_0/H_0$, respectively, apropos the classic Nusselt solution [48], and the time by $T_0 = H_0/U_0$, equations (1) and (2) can be rewritten in non-dimensional form as:

$$\mathrm{Re}\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)=-\nabla p+\nabla\cdot\boldsymbol{\tau}+\mathrm{St}\boldsymbol{g}, \tag{3}$$

$$\nabla\cdot\boldsymbol{u}=0, \tag{4}$$

where $\boldsymbol{u}=(u,v,w)$, $\boldsymbol{\tau}$ and $\boldsymbol{g}=\boldsymbol{G}/g_0$ are the dimensionless velocity, viscous stress tensor and gravity component, respectively; $\mathrm{Re}=\rho U_0 H_0/\mu$ is the Reynolds number and $\mathrm{St}=2/\sin\theta$ the Stokes number. Alternatively, the latter can be written as $\mathrm{St}=\mathrm{Re}/\mathrm{Fr}$, where $\mathrm{Fr}=U_0^2/(H_0 g_0)$ is the Froude number.

The problem is closed by imposing the required no-slip, inflow, outflow, kinematic, free-surface normal and tangential stress boundary conditions [49], namely:

$$\boldsymbol{u}|_{z=s}=0, \tag{5}$$

$$u|_{x=0,l_p;y=0,w_p}=z\,(2-z)\,,\qquad v|_{x=0,l_p;y=0,w_p}=w|_{x=0,l_p;y=0,w_p}=0, \tag{6}$$

$$\frac{\partial f}{\partial t}+u|_{z=f}\frac{\partial f}{\partial x}+v|_{z=f}\frac{\partial f}{\partial y}-w|_{z=f}=0, \tag{7}$$

$$-p|_{z=f}+(\boldsymbol{\tau}|_{z=f}\cdot\boldsymbol{n})\cdot\boldsymbol{n}=\frac{\kappa}{\mathrm{Ca}}, \tag{8}$$

$$(\boldsymbol{\tau}|_{z=f}\cdot\boldsymbol{n})\cdot\boldsymbol{t}=0, \tag{9}$$

where $\mathrm{Ca}=\mu U_0/\sigma$ is the capillary number, x,y,z,l_p,w_p,s,f correspond to their dimensional counterparts, $\boldsymbol{n}=\left(-\frac{\partial f}{\partial x},-\frac{\partial f}{\partial y},1\right)\cdot\left[\left(\frac{\partial f}{\partial x}\right)^2+\left(\frac{\partial f}{\partial y}\right)^2+1\right]^{-1/2}$ is the unit normal vector pointing outward from the free surface, $\boldsymbol{t}=\left(\alpha_t,\beta_t,\alpha_t\frac{\partial f}{\partial x}+\beta_t\frac{\partial f}{\partial y}\right)\cdot\left[\alpha_t^2+\beta_t^2+\left(\alpha_t\frac{\partial f}{\partial x}+\beta_t\frac{\partial f}{\partial y}\right)^2\right]^{-1/2}$ is the unit vector tangential to the free surface, α_t, β_t are the arbitrary constants that define the tangent vector direction in the tangential plane and $\kappa=-\nabla\cdot\boldsymbol{n}$ is the free-surface curvature.

Although in principle the above system of equations and boundary conditions, (3) to (9), could be solved using, for example, a finite element formulation, the memory and computational resources required to obtain the accuracy necessary to produce grid independent solutions remains a formidable stumbling block. In addition, this constraint becomes further exacerbated, even in the Stokes flow limit, when one has to handle very small topographical features and/or when the same are sparsely distributed [14]. Accordingly a process of depth-averaging is used to derive a new equation set, that in effect reduces the dimensionality of the problem by one and which can be solved both accurately and efficiently.

2.1 Depth-Averaged Form (DAF)

The task of solving the problem of interest is simplified greatly by adopting a long-wave approximation [8], the main assumption being that $\varepsilon=H_0/L_0\ll 1$, where L_0 is the characteristic in-plane length scale. Formulating the governing equations (3) and (4) in terms of L_0 is equivalent to the following change of non-dimensional variables $(x,y,l_p,w_p,t,p)\to(x,y,l_p,w_p,t,p)/\varepsilon$, $w\to\varepsilon w$, leading to:

$$\varepsilon\mathrm{Re}\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial p}{\partial x}+\varepsilon^2\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)+\frac{\partial^2 u}{\partial z^2}+2, \tag{10}$$

$$\varepsilon\mathrm{Re}\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=-\frac{\partial p}{\partial y}+\varepsilon^2\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+\frac{\partial^2 v}{\partial z^2}, \tag{11}$$

$$\varepsilon^3\mathrm{Re}\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=-\frac{\partial p}{\partial z}+\varepsilon^4\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}\right)+\varepsilon^2\frac{\partial^2 w}{\partial z^2}-2\varepsilon\cot\theta, \tag{12}$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \tag{13}$$

while the boundary conditions (8) and (9) become:

$$-p|_{z=f}+\left\{\frac{2\varepsilon^2\left(-\frac{\partial u}{\partial z}\frac{\partial f}{\partial x}-\frac{\partial v}{\partial z}\frac{\partial f}{\partial y}+\frac{\partial w}{\partial z}\right)+O(\varepsilon^4)}{1+\varepsilon^2\left[\left(\frac{\partial f}{\partial x}\right)^2+\left(\frac{\partial f}{\partial y}\right)^2\right]}\right\}|_{z=f}=\frac{\varepsilon^3}{\mathrm{Ca}}\nabla\frac{\nabla f}{\sqrt{1+\varepsilon^2\left[\left(\frac{\partial f}{\partial x}\right)^2+\left(\frac{\partial f}{\partial y}\right)^2\right]}}, \tag{14}$$

$$\begin{aligned}&\left(\alpha_t\frac{\partial u}{\partial z}+\beta_t\frac{\partial v}{\partial z}\right)|_{z=f}+\varepsilon^2\left\{\left(\alpha_t\frac{\partial f}{\partial x}+\beta_t\frac{\partial f}{\partial y}\right)\left(-\frac{\partial u}{\partial z}\frac{\partial f}{\partial x}-\frac{\partial v}{\partial z}\frac{\partial f}{\partial y}+2\frac{\partial w}{\partial z}\right)\right.\\&\left.+\alpha_t\left[-2\frac{\partial u}{\partial x}\frac{\partial f}{\partial x}-\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\frac{\partial f}{\partial y}+\frac{\partial w}{\partial x}\right]+\beta_t\left[-2\frac{\partial v}{\partial y}\frac{\partial f}{\partial y}-\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\frac{\partial f}{\partial x}+\frac{\partial w}{\partial y}\right]\right\}|_{z=f}+O(\varepsilon^4)=0.\end{aligned} \tag{15}$$

By neglecting all terms of $O(\varepsilon^2)$ and smaller the above system simplifies considerably and can be averaged over the depth of the film. As in the case of a lubrication approach [8] the depth-averaged form (DAF) derived below can be thought of as a second-order accurate long-wave approximation but with no Reynolds number limitation.

For thin film flows the capillary pressure is of the same order as the fluid pressure; to be consistent with [13], [31] and [50] the capillary number is defined as:

$$\mathrm{Ca}=\frac{\varepsilon^3}{6}=\frac{H_0^3}{6L_0^3}, \tag{16}$$

where $L_0=(\sigma H_0/3\rho g\sin\theta)^{1/3}$ represents the associated capillary length-scale; the resulting DAF is therefore valid for the case of small capillary numbers, $\mathrm{Ca}\sim O(\epsilon^3)\ll 1$, only.

Equation (12) results in a balance between the acceleration arising from the pressure and that from gravity, which when integrated with respect to z and applying boundary condition (14), leads to the following familiar equation [13] for pressure:

$$p=-\frac{\varepsilon^3}{\mathrm{Ca}}\nabla^2 f+2\varepsilon\,(f-z)\cot\theta. \tag{17}$$

Applying Leibniz's rule to the continuity equation (13) and using boundary conditions (5) and (7) leads to the following depth-averaged equation for the conservation of mass:

$$\int_s^f\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)dz=\frac{\partial h}{\partial t}+\frac{\partial h\bar{u}}{\partial x}+\frac{\partial h\bar{v}}{\partial y}=0, \tag{18}$$

where

$$\bar{u}=\frac{1}{h}\int_s^f u dz,\quad \bar{v}=\frac{1}{h}\int_s^f v dz, \tag{19}$$

are the x and y depth-averaged components of velocity.

The DAF of the momentum equations (10) and (11) is obtained in three stages: first the pressure gradient, then the diffusion terms and finally the advection terms are averaged. In the case of the u-momentum equation (10), making use of the boundary conditions (5), (7), (15), equation (13) and noting that fluctuations about the average are zero, this gives in order:

$$\int_s^f \frac{\partial p}{\partial x} dz = h\frac{\partial p}{\partial x}, \tag{20}$$

$$\int_s^f \frac{\partial^2 u}{\partial z^2} dz = \frac{\partial u}{\partial z}|_{z=f} - \frac{\partial u}{\partial z}|_{z=s} = -\frac{\partial u}{\partial z}|_{z=s}, \tag{21}$$

$$\begin{aligned}\int_s^f \left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}\right) dz &= \int_s^f \left(\frac{\partial u}{\partial t} + \frac{\partial uu}{\partial x} + \frac{\partial vu}{\partial y} + \frac{\partial wu}{\partial z}\right) dz \\ = h\left(\frac{\partial \bar{u}}{\partial t} + \bar{u}\frac{\partial \bar{u}}{\partial x} + \bar{v}\frac{\partial \bar{u}}{\partial y}\right) + \frac{\partial}{\partial x}\int_s^f (\bar{u}-u)^2 dz &+ \frac{\partial}{\partial y}\int_s^f (\bar{u}-u)(\bar{v}-v) dz. \end{aligned} \tag{22}$$

The DAF of the v-momentum equation (11) is derived similarly.

After substitution of the pressure equation (17) into the momentum equations and dividing through by the film thickness, the resulting governing system of equations for the unknown averaged velocities $\bar{u}(x,y,t)$, $\bar{v}(x,y,t)$ and the film thickness $h(x,y,t)$ is:

$$\begin{aligned}\varepsilon \mathrm{Re}\left[\frac{\partial \bar{u}}{\partial t} + \bar{u}\frac{\partial \bar{u}}{\partial x} + \bar{v}\frac{\partial \bar{u}}{\partial y} + \frac{1}{h}\frac{\partial}{\partial x}\int_s^f (\bar{u}-u)^2 dz + \frac{1}{h}\frac{\partial}{\partial y}\int_s^f (\bar{u}-u)(\bar{v}-v) dz\right] \\ = \frac{\partial}{\partial x}\left[\frac{\varepsilon^3}{\mathrm{Ca}}\nabla^2 (h+s) - 2\varepsilon (h+s)\cot\theta\right] - \frac{1}{h}\frac{\partial u}{\partial z}|_{z=s} + 2,\end{aligned} \tag{23}$$

$$\begin{aligned}\varepsilon \mathrm{Re}\left[\frac{\partial \bar{v}}{\partial t} + \bar{u}\frac{\partial \bar{v}}{\partial x} + \bar{v}\frac{\partial \bar{v}}{\partial y} + \frac{1}{h}\frac{\partial}{\partial x}\int_s^f (\bar{u}-u)(\bar{v}-v) dz + \frac{1}{h}\frac{\partial}{\partial y}\int_s^f (\bar{v}-v)^2 dz\right] \\ = \frac{\partial}{\partial y}\left[\frac{\varepsilon^3}{\mathrm{Ca}}\nabla^2 (h+s) - 2\varepsilon (h+s)\cot\theta\right] - \frac{1}{h}\frac{\partial v}{\partial z}|_{z=s},\end{aligned} \tag{24}$$

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} + \frac{\partial h\bar{v}}{\partial y} = 0. \tag{25}$$

The above system of equations contains four dimensionless parameters: ε, Re, Ca and θ; however, due to the nature of the length-scale L_0 it is possible to avoid one spare parameter - either Ca or ε as per equation (16). Therefore the similarity of the results obtained by solving the DAF depends on two dimensionless groupings only: an inertia parameter $\mathcal{I} = \mathrm{Ca}^{1/3} \cdot \mathrm{Re}$ and gravity parameter $\mathrm{N} = \mathrm{Ca}^{1/3} \cdot \cot\theta$.

The problem is closed in terms of specified averaged inflow conditions and the assumption of fully developed flow both upstream and downstream, namely:

$$\bar{u}|_{x=0} = 2/3, \quad \bar{v}|_{x=0} = \frac{\partial \bar{u}}{\partial x}|_{x=l_p} = \frac{\partial \bar{v}}{\partial x}|_{x=l_p} = \frac{\partial \bar{u}}{\partial y}|_{y=0,w_p} = \frac{\partial \bar{v}}{\partial y}|_{y=0,w_p} = 0. \tag{26}$$

$$h|_{x=0} = 1, \quad \frac{\partial h}{\partial x}|_{x=l_p} = \frac{\partial h}{\partial y}|_{y=0,w_p} = 0. \tag{27}$$

2.2 Friction and Dispersion Terms

The DAF of the governing equations (23) to (25) contains friction and dispersion terms of the form $\frac{\partial u}{\partial z}|_{z=s}$, $\frac{\partial v}{\partial z}|_{z=s}$ and $\int_s^f (\bar{u}-u)^2\,dz$, $\int_s^f (\bar{v}-v)^2\,dz$, $\int_s^f (\bar{u}-u)(\bar{v}-v)\,dz$, respectively. For the thin film flows of interest, these terms can be determined by assuming that the velocity profile within the film has the same and consistent self-similar form as the classical Nusselt solution [48], namely:

$$u = 3\bar{u}\left(\xi - 1/2\xi^2\right), \quad v = 3\bar{v}\left(\xi - 1/2\xi^2\right), \tag{28}$$

where $\xi = (z-s)/h$. The validity and robustness of this assumption is established in Section 4, even for flow over deep topographic features, by comparison with complementary experimentally measured and numerically predicted free-surface disturbances.

Using relations (28) and equation (18) leads to the following analytical expressions for the friction and dispersion terms:

$$\frac{\partial u}{\partial z}|_{z=s} = \frac{3\bar{u}}{h}, \tag{29}$$

$$\frac{\partial v}{\partial z}|_{z=s} = \frac{3\bar{v}}{h}, \tag{30}$$

$$\frac{\partial}{\partial x}\int_s^f (\bar{u}-u)^2\,dz + \frac{\partial}{\partial y}\int_s^f (\bar{u}-u)(\bar{v}-v)\,dz = \frac{1}{5}\left(h\bar{u}\frac{\partial \bar{u}}{\partial x} + h\bar{v}\frac{\partial \bar{u}}{\partial y} - \bar{u}\frac{\partial h}{\partial t}\right), \tag{31}$$

$$\frac{\partial}{\partial x}\int_s^f (\bar{u}-u)(\bar{v}-v)\,dz + \frac{\partial}{\partial y}\int_s^f (\bar{v}-v)^2\,dz = \frac{1}{5}\left(h\bar{u}\frac{\partial \bar{v}}{\partial x} + h\bar{v}\frac{\partial \bar{v}}{\partial y} - \bar{v}\frac{\partial h}{\partial t}\right). \tag{32}$$

Note too, that the above forms for the friction and dispersion terms ensure that the DAF of the governing equations reduces to the familiar lubrication equations [8] when $\mathrm{Re} = 0$.

2.3 Topography Definition

Attention is restricted to flows involving simple, well-defined topography, such as one-dimensional (spanwise) trench, peak, step-up, and step-down features, and in two-dimensions (localised) rectangular trenches and peaks. Note, however, that the DAF can be readily applied to flows over much more complex topographies - see for example [51].

Since the topography profile appears as a function in the governing equations, it is not possible to consider completely sharp features. Following previous authors [13, 23, 27], the topography is therefore specified via arctangent functions; for example, a rectangular trench (peak) is defined as follows:

$$\begin{aligned} s(x^*, y^*) = {} & \frac{s_0}{4\tan^{-1}\frac{l_t}{2\delta}\tan^{-1}\frac{w_t}{2\delta}}\left[\tan^{-1}\left(\frac{x^*+l_t/2}{\delta}\right) - \tan^{-1}\left(\frac{x^*-l_t/2}{\delta}\right)\right] \\ & \times\left[\tan^{-1}\left(\frac{y^*+w_t/2}{\delta}\right) - \tan^{-1}\left(\frac{y^*-w_t/2}{\delta}\right)\right], \end{aligned} \tag{33}$$

where s_0 is the dimensionless depth ($s_0 < 0$) or height ($s_0 > 0$), with l_t, w_t and δ the non-dimensional streamwise length, spanwise width and steepness factor, respectively. The coordinate system $(x^*, y^*) = (x - x_t, y - y_t)$ has its origin at the centre of the topography, (x_t, y_t).

3 Method of Solution

3.1 Spatial Discretisation

Equations (23) to (25), incorporating expressions (29) to (32), are solved, subject to boundary conditions (26) and (27), on a rectangular computational domain, $(x, y) \in \Omega = (0, l_p) \times (0, w_p)$, subdivided using a regular spatially staggered mesh arrangement of cells having sides of length Δx and width Δy. The unknown variables, film thickness, h, and the velocity components, $\bar{u}$, $\bar{v}$, are located at cell centres, (i, j), and cell faces, $(i + 1/2, j)$, $(i, j + 1/2)$, respectively. The use of a staggered mesh arrangement avoids the well known checkerboard instability [54] that results if central differencing is applied to first-order pressure term derivatives and to the terms in the continuity equation when pressure and velocity components are collocated. Solving the momentum equations (23) and (24) at cell faces with the convection and time derivative terms grouped together to simplify their numerical treatment following the inclusion of the friction and dispersion terms, the continuity equation (25) at cell centres, and omitting for the sake of convenience the overbar denoting velocity averaging, results in the following second-order accurate discretisation scheme:

$$\varepsilon \mathrm{Re}\left(\frac{\partial u}{\partial t} - \frac{u}{5h}\frac{\partial h}{\partial t} + \frac{6}{5}F[u]\right)|_{i+1/2,j} - \frac{\varepsilon^3}{\mathrm{Ca}}\left(\frac{f_{i+1,j+1} - 2f_{i+1,j} + f_{i+1,j-1} - f_{i,j+1} + 2f_{i,j} - f_{i,j-1}}{\Delta x \Delta y^2}\right.$$
$$\left. + \frac{f_{i+2,j} - 3f_{i+1,j} + 3f_{i,j} - f_{i-1,j}}{\Delta x^3}\right) + 2\varepsilon \cot\theta \frac{f_{i+1,j} - f_{i,j}}{\Delta x} + \frac{3u_{i+1/2,j}}{h^2_{i+1/2,j}} - 2 = 0, \quad (34)$$

$$\varepsilon \mathrm{Re}\left(\frac{\partial v}{\partial t} - \frac{v}{5h}\frac{\partial h}{\partial t} + \frac{6}{5}F[v]\right)|_{i,j+1/2} - \frac{\varepsilon^3}{\mathrm{Ca}}\left(\frac{f_{i+1,j+1} - 2f_{i,j+1} + f_{i-1,j+1} - f_{i+1,j} + 2f_{i,j} - f_{i-1,j}}{\Delta x^2 \Delta y}\right.$$
$$\left. + \frac{f_{i,j+2} - 3f_{i,j+1} + 3f_{i,j} - f_{i,j-1}}{\Delta y^3}\right) + 2\varepsilon \cot\theta \frac{f_{i,j+1} - f_{i,j}}{\Delta y} + \frac{3v_{i,j+1/2}}{h^2_{i,j+1/2}} = 0, \quad (35)$$

$$\frac{\partial h}{\partial t}|_{i,j} + \frac{h_{i+1/2,j}u_{i+1/2,j} - h_{i-1/2,j}u_{i-1/2,j}}{\Delta x} + \frac{h_{i,j+1/2}v_{i,j+1/2} - h_{i,j-1/2}v_{i,j-1/2}}{\Delta y} = 0, \quad (36)$$

where $F[\omega] = u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y}$ is the convective operator and the following terms are interpolated from neighbouring nodes: $h_{i\pm1/2,j} = (h_{i\pm1,j} + h_{i,j})/2$, $h_{i,j\pm1/2} = (h_{i,j\pm1} + h_{i,j})/2$.

In the above discrete DAF analogue, as is the case for all convection-diffusion problems, proper numerical treatment of the convection terms is very important [52, 53]. The mesh Péclet number, Pe, stability condition (see [54], for example), defined as the ratio of the convection to friction term in the momentum equation, is given by:

$$\mathrm{Pe} = \frac{2\varepsilon \mathrm{Re} h^2 \max(u, v)}{5\min(\Delta x, \Delta y)} \leq 2 \Rightarrow \mathrm{Re} \leq \mathrm{Re}_{cr} = \frac{15\min(\Delta x, \Delta y)}{2\varepsilon}. \quad (37)$$

For typical mesh spacings of $\Delta x = \Delta y = 0.05$ and with $\varepsilon = 0.1$ the value of the critical Reynolds number, Re_{cr}, is small and equal to 3.75, illustrating the restrictiveness of this constraint apropos the accurate solution of the thin film flows of interest. To alleviate this restriction the convective operator $F[\omega]$ is discretized using a second-order accurate total variation diminishing (TVD) scheme [55]. As such, the first term of the convective operator, $u\partial_x\omega$, takes the form:

$$\frac{\partial \omega}{\partial x}|_{i,j} = \frac{u^+_{i,j}}{4\Delta x}\left\{(\omega_{i,j} - \omega_{i-1,j})\left[2 + \psi\left(\frac{\omega_{i+1,j} - \omega_{i,j}}{\omega_{i,j} - \omega_{i-1,j}}\right)\right] - (\omega_{i-1,j} - \omega_{i-2,j})\,\psi\left(\frac{\omega_{i,j} - \omega_{i-1,j}}{\omega_{i-1,j} - \omega_{i-2,j}}\right)\right\}$$
$$+ \frac{u^-_{i,j}}{4\Delta x}\left\{(\omega_{i+1,j} - \omega_{i,j})\left[2 + \psi\left(\frac{\omega_{i,j} - \omega_{i-1,j}}{\omega_{i+1,j} - \omega_{i,j}}\right)\right] - (\omega_{i+2,j} - \omega_{i+1,j})\,\psi\left(\frac{\omega_{i+1,j} - \omega_{i,j}}{\omega_{i+2,j} - \omega_{i+1,j}}\right)\right\}, \quad (38)$$

where $u_{i,j}^{+} = u_{i,j} + |u_{i,j}|$, $u_{i,j}^{-} = u_{i,j} - |u_{i,j}|$, and $\psi(\eta) = (\eta^2 + \eta)/(\eta^2 + 1)$ is the well known van Albada flux limiter [54]; the second term in $F[\omega]$ is expressed similarly. The formulation is easily shifted to the appropriate staggered grid location to obtain $F[u]_{i+1/2,j}$ or $F[v]_{i,j+1/2}$ with the following terms interpolated from neighbouring nodes:

$$u_{i,j+1/2} = \left(u_{i-1/2,j} + u_{i+1/2,j} + u_{i-1/2,j+1} + u_{i+1/2,j+1}\right)/4, \tag{39}$$

$$v_{i+1/2,j} = \left(v_{i,j-1/2} + v_{i,j+1/2} + v_{i+1,j-1/2} + v_{i+1,j+1/2}\right)/4. \tag{40}$$

To simplify the description of the calculation procedure presented below, it is convenient to separate the leading temporal u, v and h terms from the discretized u-momentum, v-momentum and continuity operators and to express them as functions $\mathcal{M}^u_{i+1/2,j}$, $\mathcal{M}^v_{i,j+1/2}$ and $\mathcal{M}^h_{i,j}$, respectively, enabling equations (34) to (36) to be rewritten as:

$$\varepsilon \mathrm{Re}\frac{\partial u}{\partial t}|_{i+1/2,j} + \mathcal{M}^u_{i+1/2,j}(u,v,h) = 0, \tag{41}$$

$$\varepsilon \mathrm{Re}\frac{\partial v}{\partial t}|_{i,j+1/2} + \mathcal{M}^v_{i,j+1/2}(u,v,h) = 0, \tag{42}$$

$$\frac{\partial h}{\partial t}|_{i,j} + \mathcal{M}^h_{i,j}(u,v,h) = 0, \tag{43}$$

where the time derivatives of h in momentum equations (34) and (35) are expressed through the continuity operator and included in the momentum operators of equations (41) and (42), respectively. Locations of the independent variables (u, v, h) for the operators $\mathcal{M}^u_{i+1/2,j}$, $\mathcal{M}^v_{i,j+1/2}$ and $\mathcal{M}^h_{i,j}$ are shown in Figure 2.

Clearly, when $\mathrm{Re} = 0$ the solution procedure simplifies considerably since the terms containing time derivatives on the left hand side of the momentum equations (41) and (42) disappear.

3.2 Temporal Discretisation

The automatic adaptive time-stepping procedure adopted employs an estimate of the local truncation error (LTE) obtained from the difference between an explicit predictor stage and the current solution stage to optimise the size of time steps and minimise computational waste.

Using equations (41) to (43), the predicted (Pr) solution is first determined at the predictor stage, which is fully explicit and second-order accurate in time, allowing the anticipated values for u, v and h to be obtained by solving:

$$u^{n+1,Pr}_{i+1/2,j} = \gamma^2 u^{n-1}_{i+1/2,j} + \left(1-\gamma^2\right) u^n_{i+1/2,j} - \frac{\Delta t^{n+1}}{\varepsilon \mathrm{Re}}(1+\gamma)\mathcal{M}^u_{i+1/2,j}(u^n, v^n, h^n), \tag{44}$$

$$v^{n+1,Pr}_{i,j+1/2} = \gamma^2 v^{n-1}_{i,j+1/2} + \left(1-\gamma^2\right) v^n_{i,j+1/2} - \frac{\Delta t^{n+1}}{\varepsilon \mathrm{Re}}(1+\gamma)\mathcal{M}^v_{i,j+1/2}(u^n, v^n, h^n), \tag{45}$$

$$h^{n+1,Pr}_{i,j} = \gamma^2 h^{n-1}_{i,j} + \left(1-\gamma^2\right) h^n_{i,j} - \Delta t^{n+1}(1+\gamma)\mathcal{M}^h_{i,j}(u^n, v^n, h^n), \tag{46}$$

where n and $n+1$ denote values at the end of the nth and $(n+1)$st time steps, $t = t^n$ and $t = t^{n+1}$ respectively, and $\gamma = \Delta t^{n+1}/\Delta t^n = (t^{n+1} - t^n)/(t^n - t^{n-1})$.

Adaptive time-stepping is performed by keeping the LTE for u within a specified tolerance that in practice automatically restricts the LTE for v and h and provides a means of increasing the time step in a controlled manner. The LTE for u at the predictor stage can be expressed via a Taylor series expansion of equation (44) in the form:

$$(\mathrm{LTE})^{Pr}_{i+1/2,j} = \frac{(\Delta t^{n+1})\Delta t^n(1+\gamma)}{6}\frac{\partial^3 u}{\partial t^3}|_{i+1/2,j,t=t_p}, \tag{47}$$

with the third-order time derivative term evaluated at time $t_p \in (t^n, t^{n+1})$.

An implicit β-method [55] is used to advance the solution in time:

$$\begin{aligned}
u^{n+1}_{i+1/2,j} &+ \frac{\beta \Delta t^{n+1}}{\varepsilon \mathrm{Re}} \mathcal{M}^u_{i+1/2,j}\left(u^{n+1}, v^{n+1}, h^{n+1}\right) \\
&= u^n_{i+1/2,j} + \frac{(\beta - 1)\,\Delta t^{n+1}}{\varepsilon \mathrm{Re}} \mathcal{M}^u_{i+1/2,j}\left(u^n, v^n, h^n\right), \qquad (48)\\
v^{n+1}_{i,j+1/2} &+ \frac{\beta \Delta t^{n+1}}{\varepsilon \mathrm{Re}} \mathcal{M}^v_{i,j+1/2}\left(u^{n+1}, v^{n+1}, h^{n+1}\right) \\
&= v^n_{i,j+1/2} + \frac{(\beta - 1)\,\Delta t^{n+1}}{\varepsilon \mathrm{Re}} \mathcal{M}^v_{i,j+1/2}\left(u^n, v^n, h^n\right), \qquad (49)\\
h^{n+1}_{i,j} &+ \beta \Delta t^{n+1} \mathcal{M}^h_{i,j}\left(u^{n+1}, v^{n+1}, h^{n+1}\right) \\
&= h^n_{i,j} + (\beta - 1)\,\Delta t^{n+1} \mathcal{M}^h_{i,j}\left(u^n, v^n, h^n\right). \qquad (50)
\end{aligned}$$

Note that for $\beta = 1/2$ the method reduces to the second order accurate in time, but conditionally stable Crank-Nicolson scheme, whereas $\beta = 1$ leads to the fully implicit first order accurate in time unconditionally stable Laasonen method.

Similarly, the LTE for u at the solution stage is given by a Taylor series expansion of equation (48):

$$(\mathrm{LTE})_{i+1/2,j} = -\frac{(\Delta t^{n+1})^3}{12} \frac{\partial^3 u}{\partial t^3}|_{i+1/2,j,t=t_s}, \quad t_s \in (t^n, t^{n+1}). \qquad (51)$$

As described in [56], the assumption that the third order derivative term varies by only a small amount over the time step enables the LTE to be estimated as:

$$(\mathrm{LTE})_{i+1/2,j} = \frac{u^{n+1}_{i+1/2,j} - u^{n+1,Pr}_{i+1/2,j}}{1 + 2[(1+\gamma)/\gamma]}\ , \qquad (52)$$

which, following [57], is used to obtain an estimate of the overall truncation error by finding its Euclidean norm that, in turn, is used to specify the next time step Δt^{n+2} via:

$$\Delta t^{n+2} = 0.9 \Delta t^{n+1} \left(\frac{\mathrm{TOL}}{||\mathrm{LTE}||} \right)^{1/3}, \qquad (53)$$

if $||\mathrm{LTE}|| \leq \mathrm{TOL}$. The iteration is restarted with half the current time step if $||\mathrm{LTE}|| > \mathrm{TOL}$, where TOL is a user prescribed tolerance.

3.3 Multigrid Solver

At the solution stage of the temporal discretisation, the system of the equations (48) to (50) is solved using a multigrid formulation that enables a system with N unknowns to be solved in only $O\,(\mathrm{N})$ operations. The basis of this approach, as described in several comprehensive texts – see for example [54], exploits the convergence rates of iterative solvers, such as Gauss-Seidel or Jacobi smoothers, to effectively reduce local (high-frequency) errors present in the solution on a particular computational grid, while global (low-frequency) errors are reduced by employing a hierarchy of successively finer grids, $G^0, \ldots, G^k, \ldots, G^K$, where G^0 denotes the coarsest and G^K the finest grid level.

For a specified number of cells on the coarsest grid G^0, n^0_x and n^0_y in the x and y directions respectively, the number of cells on an arbitrary grid G^k say, is $n^k_x = n^0_x 2^k$, $n^k_y = n^0_y 2^k$. This results in grid spacings on G^k of $\Delta x^k = l_p/n_x^k = \Delta x^0 2^{-k}$, $\Delta y^k = w_p/n_y^k = \Delta y^0 2^{-k}$, where $\Delta x^0 = l_p/n_x^0$ and $\Delta y^0 = w_p/n_y^0$ are the grid spacings on G^0.

To simplify the explanation and the steps taken in the multigrid process, the system of discrete equations (48) to (50) is rewritten in the following way:

$$\mathcal{N}^u_{i+1/2,j}\left(u^{n+1}, v^{n+1}, h^{n+1}\right) = \mathcal{F}^u_{i+1/2,j}\left(u^n, v^n, h^n\right), \tag{54}$$

$$\mathcal{N}^v_{i,j+1/2}\left(u^{n+1}, v^{n+1}, h^{n+1}\right) = \mathcal{F}^v_{i,j+1/2}\left(u^n, v^n, h^n\right), \tag{55}$$

$$\mathcal{N}^h_{i,j}\left(u^{n+1}, v^{n+1}, h^{n+1}\right) = \mathcal{F}^h_{i,j}\left(u^n, v^n, h^n\right), \tag{56}$$

where $\mathcal{N}^u_{i+1/2,j}$, $\mathcal{N}^v_{i,j+1/2}$ and $\mathcal{N}^h_{i,j}$ are the time-dependent nonlinear operators and $\mathcal{F}^u_{i+1/2,j}$, $\mathcal{F}^v_{i,j+1/2}$ and $\mathcal{F}^h_{i,j}$ are the right-hand side functions that are defined by the solution on the previous time step.

In the present work a combination of the Full Approximation Storage (FAS) and full multigrid (FMG) technique is employed. The main advantage of the FMG technique is based on the fact that an initial guess (Gs) for the multigrid solver on each grid $k \in [1, K]$ is provided by FMG interpolation of the solution (Sl) from the coarser grid $k-1$ (see Figure 3) using bilinear interpolation operators on a staggered grid system $I^u_{k-1\to k}$, $I^v_{k-1\to k}$, $I^h_{k-1\to k}$ (see Appendix A):

$$u_k^{Gs} = I^u_{k-1\to k}\left(u^{Sl}_{k-1}\right), \quad v_k^{Gs} = I^u_{k-1\to k}\left(v^{Sl}_{k-1}\right), \quad h_k^{Gs} = I^h_{k-1\to k}\left(h^{Sl}_{k-1}\right), \tag{57}$$

where, for the sake of simplicity, the coordinate and time indices have been omitted.

The solution process consists of performing a fixed number of FAS V-cycles on intermediate grid levels $k \in [1, K-1]$ (usually 1 to 3 V-cycles) and up to 10 V-cycles on the finest grid level K (that is, sufficient V-cycles are executed until the residuals have been reduced to a specified tolerance). The structure of a single FAS multigrid V-cycle on an arbitrary grid level k may be described in the same pseudo-code formalism as in [12]:

$$\left(u_k^{Sl}, v_k^{Sl}, h_k^{Sl}\right) = \text{FASCYC}\left(k, u_k^{Gs}, v_k^{Gs}, h_k^{Gs}, \mathcal{F}^u_k, \mathcal{F}^v_k, \mathcal{F}^h_k, \nu_{pre}, \nu_{post}\right), \tag{58}$$

where ν_{pre} and ν_{post} are number of pre- and post-relaxations of the multigrid cycle (usually $\nu_{pre} = \nu_{post} = 2$).

1. Pre-smoothing stage

- Apply the relaxation scheme (see next subsection) ν_{pre} times to obtain first corrected appproximation (Rl):

$$\left(u_k^{Rl}, v_k^{Rl}, h_k^{Rl}\right) = \text{RELAX}^{\nu_{pre}}\left(u_k^{Gs}, v_k^{Gs}, h_k^{Gs}, \mathcal{F}^u_k, \mathcal{F}^v_k, \mathcal{F}^h_k\right), \tag{59}$$

2. Coarse-grid correction stage

- Compute the defects:

$$d^u_k = \mathcal{F}^u_k - \mathcal{N}^u_k\left(u_k^{Rl}, v_k^{Rl}, h_k^{Rl}\right), \quad d^v_k = \mathcal{F}^v_k - \mathcal{N}^v_k\left(u_k^{Rl}, v_k^{Rl}, h_k^{Rl}\right), \quad d^h_k = \mathcal{F}^h_k - \mathcal{N}^h_k\left(u_k^{Rl}, v_k^{Rl}, h_k^{Rl}\right), \tag{60}$$

- Restrict the defects to the next coarser grid level using full-weighting restriction operators for staggered grids $R^u_{k\to k-1}$, $R^v_{k\to k-1}$, $R^h_{k\to k-1}$ (see Appendix A):

$$d^u_{k-1} = R^u_{k\to k-1}\left(d^u_k\right), \quad d^v_{k-1} = R^v_{k\to k-1}\left(d^v_k\right), \quad d^h_{k-1} = R^h_{k\to k-1}\left(d^h_k\right), \tag{61}$$

- Restrict the solution to get the initial guess for the next coarser grid level:

$$u_{k-1}^{Gs} = R_{k\to k-1}^{u}\left(u_k^{Rl}\right), \quad v_{k-1}^{Gs} = R_{k\to k-1}^{v}\left(v_k^{Rl}\right), \quad h_{k-1}^{Gs} = R_{k\to k-1}^{h}\left(h_k^{Rl}\right), \tag{62}$$

- Compute the right-hand side on the next coarser grid level:

$$\mathcal{F}_{k-1}^{u} = d_{k-1}^{u} + \mathcal{N}_{k-1}^{u}\left(u_{k-1}^{Gs}, v_{k-1}^{Gs}, h_{k-1}^{Gs}\right), \quad \mathcal{F}_{k-1}^{v} = d_{k-1}^{v} + \mathcal{N}_{k-1}^{v}\left(u_{k-1}^{Gs}, v_{k-1}^{Gs}, h_{k-1}^{Gs}\right),$$

$$\mathcal{F}_{k-1}^{h} = d_{k-1}^{h} + \mathcal{N}_{k-1}^{h}\left(u_{k-1}^{Gs}, v_{k-1}^{Gs}, h_{k-1}^{Gs}\right), \tag{63}$$

If $k = 0$ a coarsest grid solver is employed (equations (54) to (56) can be solved directly or, as is the case here, using relaxation – see section 3.4). If $k > 0$ the FAS cycle is used to update the next $k-1$ coarser grid solution:

$$\left(u_{k-1}^{Sl}, v_{k-1}^{Sl}, h_{k-1}^{Sl}\right) = \text{FASCYC}\left(k-1, u_{k-1}^{Gs}, v_{k-1}^{Gs}, u_{k-1}^{Gs}, \mathcal{F}_{k-1}^{u}, \mathcal{F}_{k-1}^{v}, \mathcal{F}_{k-1}^{h}, \nu_{pre}, \nu_{post}\right), \tag{64}$$

- Compute the corrections:

$$e_{k-1}^{u} = u_{k-1}^{Sl} - u_{k-1}^{Gs}, \quad e_{k-1}^{v} = v_{k-1}^{Sl} - v_{k-1}^{Gs}, \quad e_{k-1}^{h} = h_{k-1}^{Sl} - h_{k-1}^{Gs}, \tag{65}$$

- Interpolate the corrections on the fine grid level using bilinear interpolation operators for staggered grids $I_{k-1\to k}^{u}, I_{k-1\to k}^{v}, I_{k-1\to k}^{h}$ (see Appendix A):

$$e_k^{u} = I_{k-1\to k}^{u}\left(e_{k-1}^{u}\right), \quad e_k^{v} = I_{k-1\to k}^{v}\left(e_{k-1}^{v}\right), \quad e_k^{h} = I_{k-1\to k}^{h}\left(e_{k-1}^{h}\right), \tag{66}$$

- Compute the second corrected approximation (Cr):

$$u_k^{Cr} = u_k^{Rl} + e_k^{u}, \quad v_k^{Cr} = v_k^{Rl} + e_k^{v}, \quad h_k^{Cr} = h_k^{Rl} + e_k^{h}, \tag{67}$$

3. Post-smoothing stage

- Apply the relaxation scheme ν_{post} times to get the final solution (Sl):

$$\left(u_k^{Sl}, v_k^{Sl}, h_k^{Sl}\right) = \text{RELAX}^{\nu_{post}}\left(u_k^{Cr}, v_k^{Cr}, h_k^{Cr}, \mathcal{F}_k^{u}, \mathcal{F}_k^{v}, \mathcal{F}_k^{h}\right). \tag{68}$$

3.4 Relaxation Methodology

Due to the staggered nature of the discretisation involved, the relaxation methodology employs a lexicographic box smoothing Gauss-Seidel scheme [54] to define a collective local relaxation which encompasses the associated variables u, v and h; this efficiently retains the diagonal dominance of the relaxation scheme. The set of algebraic equations (54) to (56) is written in a linearised form using the Newton-Raphson method. On each cell, see Figure 2, five coupled equations (two each from the u-momentum and v-momentum equations and one from the continuity equation, given in Appendix B) are solved for the unknown increments $\Delta u_{i+1/2,j}$, $\Delta u_{i-1/2,j}$, $\Delta v_{i,j+1/2}$, $\Delta v_{i,j-1/2}$, $\Delta h_{i,j}$ with the new approximations given by:

$$\begin{aligned} \tilde{u}_{i+1/2,j} &= u_{i+1/2,j} + \Delta u_{i+1/2,j}, \\ \tilde{u}_{i-1/2,j} &= u_{i-1/2,j} + \Delta u_{i-1/2,j}, \\ \tilde{v}_{i,j+1/2} &= v_{i,j+1/2} + \Delta v_{i,j+1/2}, \\ \tilde{v}_{i,j-1/2} &= v_{i,j-1/2} + \Delta v_{i,j-1/2}, \\ \tilde{h}_{i,j} &= h_{i,j} + \Delta h_{i,j}, \end{aligned} \tag{69}$$

updated simultaneously; and where each velocity component is updated twice, while the film thickness is updated only once per relaxation sweep. Dirichlet boundary conditions are assigned as exact values at the boundary points, whereas Neumann boundary conditions are implemented by employing ghost nodes at the edge of the computational domain.

4 Results

All of the steady-state results generated were obtained using the implicit time-stepping scheme described above, with $\beta = 3/4$, starting with the initial condition of a flat free-surface ($h = 1-s$) and velocity profile $u = \frac{2}{3}h^2$, $v = 0$ (commensurate with Re = 0). Solutions were obtained on a computational domain with $l_p = w_p = 100$, chosen to be large enough to ensure fully developed flow both upstream and downstream of the topography and of sufficient width to negate edge effects. The multigrid algorithm employs a coarsest grid level G^0 with $n_x^0 = n_y^0 = 64$ ($n_x^0 = 64$ in one-dimension) and a finest grid level G^4 with $n_x^4 = n_y^4 = 1024$ (G^5 with $n_x^5 = 2048$ in one-dimension) uniformly spaced cells. At each time step sufficient multigrid V-cycles are performed to reduce residuals on the finest mesh level to below 10^{-6}. Dependence of CPU time for a typical time step as a function of the total number of unknowns for a flow over a localised (two-dimensional) square trench topography is illustrated in Figure 4. A typical value of the time adaptive tolerance used in the computations is TOL $\approx 10^{-3}$. The choice of topography steepness parameter, δ, is also important in ensuring grid independence of solutions and for all types of topographies (one-dimensional trench, step-up, step-down, two-dimensional trench and peak) solutions are found to be independent of δ provided $\delta \leq \delta_{cr} = 10^{-3}$.

In order to facilitate direct comparison with experiment [31], the focus of the ensuing investigation is that of gravity-driven flow of thin water films with fixed fluid properties $\rho = 1000\text{kg}\cdot\text{m}^{-3}$, $\mu = 0.001\text{Pa}\cdot\text{s}$ and $\sigma = 0.07\text{N}\cdot\text{m}^{-1}$. Accordingly, $\theta = 30°$ unless stated otherwise, with spanwise topography located with its centre at $x_t = 50$ and localised topography shifted upstream slightly and centred on $(x_t, y_t) = (30.77, 50)$. Consequently, for specified values of θ and Re the other parameters appearing in the calculation can be easily derived in terms of them and the fixed fluid properties; for example, H_0 and Ca, can be written as:

$$H_0 = \left(\frac{2\mu^2}{\rho^2 g_0}\right)^{1/3}\left(\frac{\text{Re}}{\sin\theta}\right)^{1/3}, \quad \text{Ca} = \left(\frac{g_0\mu^4}{2\rho\sigma^3}\right)^{1/3}\left(\text{Re}^2\sin\theta\right)^{1/3}. \tag{70}$$

Two sets of results are presented, for the parameter values shown in Table 1. In the first set, DAF predictions are compared with experimental data and lubrication predictions [14] and the accuracy of the DAF method is assessed. In the second set, the influence of varying inertia, Re, and/or inclination angle, θ, is investigated for flow over a topography of fixed physical dimensions, with the result that both the asymptotic film thickness and capillary length vary; also explored is the effect of topography aspect ratio on the free-surface disturbance when $\theta = 30°$. In these cases, results are presented more clearly in terms of coordinates scaled by the fixed streamwise dimension of the topography: $(x^o, y^o) = (x^*, y^*)/l_t$, while the substrate and free-surface locations are scaled with respect to the fixed height/depth of the topography, namely $s^* = s/s_0$ and $f^* = (f-1)/s_0$, respectively.

4.1 Thin film flow over spanwise topography

Two-dimensional flow over spanwise (one-dimensional) topography is considered first. The accuracy of the DAF predictions is quantified by comparison with experimental data [31] and accurate finite element solutions of the full Navier-Stokes (N-S) problem – see [58] for a description of the methodology involved. Figure 5 shows the effect of Re on the streamwise free-surface profile for the flow of a thin water film over a spanwise trench topography of width L_t =1.2mm and depth $S_0 = 20\mu$m. Figures 5(a) and 5(b) show the evolution of the solution towards steady state for (a) Re = 5 and (b) Re = 15. Such solutions are obtained in a matter of minutes, with higher Reynolds number flows taking longer to reach a steady-state due to the increased inherent non-linearity. Figure 5(c) demonstrates the influence of inertia on the free-surface profile, showing predictions for the cases Re = 5, 15 and 30, corresponding to H_0 = 126.8, 182.9 and 230.5 μm, respectively. They reveal that increasing Re leads to amplification and widening of both the capillary ridge and the free-surface depression over the trench. Note also the exacerbated free-surface disturbance upstream of the capillary ridge with increasing Re.

Figure 6 compares steady-state free-surface profiles obtained using the DAF and corresponding FE solutions for the experimental cases considered by Decre & Baret [31]. Figures 6(a) and 6(b) consider flow of a thin water film, with Re = 2.45, over spanwise step-up and step-down topographies respectively of depth/height $|s_0| = 0.2$, while figure 6(c) considers flow with Re = 2.84 over a spanwise trench of depth $s_0 = 0.19$ and width l_t=1.51. In all three cases, the DAF and FE predictions are indistinguishable from each other, while the agreement with their experimentally measured counterparts is excellent as exemplified in the blown-up insert of Figure 6(c) showing the free-surface shape across and upstream of the capillary ridge. Indeed the r.m.s. error between the predicted DAF and experimentally obtained free-surface profiles is approximately 1.5% for all three spanwise topographies, which lies well within the reported experimental accuracy of 2% [31].

A wider range of parameter space is now considered by retaining the same fluid properties as used by [31], i.e. those of water, while changing Re, H_0 and Ca according to equation (70). Figures 7 and 8 show the effect of increasing inertia and/or topography amplitude on the free surface profiles for flow over step-up and step-down topography, respectively, for cases with Re = 15 and Re = 30 and $|s_0| = 0.2$ and $|s_0| = 1.0$. The corresponding predictions from lubrication theory [14] are also given for comparison purposes. These show that increasing inertia results in a widening and amplification of the free-surface disturbance, leading to larger free-surface depressions and capillary ridges upstream of the step-up and step-down topography respectively. It is evident that: (i) the DAF and FE predictions are in close agreement; (ii) lubrication theory, although capturing the essential features, significantly under predicts the associated capillary ridges and depressions; (iii) the discrepancy between the lubrication predictions and the DAF and FE ones is exacerbated by increasing either Re or $|s_0|$.

These findings are quantified in greater detail in Figure 9, which shows contour plots of the discrepancy between lubrication [14] and DAF predictions and corresponding FE solutions of the full N-S equations. Following [13], the error is quantified by the maximum percentage discrepancy between the lubrication or DAF predictions, measured normal to the N-S profile. This measure is preferred to a r.m.s. error since the latter would be unduly biased by the extensive asymptotic flow regions where all free-surface profiles are indistinguishable. Note that the maximum error occurs close to the peak of the topography, over the steeply sloping section of the free surface, whereas the predicted errors in the vicinity of the free surface depression (step-up) and capillary ridge (step-down) are typically only 25% of these maximum values.

For both sets of contours, the discrepancies associated with the step-down flow become larger once the values of Re and $|s_0|$ become significant. The errors in the lubrication predictions are consistently greater than those obtained with the DAF, being typically 3 times and 1.5 times larger for the step-up and step-down cases, respectively. For example, for the extreme step-up case with Re = 30 and $|s_0| = 1.0$, the DAF error is only 5.5% compared to lubrication theory's 16%, while for a step-down these errors are 12% and 22% respectively.

Although different in magnitude, the upper two discrepancy contours have roughly the same shape suggesting that the source of error for both step-up and step-down configurations is predominately one of the neglect of inertia, consistent with the basis of lubrication theory. The lower discrepancy contours paint a different picture; the step-up ones being much steeper but lower in magnitude than the step-down ones (which are consistent in shape and form, though not magnitude, with their lubrication counterpart) suggesting that for the former the relative step height is the more dominate cause of discrepancy.

The source of the greater discrepancy associated with the step-down can be traced to the underlying flow structure as Re and $|s_0|$ are increased. Under Stokes flow, Re = 0 conditions the eddy structure associated with an equivalent step-up and step-down would be mirror images of each other. Figures 10 and 11 show that increasing Re slowly *reduces* the lateral extent of the corner eddy which is present in the case of a step-up; whereas for the step-down it results in a more rapid *enlargement* of the size and extent of the existing corner eddy. Accordingly, it is arguably the neglect of vertical velocity terms of the $O(\varepsilon^2)$ and the use of the classical Nusselt solution in determining the friction and dispersion terms in regions of the flow where a large eddy exists that leads to greater discrepancy. That said, except for extreme values of Re and $|s_0|$ over the range considered, the free-surface profiles obtained via the DAF and from FE solutions of the full N-S equations are comparable and encouragingly good.

4.2 Thin film flow over localised topography

The DAF is now used to predict the effect of inertia on three-dimensional thin film flow over localised (two-dimensional) topography based on the square trench used by [31] with $L_t = W_t = 1.2mm$ and $|S_0| = 25\mu m$. For a topography of this depth and the Re range considered ($|s_0| = 0.197$ for Re = 5 and $|s_0| = 0.092$ for Re = 50), according to Figure 9 the maximum discrepancy in the predicted free-surface profiles is expected to be of the order of 1% only.

Figure 12 shows the effect of Re on the three-dimensional free-surface disturbance caused by this square trench. Each case exhibits a characteristic 'horseshoe'-shaped 'bow-wave', free-surface depression over the trench, a downstream peak or 'surge' caused by the fact that, for three-dimensional flow, liquid exits the trench across a narrower length than across which it enters [13], and 'comet-tail'. Note that no such 'surge' mechanism exists for two-dimensional flow over a completely spanwise trench, which explains the lack of a downstream surge in the profiles given in Figures 5(c) and 6(c). Increasing inertia causes a gradual amplification and widening of the free surface disturbance and reduction in the extent of the 'comet-tail'. These effects are seen more clearly in Figure 13 which gives the corresponding streamwise and spanwise free-surface profiles through the centre of the topography. Figure 13(a) shows that increasing Re from 5 to 50 more than doubles the magnitude of the capillary ridge ($f^* = 0.015$ compared with $f^* = 0.037$) and roughly trebles the size of the downstream surge ($f^* = 0.023$ compared to $f^* = 0.067$).

The effect of inertia on the downstream surge can be explored in more detail as follows. For small Re, fluid enters the trench across its upstream side and both spanwise sides due to lateral pressure gradients resulting from the spanwise curvature of the free-surface. Since the flow is steady, fluid entering the trench must leave it on the downstream side. As the Re is increased the downstream surge becomes more focused; by the time Re = 50 it creates a free-surface disturbance larger than that of the downstream capillary ridge, Figure 13(a); in addition it is positioned further upstream. A plausible explanation for what is observed is that increasing inertia gradually overcomes the lateral pressure gradients causing the flow to become essentially streamwise; in which case fluid enters and exits the trench topography principally across its upstream and downstream sides respectively, and only fractionally if at all via its spanwise sides.

Figures 14 and 15 analyse how inertia affects the transition to two-dimensional, spanwise flow as the trench width in the spanwise direction, W_t, is increased for fixed L_t=1.2mm. The free-surface profiles given in Figure 14, viewed from the downstream side, show that increasing trench aspect ratio $A = W_t/L_t$, causes the bow wave to broaden while increasing Re leads to larger free-surface disturbances that are more sharply focussed around the streamwise centreline. For the cases shown, increasing A from 5 to 10 causes the downstream surge to bifurcate into two smaller ones lying either side of the streamwise centreline. The progression to two-dimensional flow can be seen more clearly by the streamwise and spanwise free-surface profiles shown in Figure 15 for Re = 5 and 50 and trench aspect ratio $A = 1$, 5, 10 and ∞ (i.e. spanwise topography). Increasing A from 1 to 5 has a dramatic effect on the free surface depression and on the upstream capillary ridge, while for $A = 10$ the streamwise profiles have much reduced downstream surges. The sharper focus of the Re = 50 flow around the streamwise centreline is shown by the spanwise free-surface profiles in Figure 15(d) and by the fact that a larger aspect ratio is needed for its streamwise profile to approximate that of the two-dimensional case shown in Figure 5. This is reinforced by calculating the difference in the streamwise free-surface profiles obtained for finite A and the case $A \to \infty$ in the same way as the discrepancy contours of Figure 9 were generated. For Re = 5, these are found to be 0.74% and 0.24% for $A = 5$ and $A = 10$, respectively; whereas for Re = 50 they are 0.97% and 0.31%, respectively. This behaviour can be explained in physical terms by noting that the Re = 50 case has larger streamwise inertia and therefore will have less of a tendency than the Re = 5 case to spread across a given trench geometry.

The final figure considers the competing effects of inertia and the normal component of gravity on the free-surface disturbance induced by the square trench topography considered above with $L_t = W_t = 1.2mm$ and $S_0 = 25\mu m$. In the DAF the parameter controlling the relative strength of the gravity component is $\mathrm{N} = \mathrm{Ca}^{1/3} \cot\theta$ and since the fluid properties are fixed, the effect of N is explored via changes to the substrate inclination angle θ. Table 1 summaries the changes to N and $\mathcal{I}$ and the other dependent parameters H_0, L_0, U_0 and Ca. Figure 16 shows that increasing N (by decreasing θ) suppresses all free surface disturbances and reduces considerably the magnitude of the bow wave, downstream surge and free-surface depression over the trench. The streamwise and spanwise free-surface profiles given in Figure 17 show more clearly that the bow wave migrates upstream as N increases, while the downstream surge is more resistant to increasing N and its location remains effectively constant.

5 Conclusions

Inertial thin film flow over various one- and two-dimensional topographies has been investigated by means of solving of a depth-averaged form of the governing unsteady Navier-Stokes equations. Steady-state, mesh independent multigrid solutions of a discrete analogue to this coupled equation set have been generated both efficiently and accurately using adaptive time-stepping, a staggered grid arrangement for the dependent variables and proper treatment of the nonlinear convective terms via a second order accurate TVD scheme in conjunction with a suitable flux limiter.

DAF solutions of the spanwise topographies and flow conditions explored by [31] show very good agreement with their experimentally measured free-surface disturbances and with predictions of the same from corresponding FE solutions of the full Navier-Stokes problem. The flow over step-up and step-down geometries was then explored in more detail in order to quantify the accuracy of the DAF relative to Navier-Stokes calculations for a range of step heights/depths and Reynolds numbers. The discrepancy contours generated reveal that even when the step height/depth is equal to the film thickness, the DAF predicts maximum profile errors of 5.5% and 12% for a step-up and step-down, respectively, when Re = 30. These results are very encouraging when compared with the level of accuracy obtained using lubrication theory relative to Navier-Stokes calculations, which lead to corresponding maximum errors of 16% and 22%, respectively. Furthermore, investigation of the underlying flow structure in the form of streamline plots reveal why the step-down topography leads to a greater maximum error as the step height/depth and Reynolds number becomes significant, compared to the step-up topography.

The exploration of three-dimensional flow is centred on that over a square trench topography as utilised in the experiments of [31]. It is found that the general shape of the predicted free-surface disturbance agrees well with the profile obtained by the latter, while revealing the subtle effects of increasing inertia. Particular attention was given to changes in the characteristic 'horseshoe'-shaped 'bow-wave' and 'comet-tail' free-surface disturbance with inertia and the effect it has on the accompanying downstream surge, a feature that is not present in the flow over spanwise topography. Increasing flow inertia leads to amplification and a sharper focussing of free-surface disturbances in the vicinity of the topography, since streamwise inertia reduces the tendency of disturbances to propagate in the spanwise direction. These findings are consistent with the practical experience that free-surface instabilities arise at critical values of the Reynolds number.

Considered also is the effect of the trench aspect ratio and substrate inclination angle on the resulting free-surface disturbance as the Reynolds number is increased. The results show that despite the tendency of increasing inertia to amplify and focus features of the free-surface disturbance, decreasing the inclination angle, and hence the normal component of gravity, suppresses them, with the downstream surge proving to be more resilient to decreasing inclination angle than the upstream bow-wave. Increasing the trench aspect ratio leads to a broadening of the upstream capillary ridge and an eventual bifurcation of the associated downstream surge; the latter divides to form two decoupled surges and when the aspect ratio is large enough the mid-plane streamwise free-surface profile approaches its one-dimensional (spanwise) equivalent.

Based on the above systematic application of the DAF to the problem of thin film flow over one- and two-dimensional topographies, together with its accurate and efficient numerical solution, it can be considered to represent an important means for investigating a wealth of other important inertial effects in related to the deposition of fluid layers and associated phenomena; for example, free-surface planarization in photolithography and droplet spreading and coalescence [59]. Furthermore, it is a relatively simple task to include additional physics such as evaporation [16] and thermal effects.

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Appendix A

Full weighting restriction operators $R^u_{k\to k-1}$ (for u), $R^v_{k\to k-1}$ (for v), $R^h_{k\to k-1}$ (for h):

$$u^{k-1}_{i+1/2,j} = \frac{1}{32}\left[u^k_{2i-1/2,2j-1} + u^k_{2i-1/2,2j+2} + u^k_{2i+3/2,2j-1} + u^k_{2i+3/2,2j+2} + 2\left(u^k_{2i+1/2,2j-1} + u^k_{2i+1/2,2j+2}\right)\right.$$

$$\left. +3\left(u^k_{2i-1/2,2j} + u^k_{2i+3/2,2j} + u^k_{2i-1/2,2j+1} + u^k_{2i+3/2,2j+1}\right) + 6\left(u^k_{2i+1/2,2j} + u^k_{2i+1/2,2j+1}\right)\right],$$

$$v_{i,j+1/2}^{k-1} = \frac{1}{32}\left[v_{2i-1,2j-1/2}^k + v_{2i+2,2j-1/2}^k + v_{2i-1,2j+3/2}^k + v_{2i+2,2j+3/2}^k + 2\left(v_{2i-1,2j+1/2}^k + v_{2i+2,2j+1/2}^k\right)\right.$$

$$\left.+3\left(v_{2i,2j-1/2}^k + v_{2i,2j+3/2}^k + v_{2i+1,2j-1/2}^k + v_{2i+1,2j+3/2}^k\right) + 6\left(v_{2i,2j+1/2}^k + v_{2i+1,2j+1/2}^k\right)\right], \qquad (71)$$

$$h_{i,j}^{k-1} = \frac{1}{64}\left[h_{2i-1,2j-1}^k + h_{2i-1,2j+2}^k + h_{2i+2,2j-1}^k + h_{2i+2,2j+2}^k + 3\left(h_{2i,2j-1}^k + h_{2i,2j+2}^k\right.\right.$$

$$\left.+h_{2i+1,2j-1}^k + h_{2i+1,2j+2}^k h_{2i-1,2j}^k + h_{2i-1,2j+1}^k + h_{2i+2,2j}^k + h_{2i+2,2j+1}^k\right)$$

$$\left.+9\left(h_{2i,2j}^k + h_{2i+1,2j}^k + h_{2i,2j+1}^k + h_{2i+1,2j+1}^k\right)\right].$$

Bilinear interpolation operators $I_{k-1\to k}^u$ (for u), $I_{k-1\to k}^v$ (for v), $I_{k-1\to k}^h$ (for h):

$$u_{2i+1/2,2j}^k = \frac{1}{4}\left[3u_{i+1/2,j}^{k-1} + u_{i+1/2,j-1}^{k-1}\right],$$

$$u_{2i+3/2,2j}^k = \frac{1}{8}\left[3\left(u_{i+1/2,j}^{k-1} + u_{i+3/2,j}^{k-1}\right) + u_{i+1/2,j-1}^{k-1} + u_{i+3/2,j-1}^{k-1}\right],$$

$$u_{2i+1/2,2j+1}^k = \frac{1}{4}\left[3u_{i+1/2,j}^{k-1} + u_{i+1/2,j+1}^{k-1}\right],$$

$$u_{2i+3/2,2j+1}^k = \frac{1}{8}\left[3\left(u_{i+1/2,j}^{k-1} + u_{i+3/2,j}^{k-1}\right) + u_{i+1/2,j+1}^{k-1} + u_{i+3/2,j+1}^{k-1}\right],$$

$$v_{2i,2j+1/2}^k = \frac{1}{4}\left[3v_{i,j+1/2}^{k-1} + v_{i-1,j+1/2}^{k-1}\right],$$

$$v_{2i+1,2j+1/2}^k = \frac{1}{4}\left[3v_{i,j+1/2}^{k-1} + v_{i+1,j+1/2}^{k-1}\right], \qquad (72)$$

$$v_{2i,2j+3/2}^k = \frac{1}{8}\left[3\left(v_{i,j+1/2}^{k-1} + v_{i,j+3/2}^{k-1}\right) + v_{i-1,j+1/2}^{k-1} + v_{i-1,j+3/2}^{k-1}\right],$$

$$v_{2i+1,2j+3/2}^k = \frac{1}{8}\left[3\left(v_{i,j+1/2}^{k-1} + v_{i,j+3/2}^{k-1}\right) + v_{i+1,j+1/2}^{k-1} + v_{i+1,j+3/2}^{k-1}\right],$$

$$h_{2i,2j}^k = \frac{1}{16}\left[9h_{i,j}^{k-1} + 3\left(h_{i-1,j}^{k-1} + h_{i,j-1}^{k-1}\right) + h_{i-1,j-1}^{k-1}\right],$$

$$h_{2i+1,2j}^k = \frac{1}{16}\left[9h_{i,j}^{k-1} + 3\left(h_{i+1,j}^{k-1} + h_{i,j-1}^{k-1}\right) + h_{i+1,j-1}^{k-1}\right],$$

$$h_{2i,2j+1}^k = \frac{1}{16}\left[9h_{i,j}^{k-1} + 3\left(h_{i-1,j}^{k-1} + h_{i,j+1}^{k-1}\right) + h_{i-1,j+1}^{k-1}\right],$$

$$h_{2i+1,2j+1}^k = \frac{1}{16}\left[9h_{i,j}^{k-1} + 3\left(h_{i+1,j}^{k-1} + h_{i,j+1}^{k-1}\right) + h_{i+1,j+1}^{k-1}\right].$$

Appendix B

Coupled equation set solved for the unknown increments $\Delta u_{i+1/2,j}$, $\Delta u_{i-1/2,j}$, $\Delta v_{i,j+1/2}$, $\Delta v_{i,j-1/2}$, $\Delta h_{i,j}$.

$$
\begin{aligned}
\frac{\partial \mathcal{N}^u_{i+1/2,j}}{\partial u_{i+1/2,j}}\Delta u_{i+1/2,j} + \frac{\partial \mathcal{N}^u_{i+1/2,j}}{\partial u_{i-1/2,j}}\Delta u_{i-1/2,j} + \frac{\partial \mathcal{N}^u_{i+1/2,j}}{\partial v_{i,j+1/2}}\Delta v_{i,j+1/2} & \\
+ \frac{\partial \mathcal{N}^u_{i+1/2,j}}{\partial v_{i,j-1/2}}\Delta v_{i,j-1/2} + \frac{\partial \mathcal{N}^u_{i+1/2,j}}{\partial h_{i,j}}\Delta h_{i,j} &= d^u_{i+1/2,j} \\
\frac{\partial \mathcal{N}^u_{i-1/2,j}}{\partial u_{i+1/2,j}}\Delta u_{i+1/2,j} + \frac{\partial \mathcal{N}^u_{i-1/2,j}}{\partial u_{i-1/2,j}}\Delta u_{i-1/2,j} + \frac{\partial \mathcal{N}^u_{i-1/2,j}}{\partial v_{i,j+1/2}}\Delta v_{i,j+1/2} & \\
+ \frac{\partial \mathcal{N}^u_{i-1/2,j}}{\partial v_{i,j-1/2}}\Delta v_{i,j-1/2} + \frac{\partial \mathcal{N}^u_{i-1/2,j}}{\partial h_{i,j}}\Delta h_{i,j} &= d^u_{i-1/2,j} \\
\frac{\partial \mathcal{N}^v_{i,j+1/2}}{\partial u_{i+1/2,j}}\Delta u_{i+1/2,j} + \frac{\partial \mathcal{N}^v_{i,j+1/2}}{\partial u_{i-1/2,j}}\Delta u_{i-1/2,j} + \frac{\partial \mathcal{N}^v_{i,j+1/2}}{\partial v_{i,j+1/2}}\Delta v_{i,j+1/2} & \\
+ \frac{\partial \mathcal{N}^v_{i,j+1/2}}{\partial v_{i,j-1/2}}\Delta v_{i,j-1/2} + \frac{\partial \mathcal{N}^v_{i,j+1/2}}{\partial h_{i,j}}\Delta h_{i,j} &= d^v_{i,j+1/2} \\
\frac{\partial \mathcal{N}^v_{i,j-1/2}}{\partial u_{i+1/2,j}}\Delta u_{i+1/2,j} + \frac{\partial \mathcal{N}^v_{i,j-1/2}}{\partial u_{i-1/2,j}}\Delta u_{i-1/2,j} + \frac{\partial \mathcal{N}^v_{i,j-1/2}}{\partial v_{i,j+1/2}}\Delta v_{i,j+1/2} & \\
+ \frac{\partial \mathcal{N}^v_{i,j-1/2}}{\partial v_{i,j-1/2}}\Delta v_{i,j-1/2} + \frac{\partial \mathcal{N}^v_{i,j-1/2}}{\partial h_{i,j}}\Delta h_{i,j} &= d^v_{i,j-1/2} \\
\frac{\partial \mathcal{N}^h_{i,j}}{\partial u_{i+1/2,j}}\Delta u_{i+1/2,j} + \frac{\partial \mathcal{N}^h_{i,j}}{\partial u_{i-1/2,j}}\Delta u_{i-1/2,j} + \frac{\partial \mathcal{N}^h_{i,j}}{\partial v_{i,j+1/2}}\Delta v_{i,j+1/2} & \\
+ \frac{\partial \mathcal{N}^h_{i,j}}{\partial v_{i,j-1/2}}\Delta v_{i,j-1/2} + \frac{\partial \mathcal{N}^h_{i,j}}{\partial h_{i,j}}\Delta h_{i,j} &= d^h_{i,j}
\end{aligned}
\qquad (73)
$$

Tables

Table 1: The dependence of different parameters of the thin film flow on inclination angle and Reynolds number. The fluid properties are fixed.

θ,°	Re	$H_0, \mu m$	L_0, mm	$U_0, mm/s$	Ca, 10^{-3}	N	$\mathcal{I}$
30	0.15	39.4	0.572	3.8	0.05	0.07	0.01
30	2.45	100.0	0.781	24.5	0.35	0.12	0.17
30	2.84	105.0	0.794	27.0	0.39	0.13	0.21
30	5	126.8	0.845	39.4	0.56	0.14	0.41
30	15	182.9	0.955	82.0	1.17	0.18	1.58
30	30	230.5	1.032	130.2	1.86	0.21	3.69
30	50	273.3	1.092	183.0	2.61	0.24	6.88
10	5	180.5	1.353	27.7	0.40	0.42	0.37
10	50	388.8	1.747	128.6	1.84	0.69	6.13
5	5	227.0	1.838	22.0	0.31	0.78	0.34
5	50	489.2	2.373	102.2	1.46	1.30	5.67
1	5	388.0	3.754	12.9	0.18	3.25	0.28
1	50	836.0	4.848	59.8	0.85	5.44	4.74

Figures

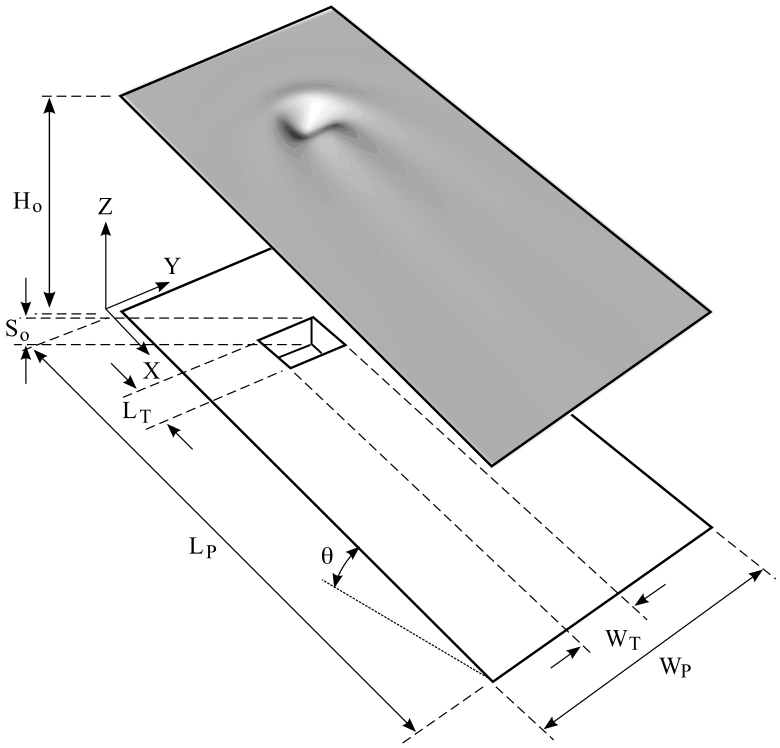

Figure 1: Schematic diagram of gravity-driven flow over a well-defined trench topography, showing the coordinate system adopted and surface geometry.

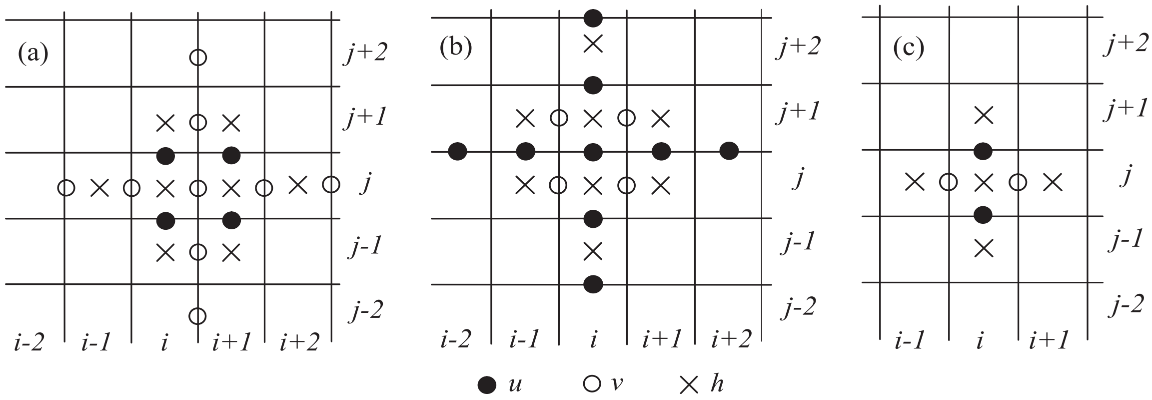

Figure 2: Location of the independent variables for (a) the u-momentum operator $\mathcal{M}^u_{i+1/2,j}$, (b) the v-momentum operator $\mathcal{M}^v_{i,j+1/2}$, (c) the continuity operator $\mathcal{M}^h_{i,j}$ (c). Positions of u, v and h are denoted by open circles, filled circles and crosses, respectively.

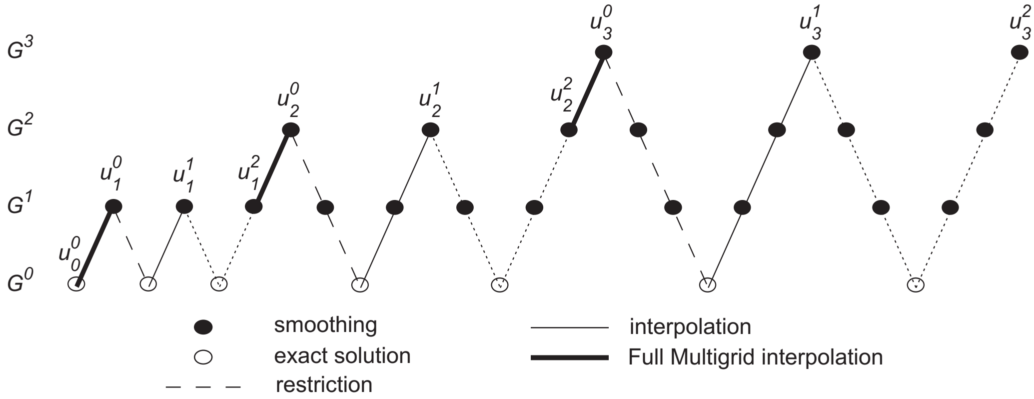

Figure 3: The Full Multigrid structure based, for illustration purposes, on 4 grid levels. u_0^0 is the initial solution on the coarsest grid provided by the predictor stage, u_k^0 is the solution on the $k \in [1,3]$ grid provided by FMG interpolation; while u_k^1 and u_k^2 is the solution on the $k \in [1,3]$ grid after the first and second FAS V-cycle, respectively.

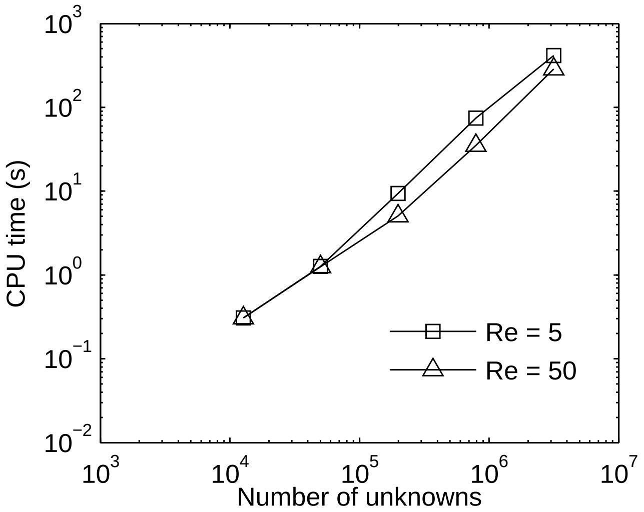

Figure 4: Dependence of CPU time for a typical time step as a function of the total number of unknowns for a flow over a localised (two-dimensional) square trench topography for (a) Re = 5 and (b) Re = 50.

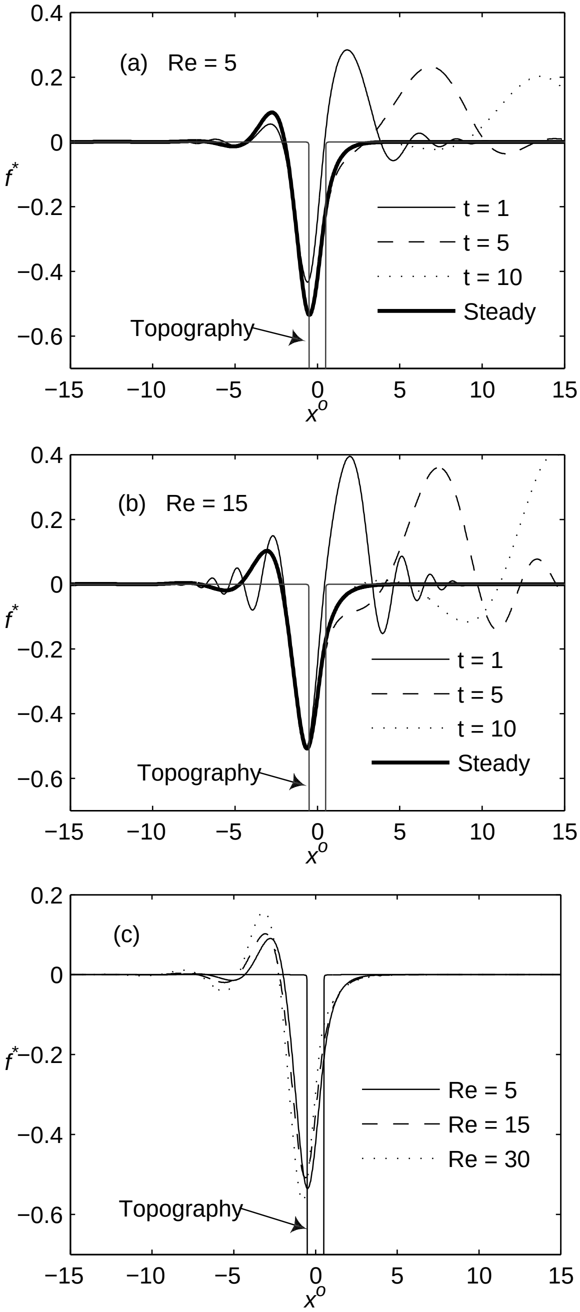

Figure 5: DAF predictions of free-surface profiles for thin film flow over a spanwise trench (width $L_t = 1.2$ mm, depth $S_0 = 20\mu m$): progression from an initial flat surface to predicted steady-state for (a) Re = 5, (b) Re = 15; (c) steady-state solutions for Re = 5, 15, 30. The shape and location of the associated trench topography is indicated in each case.

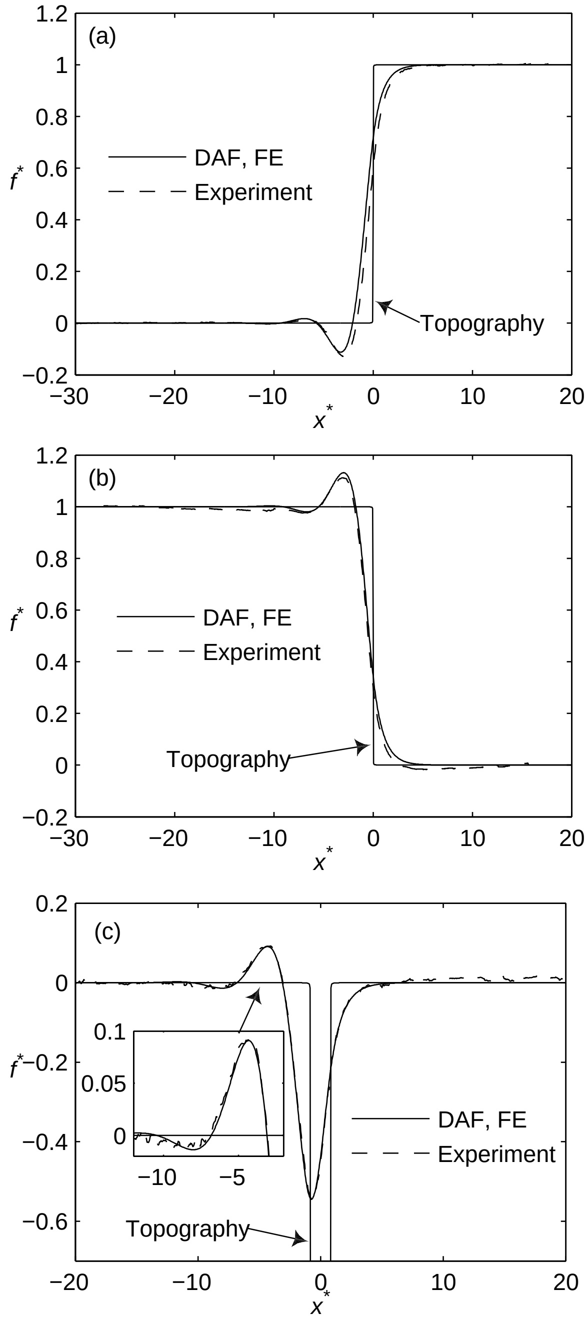

Figure 6: Comparison between predicted (DAF and FE) and experimentally obtained [31] free-surface profiles for thin film flow over a spanwise: (a) step-up (height $|s_0| = 0.2$ and $\mathrm{Re} = 2.45$); (b) step-down (depth $|s_0| = 0.2$ and $\mathrm{Re} = 2.45$); (c) trench topography (depth $s_0 = 0.19$, width $l_t = 1.51$ and $\mathrm{Re} = 2.84$). The shape and location of the associated topography is indicated in each case.

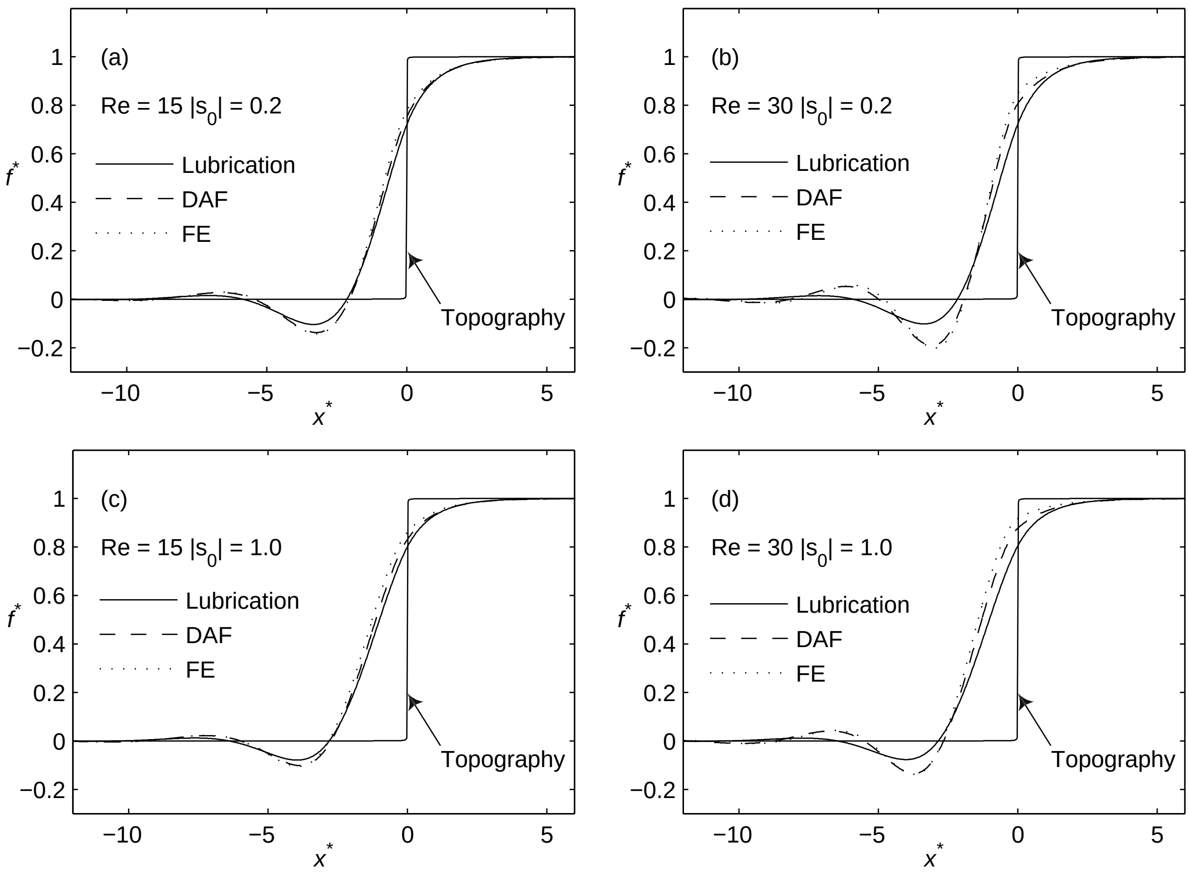

Figure 7: Comparison between predicted (DAF and FE) free-surface profiles for thin film flow over a step-up topography when Re = 15 (left) and 30 (right) for two step heights, $|s_0| = 0.2$ (top) and 1.0 (bottom). The corresponding prediction given by lubrication theory [14] and the location of the associated topography is indicated in each case.

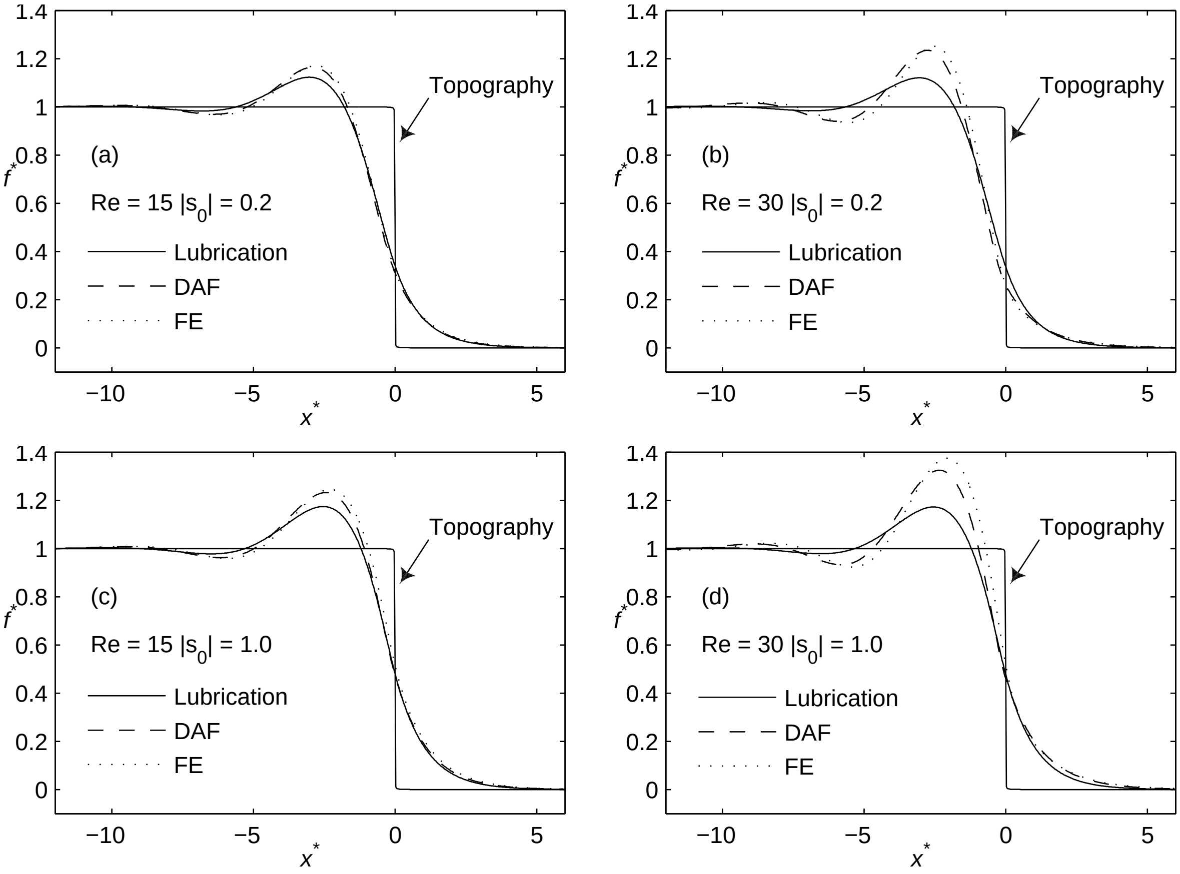

Figure 8: Comparison between predicted (DAF and FE) free-surface profiles for thin film flow over a step-down topography when Re = 15 (left) and 30 (right) for two step heights, $|s_0| = 0.2$ (top) and 1.0 (bottom). The corresponding prediction given by lubrication theory [14] and the location of the associated topography is indicated in each case.

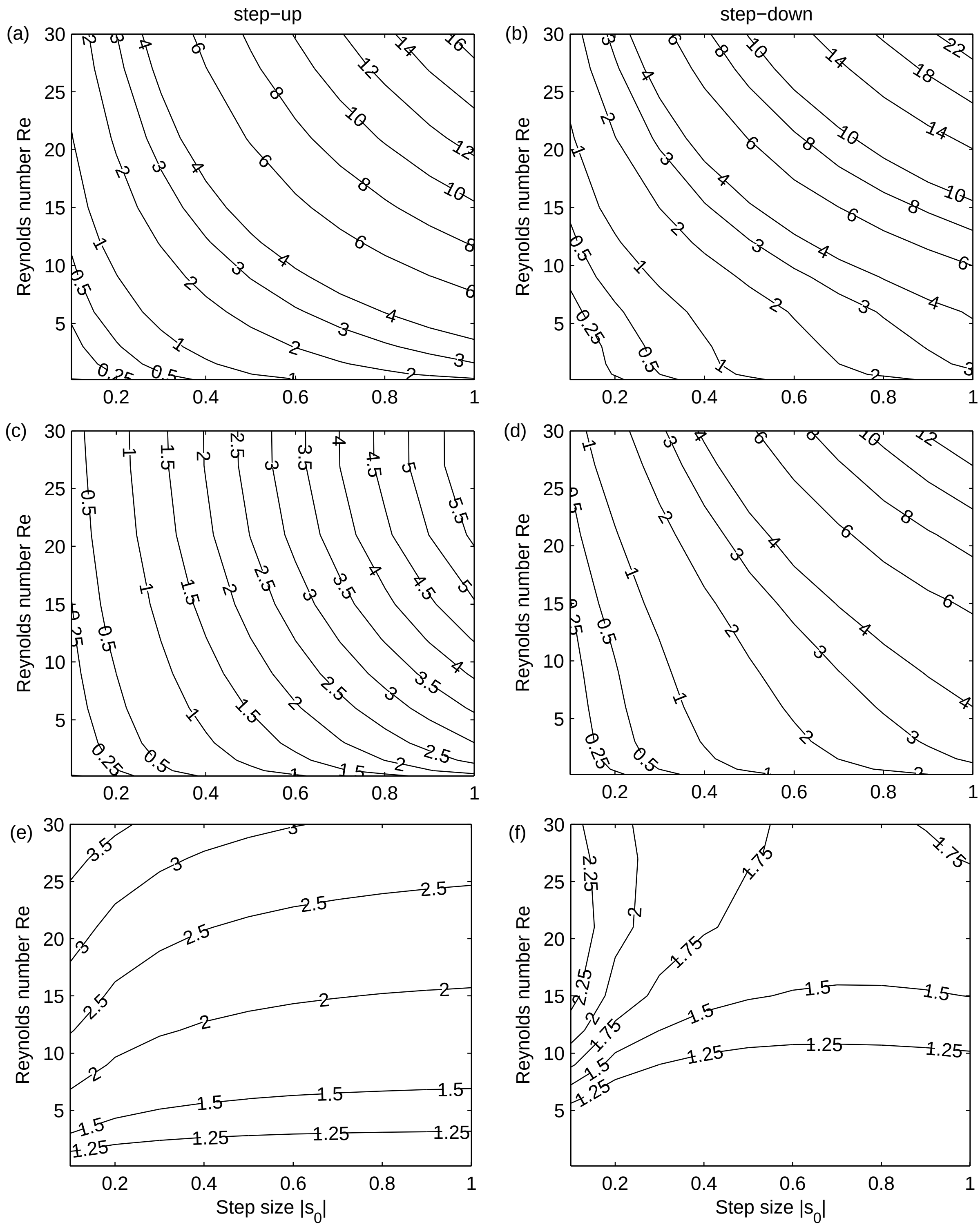

Figure 9: Contours illustrating the maximum percentage discrepancy in predicted free-surface profiles between lubrication theory [14], DAF and Navier-Stokes solutions of flow over step-up and step-down topographies with Re $\in [0.15, 30]$ and $|s_0| \in [0.1, 1]$. Comparison between lubrication and FE N-S solutions for (a) step-up, (b) step-down topography (top), and between DAF and FE N-S solutions for (c) step-up and (d) step-down topography (middle). Improvement of the accuracy of the DAF compared to the lubrication for (e) step-up and (f) step-down is presented as well (bottom).

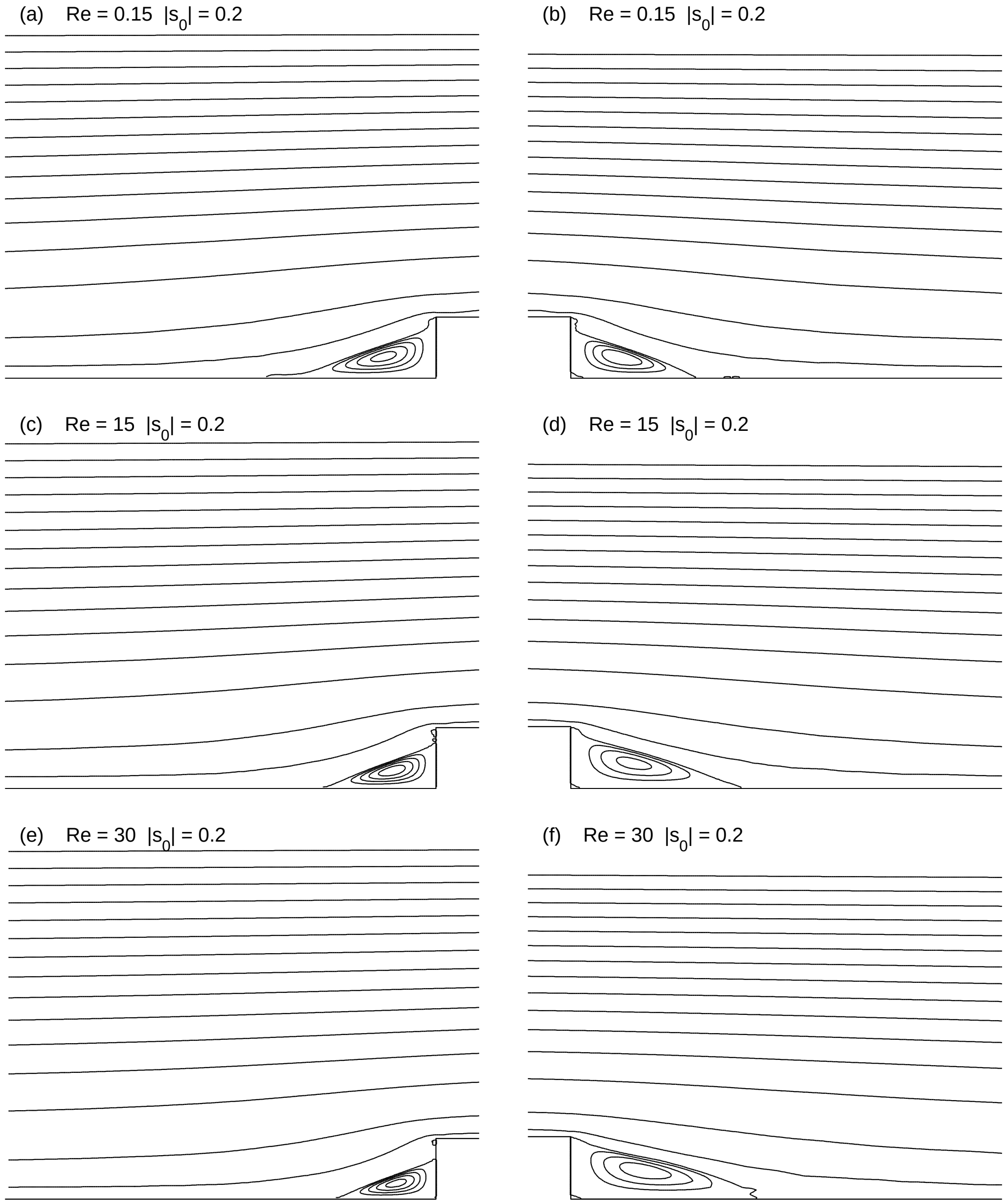

Figure 10: Streamlines showing the effect of inertia on two-dimensional flow over a step-up (left) and a step-down (right) topography, $|s_0| = 0.2$, for: (a),(b) Re $= 0.15$; (c),(d) Re $= 15$; (e),(f) Re $= 30$. Flow is from left to right.

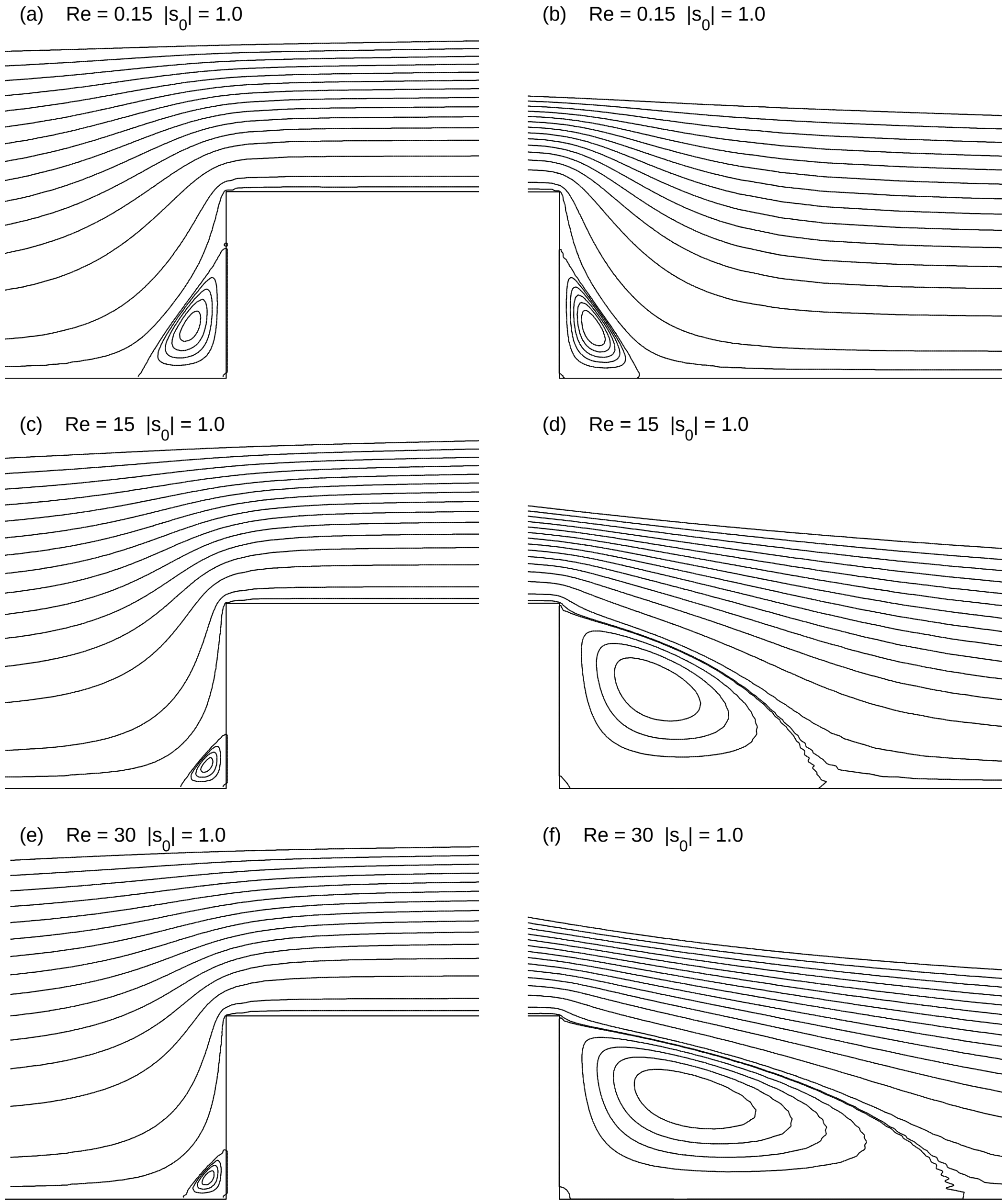

Figure 11: Streamlines showing the effect of inertia on two-dimensional flow over a step-up (left) and a step-down (right) topography, $|s_0| = 1.0$, for: (a),(b) Re $= 0.15$; (c),(d) Re $= 15$; (e),(f) Re $= 30$. Flow is from left to right

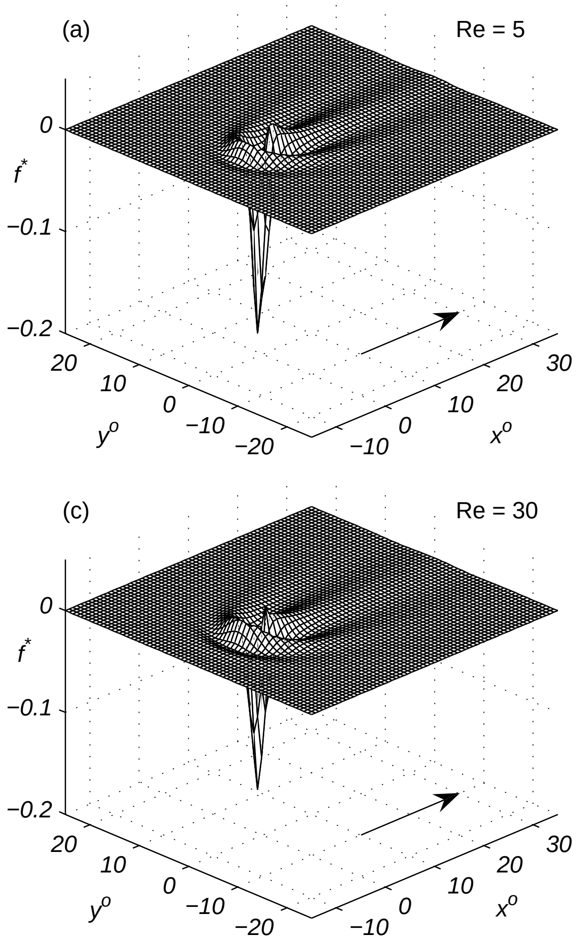

Figure 12: Three-dimensional free-surface plots for flow over a localised (two-dimensional) square trench topography ($L_t = W_t = 1.2mm$, $S_0 = 25\mu m$): (a) Re = 5; (b) Re = 15; (c) Re = 30; (d) Re = 50. The arrow shows the direction of flow.

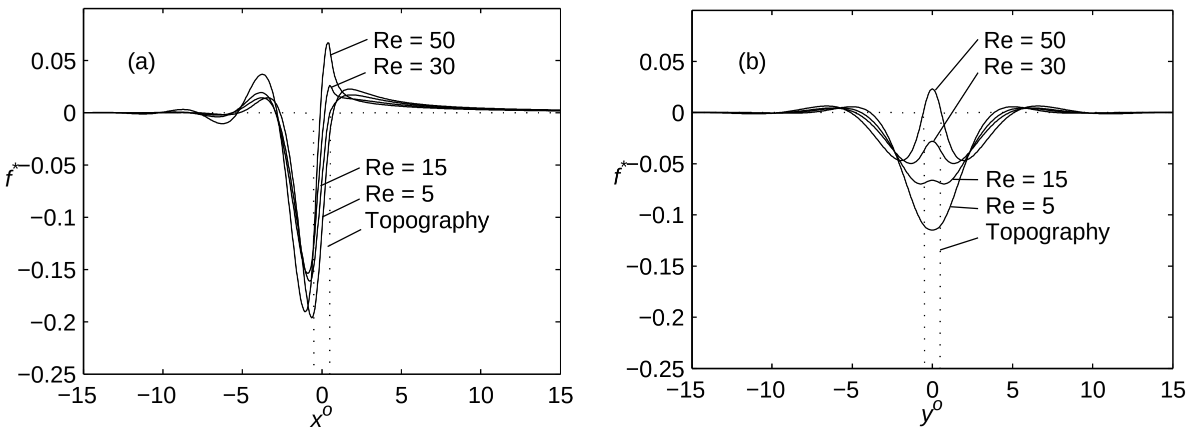

Figure 13: Flow over a localised (two-dimensional) square trench topography ($L_t = W_t = 1.2mm$, $S_0 = 25\mu m$. Streamwise (left) and spanwise (right) free-surface profiles through the centre ($x^o = 0, y^o = 0$) of the topography for Re = 5, 15, 30 and 50. The position of the topography side-walls is as indicated.

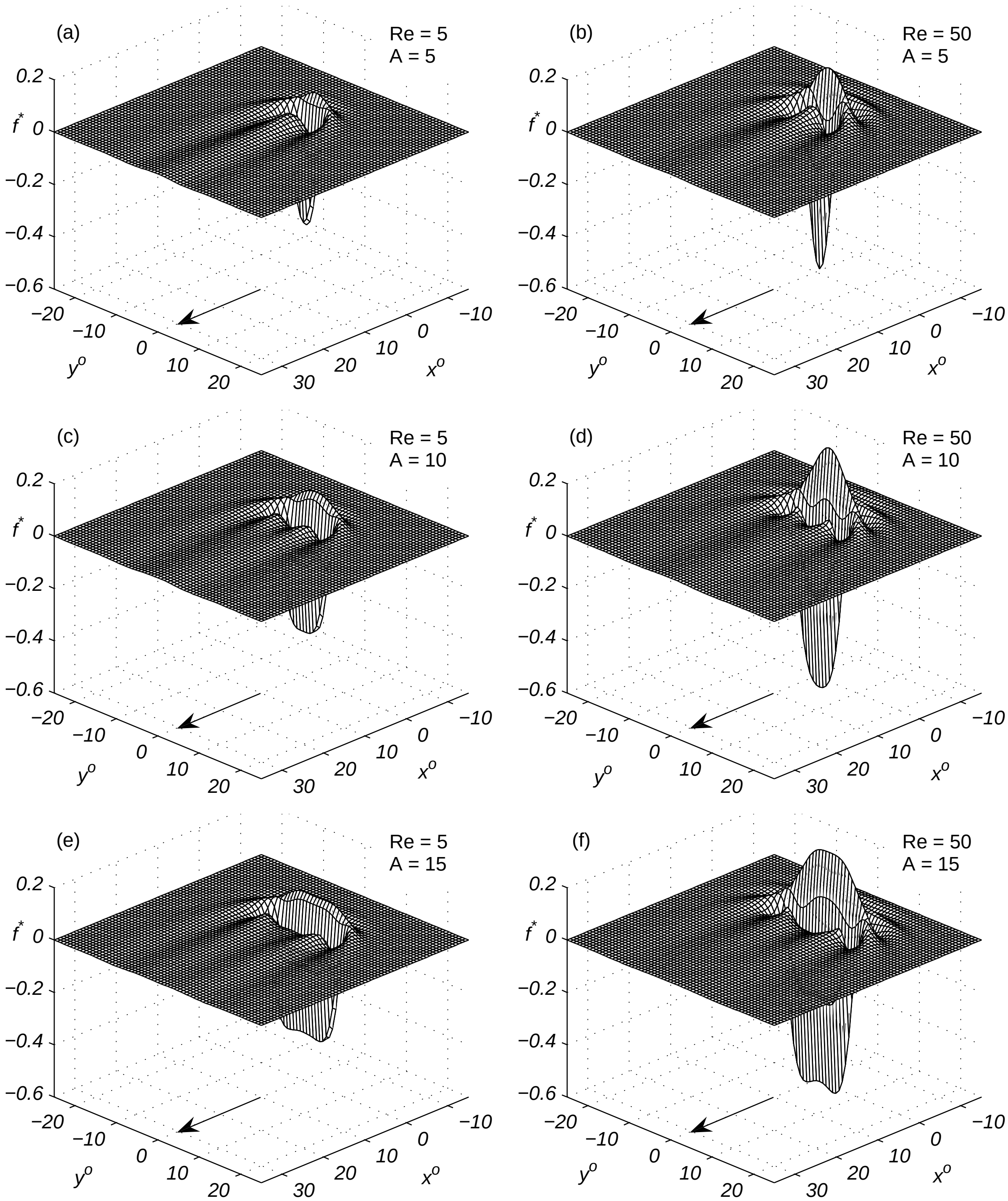

Figure 14: Three-dimensional free-surface plots for flow over a localised trench topography ($L_t = 1.2mm$, $S_0 = 25\mu m$) showing the effect of aspect ratio, $A = W_t/L_t$, on the resulting free surface disturbance. From top to bottom, $A = 5$, 10 and 15; Re = 5 (left) and Re = 50 (right). The arrow shows the direction of flow and the case when $A = 1$ can be viewed in Figures 11(a) and 11(d).

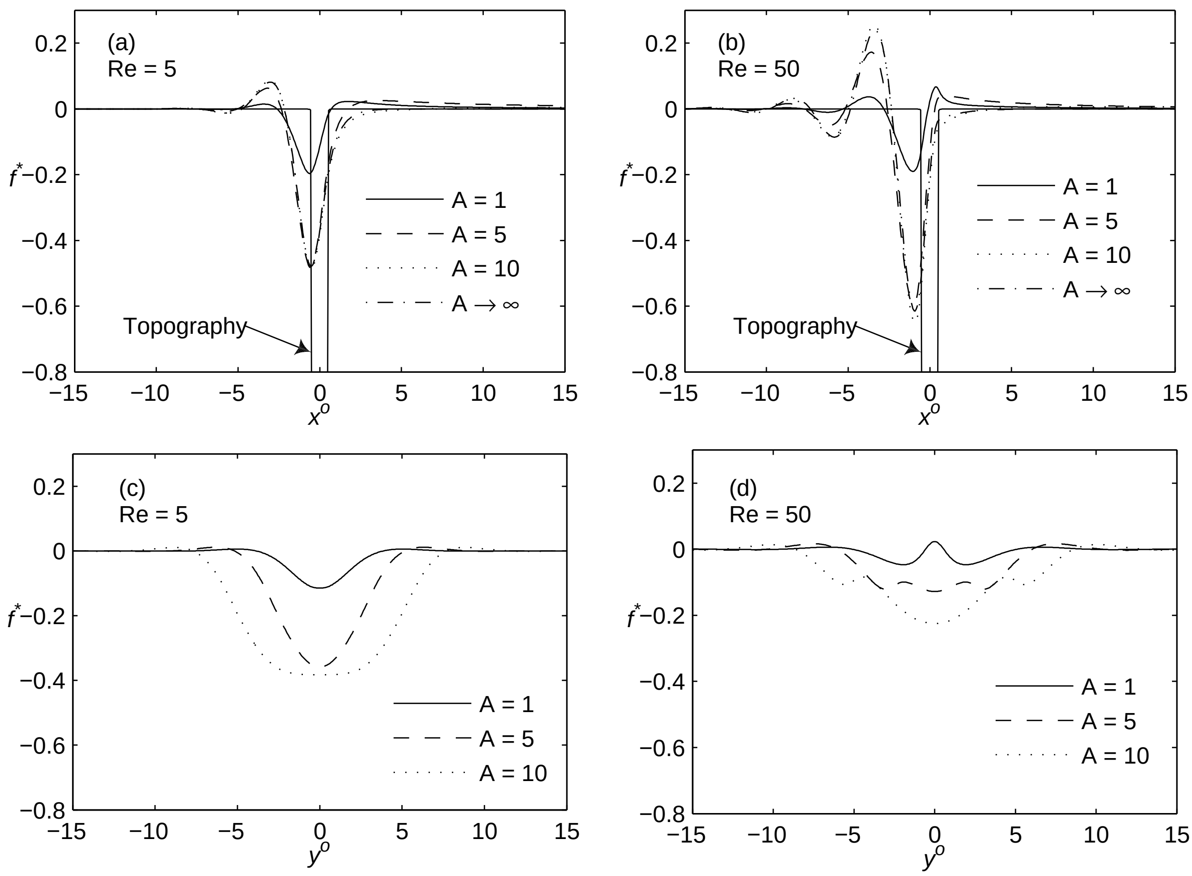

Figure 15: Streamwise (top) and spanwise (bottom) free-surface profiles through the centre of the topography ($x^o = 0, y^o = 0$) for flow over a localised trench topography ($L_t = 1.2mm$, $S_0 = 25\mu m$) showing the effect of aspect ratio, $A = W_t/L_t$ for Re = 5 (left) and Re = 50 (right). The position of the topography side-walls is as indicated in the upper figures

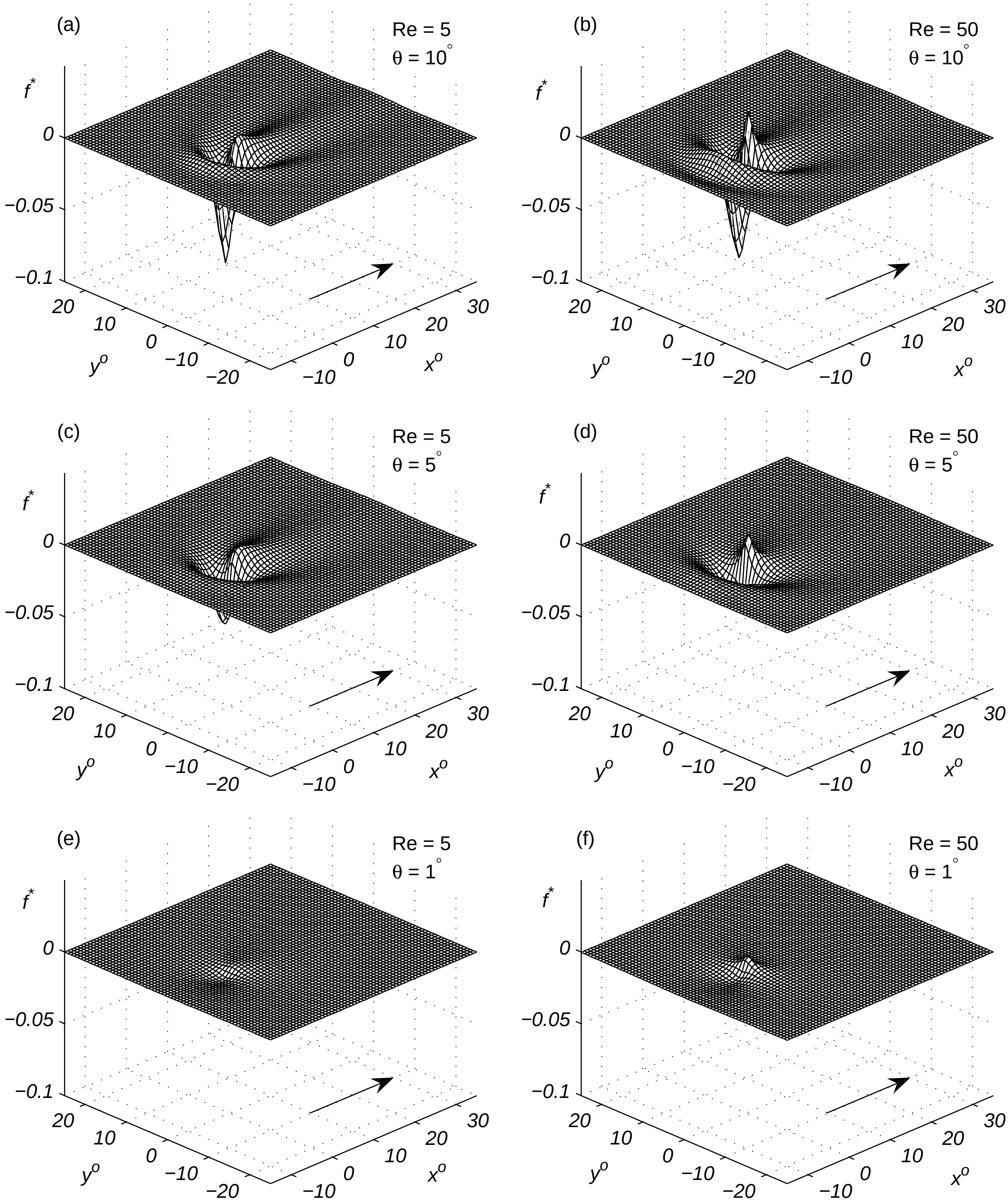

Figure 16: Three-dimensional free surface plots for flow over a localised square trench topography ($L_t = W_t = 1.2mm$, $S_0 = 25\mu m$) showing the effect of θ on the resulting free surface disturbance. From top to bottom, $\theta = 10^\circ$, 5° and 1°; $\mathrm{Re} = 5$ (left) and $\mathrm{Re} = 50$ (right). The arrow shows the direction of flow and the corresponding free-surface disturbances when $\theta = 30^\circ$ can be viewed in Figures 11 (a) and 11 (d).

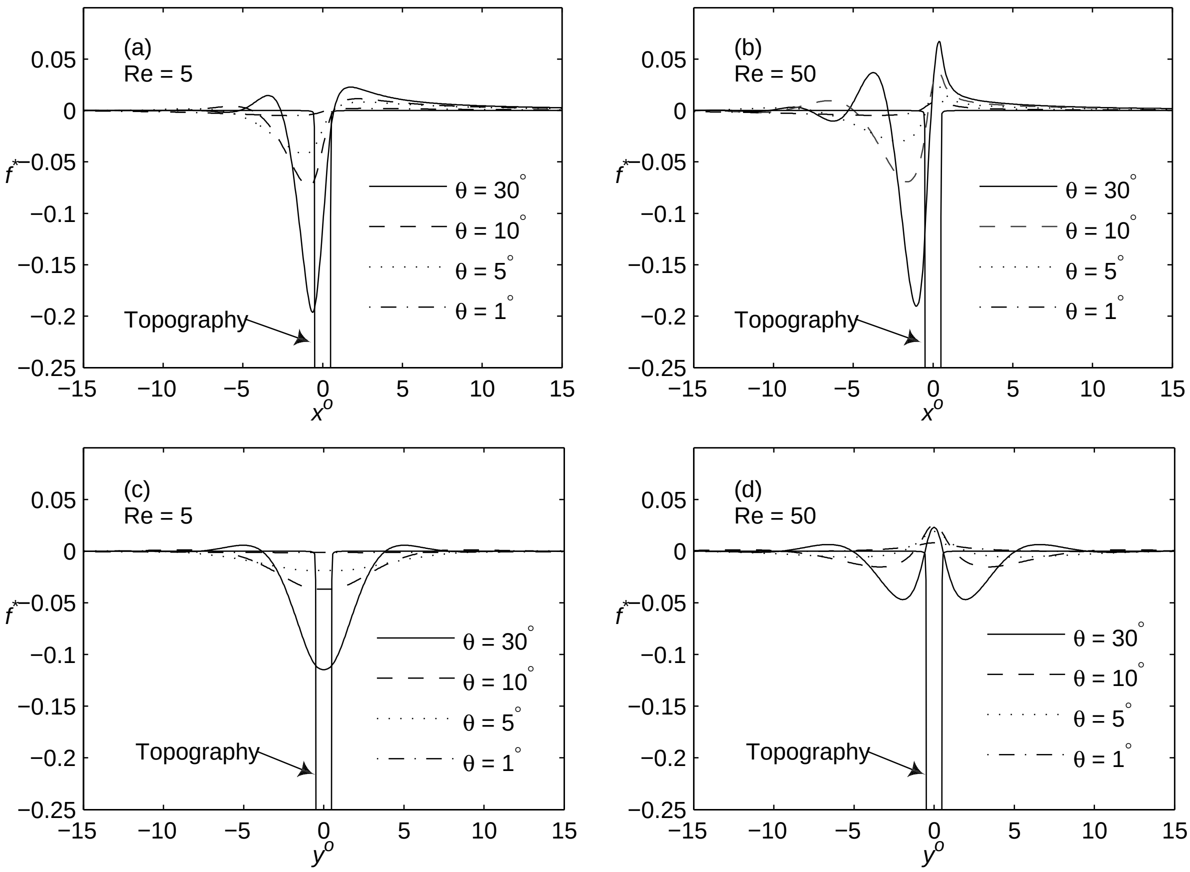

Figure 17: Streamwise (top) and spanwise (bottom) free-surface profiles through the centre of the topography ($x^o = 0, y^o = 0$) for flow over a localised square trench topography ($L_t = W_t = 1.2mm$, $S_0 = 25\mu m$) for four different inclination angles θ; Re = 5 (left) and Re = 50 (right). The position of the topography side-walls is as indicated.

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