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Direct numerical simulation of turbulent free convection in the presence of a surfactant

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ABSTRACT

The effects of surfactants on the turbulent flow of a liquid cooled from above and driven by buoyant convection, are explored using direct numerical simulations. The limiting case of zero surface stress and an insoluble surfactant is investigated. It is found that relatively small amounts of surfactant can have a significant effect on the flow, and that these effects can be accounted for by using a turbulence–surfactant interaction number, which expresses the ratio of surface elastic forces to inertial forces. Emphasis in this work is placed on the effects of surfactants on heat transfer, and the structure of the surface temperature field. As surface elasticity is increased, the surface temperature is found to decrease, the thermal boundary layer thickness is found to increase, and the Nusselt number based on the domain depth is found to decrease by as much as 43%. With increasing surface elasticity, Fourier spectra of the surface temperature show increased spectral energy in the inertial region, and decreased energy at high wavenumbers. We also explore the formation and evolution of surface normal vortices, which are found to be always associated with cold cores, and suggest a simple explanation for their formation and ubiquity.

1. Introduction

It is well known that relatively small amounts of surface active chemical agents, which are often found at air–water or ocean–atmosphere interfaces and are commonly referred to as surfactants, can have significant and surprisingly strong effects on the dynamics of flows at such interfaces. The principal reason for this is that gradients in surfactant concentration at an interface generate corresponding surface tension gradients. These spatially and temporally varying gradients offer a resistance to subsurface motions, thereby producing extra interfacial viscous dissipation. It should be noted that surfactants will affect the flow even in the case of a relatively undeformed free-surface, in contrast to a surfactant–free interface subject only to a spatially and temporally constant surface tension. In the latter case, surface tension will have important effects only for deformed free-surfaces.

Surfactants can affect a wide variety of free-surface phenomena and processes, which include surface waves, electromagnetic surface signatures of ship wakes and mesoscale geophysical flows, small scale laminar and turbulent vortical flows, the thermal (infrared) signature of the ocean surface, and gas transport across the air–ocean interface. Early work by Lucassen [1] showed that surfactants can dampen capillary waves, the greatest damping rate occurring at wavelengths associated with the so-called Marangoni resonance, an interaction of capillary waves with longitudinal waves. More recent work by Alpers and Huhnerfuss [2] indicated that this Marangoni resonance can significantly damp larger gravity waves through non-linear wave–wave interactions. Recent work by Liu and Duncan [3] has shown that surfactants can play a significant role in the dynamics of breaking waves. Surfactants are also known to affect the radar and optical signatures of ship wakes [4,5], and are also important in the identification of oceanic surface flows such as the so-called spiral eddies observed by Munk et al. [6] and investigated numerically by Shen and Evans [7] and Cooper et al. [8]. On much smaller scales, surfactants have been found to affect laminar vortex–free surface interactions [9–12] and the interaction of small-scale turbulence with free surfaces [13,14].

At the ocean surface, surfactants are often generated by biological activity, and are therefore almost always present. As a result, they play a role in not only affecting the ocean surface dynamics, but also in altering the ocean surface temperature [15]. The ocean surface temperature is frequently somewhat cooler than the temperature of the bulk. For example, at night there is often an outward radiative heat flux, and in other circumstances, latent heat transfer may be the dominant source of surface heat flux. As a result, there is often a thin thermal boundary layer at the ocean surface, commonly known as the 'cool-skin' [16,17]. Recent

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Nomenclature

c_p	heat capacity
E	surface elasticity
$\hat{e}_y$	vertical (y direction) unit vector
g	gravitational acceleration
k	thermal conductivity
L_y	domain depth
L^+	length scale
L^*	length scale
Ma	Marangoni number
nx, ny, nz	grid resolution
Nu_0	Nusselt number across the domain
Nu_1	Nusselt number across the thermal boundary layer
Pe	Peclet number
Pr	Prandtl number
P^+	pressure scale
Q	heat flux
Ra_q	flux based Rayleigh number
Re	Reynolds number
T	temperature
T_0	reference temperature
t	time
t^+	time scale
t^*	time scale
U_{pist}	piston velocity
u_S, w_S	surface velocity components
u, v, w	velocity components
U^+	velocity scale
U^*	velocity scale
$\vec{V}_S$	surface velocity vector
$\vec{V}$	velocity vector
We	Weber number
x, y, z	Cartesian coordinates
$(u_\tau)_{rms}$	rms tangential velocity
v_{rms}	rms normal velocity

Greek letters

α	thermal diffusivity
α_S	interfacial diffusivity of surfactant
β	thermal expansion coefficient
β_E	turbulence - surfactant interaction parameter
γ	surfactant concentration
γ_0	initial surfactant concentration
γ^+	surfactant concentration scale
Δ	length scale from surface strain model
$\Delta\theta_0$	mean temperature difference across the domain
$\Delta\theta_1$	mean temperature difference from surface to bulk
δ_{peak}	peak to surface distance of rms temperature
Δt	sampling time
δ_{bl}	thermal boundary layer thickness
θ	temperature
$\bar{\theta}$	mean temperature
θ_{bot}	mean temperature at bottom of the domain
θ_{bl}	mean temperature at bulk
θ_{top}	mean temperature at surface
θ_{rms}	rms temperature
θ^+	temperature scale
θ^*	temperature scale
κ	wave number
λ	wavelength
ν	kinematic viscosity
Π	modified pressure
ρ	density
σ_0	initial surface tension
σ	surface tension
$\bar{\Omega}$	vorticity vector
Ω_x, Ω_x, Ω_z	vorticity components
Ω^+	vorticity scale
$(\Omega)_y)_{rms}$	rms normal vorticity
$(\Omega_\tau)_{rms}$	rms tangential vorticity

experiments using high resolution infrared (IR) imagery [15,18] have shown that surfactants, in cases where a cool-skin exists, actually decrease the average temperature of the liquid surface. This was also confirmed by recent simulations by Handler et al. [14], who showed that this surface cooling was due to a thickening of the thermal boundary layer caused by surfactant damping of near-surface turbulence. Recent attention has also been given to the effects of surfactants on air–sea gas transport [19].

The principal objective of the current work is to investigate, through means of direct numerical simulations (DNS), the effects of surfactants on the turbulent flow of fluid at an undeformed interface subject to zero stress. In the flows to be discussed here, the turbulence is driven solely by thermally induced buoyancy forces generated by an outward (from the water to the air) pointing heat flux. These flows, without surfactant effects (clean case), were originally studied theoretically by Foster [20], and via DNS by Leighton et al. [21]. Experimental work on the clean case was investigated first by Katsaros et al. [22], and subsequently by Saylor et al. [23], who used IR imagery to characterize the effects of surfactants on the surface temperature. We have also further simplified the situation by using a model for an insoluble surfactant. In this way, the effects of surfactants on the flow will tend to be maximized in contrast to the case of a soluble surfactant, where surface material can diffuse into the bulk and thereby lessen surfactant surface concentrations.

Our interest in this particular flow stems from the fact that it represents the limiting case of what would be observed at very low wind speeds in oceans or lakes. In this sense, the results of this investigation should provide some basis for theories that may be developed for these flows, since any such models must asymptotically approach this limit as the surface stress goes to zero. In addition, we suspect that this is a fairly common case encountered in nature, and as such should be investigated in some detail. The emphasis here is on the effects of surfactants on the thermal field, particularly at the surface itself. This is due in part to the recent use of highly sensitive IR imagers which are now being used to investigate both laboratory scale flows [24,25] and geophysical flows [26]. In many of these flows, the interface between air and water is almost always contaminated to some degree with surfactants, unless considerable effort is employed. For example, in laboratory environments, bubble sparging or other techniques are used to eliminate these naturally occurring chemical agents. Also, it is interesting to note that since heat diffuses relatively slowly in water, the Prandtl number (Pr) of heat in water being significantly greater than one (Pr = 5–7), the surface thermal fields determined by such IR imagery can be used to determine the surface velocities [27]. An understanding of the role being played by surfactants on the surface thermal fields is therefore of importance in the interpretation of surface thermal field maps obtained by advanced IR imagers. Finally, the direct numerical simulations used here provide highly resolved, in space and time, velocity, temperature, and surfactant concentrations fields – information which would be difficult to obtain experimentally.

2. Problem formulation and numerical methods

2.1. Problem formulation

The fluid flows considered here are governed by the Boussinesq form of Navier–Stokes equations given by: