

Three-dimensional modeling of small-scale processes in the upper boundary layer bounded by a dynamic ocean surface

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[1] We present a numerical model for simulating boundary-layer turbulence bounded by a dynamic ocean surface and driven by wind stresses. The nonlinear boundary conditions are satisfied on the freely moving surface exactly without any approximation. The time-dependent physical space is mapped onto a rectangular computational domain where the momentum equations are integrated in time for the velocity field and the solenoidal condition is satisfied by solving the transformed pressure Poisson equation. The developed model is validated with a progressive gravity wave and with a gravity-capillary wave. The model capabilities for resolving surface waves of various length scales, ranging from the gravity waves to the capillary ripples, and the nonlinear interactions among the waves are highlighted by simulating the evolution of two-dimensional short-crested gravity-capillary waves and the development of a gravity wave train into crescent patterns. The potential applicability of the model for studying the wind-driven aqueous near-surface layer is then demonstrated. The simulation results reveal fine surface structures, including microscale breaking waves and streamwise velocity streaks, which have been observed in the laboratory and field experiments.

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1. Introduction

[2] The interaction between the ocean surface and the underlying aqueous turbulence plays a significant role in characterizing the surface features that can be detected by remote sensing instruments. The coupling dynamics are also among the major processes that control the transport of momentum, heat, gases and water vapors between the atmosphere and the ocean. It has been recognized that the energetic, coherent vortical motions within the aqueous turbulent boundary layer, or known as the surface renewal eddies, account for the effectiveness of transport across the air-water interface. On the basis of the finding, a popular approach in recent years for measuring the air-water transfer rate is to infer the renewal events from infrared images of water surface [e.g., *Asher et al.*, 2004; *Garbe et al.*, 2004; *Schimpf et al.*, 2004]. The accuracy of the technique thus relies on better understanding of the physical processes of wave-turbulence interaction, and also on relating quantitatively the surface thermal imagery to the aqueous turbulence processes and structures.

[3] Owing to the profound difficulties in conducting in situ measurements, most of the experimental studies on the aqueous near-surface layer have been conducted in labora-

tory wind-wave flumes, such as those of *Okuda* [1982], *Ebuchi et al.* [1987], *Banner and Peirson* [1998], *Caulliez and Collard* [1999], *Veron and Melville* [2001], among many others. Although the processes have been studied extensively, there are still uncertainties in understanding the physics involved due to the strong nonlinear complexities implicit in both the surface waves and the underlying turbulence. Numerical simulations offer a means for improving the understanding of the complex interactions of the processes, but only recently have computing resources advanced to make sufficiently large-scale simulations possible.

[4] The current development of numerical model concerning the interaction between the ocean surface and the underlying turbulence employs, to a certain degree, approximation or parameterization of the surface boundary conditions. One class of model considers the weakly nonlinear conditions satisfied on the mean ocean surface [e.g., *Borue et al.*, 1995; *Tsai*, 2001; *Tsai et al.*, 2003]. As such, the models are only applicable for small-amplitude surface motions; and the simulations primarily focus on the boundary effect of water surface on the underlying turbulence [see, e.g., *Teixeira and Belcher*, 2000]. A recent simulation conducted by *Sullivan et al.* [2004] also considers the mean ocean surface as the upper boundary; the dynamics of the surface waves are then parameterized as exerted forcing on the surface boundary. Accordingly, the evolutions of the underlying turbulent boundary layer depend on the parameterized surface forcing. Idealization of the surface-wave boundary in these models considers only one-way interaction between the water surface

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and the flow underneath; thus inhibiting the possible modulation of the surface roughness by the underlying flow and vice versus.

[5] The present work has been undertaken to develop a numerical model for process-oriented studies of three-dimensional turbulent flow bounded by a nonlinearly evolving ocean surface. Specifically, the developed model will be applied to the study of hydrodynamic processes concerning the immediate transport next to the ocean surface. The underlying numerics of the present model are based on that of Tsai *et al.* [2005], which considers incompressible and nonhydrostatic flow, and employs the mixed pseudo-spectral and finite-difference method. The present model, however, imposes the fully nonlinear boundary conditions of mass and momentum conservations on the exact ocean surface; and is capable of resolving surface dynamics ranging from gravity to capillary waves. This requires tracking the free-surface Lagrangian boundary and solving the governing equations in a time-dependent domain. Consequently, the computational demand of the present “free-surface” simulation exceeds greatly that of models employing boundary approximation or parameterization.

[6] The paper is organized as follows. The mathematical formulation of the model is described in section 2, followed by a detailed description of the numerical algorithms in section 3. Validation simulations of progressive gravity and gravity-capillary waves are presented in section 4. In section 5, the model’s capability of resolving surface waves of various length scales and of modeling the nonlinear interactions among the waves are highlighted by computing the evolution of a short-crested gravity-capillary wave and the development of the crescent pattern of a steep wave train. The potential applicability of the model for simulating the flow coupling the surface waves and the underlying turbulent boundary layer is then demonstrated. The simulation results reveal surface structures of microscale breaking and streaky velocity patterns that have been commonly observed in the laboratory experiments, such as those of Caulliez and Collard [1999], Ebuchi *et al.* [1987] and Veron and Melville [2001]. The paper concludes with a discussion of further extending the developed model for large-eddy and large-wave simulations.

2. Mathematical Formulation

2.1. Governing Equations and Boundary Conditions

[7] We consider a three-dimensional flow of a viscous fluid bounded by a free-moving water surface and a free-slip bottom at a depth of h . The coordinate axes $\mathbf{x} = (x, y, z)$ are in the two horizontal directions and the upward vertical direction, respectively, with the corresponding velocities $\mathbf{v} = (u, v, w)$. The instantaneous free surface is represented by the vertical deformation function, $z = \eta(x, y, t)$, with its mean vertical position at $z = 0$. The fluid is assumed to be incompressible and Newtonian, such that the velocity $\mathbf{v}$ and the dynamic pressure p are governed by the solenoidal condition and the Navier-Stokes equations,

$$\nabla \cdot \mathbf{v} = 0 \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{v}) = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}, \quad (2)$$

where p is the dynamic pressure, ρ and ν are density and kinematical viscosity of the fluid, respectively. For an incompressible fluid, the pressure can be considered as an unknown to be determined for projecting the velocity onto a solenoid field. Taking the divergence of the momentum equation (2), we can obtain a Poisson equation for the pressure field.

[8] At the water surface, $\mathcal{F} \equiv z - \eta(x, y, t)$, the free-surface boundary moves as a material surface which results in the kinematical boundary condition,

$$\frac{\partial \eta}{\partial t} + u\eta_x + v\eta_y - w = 0. \quad (3)$$

The kinematical surface condition also serves as an evolution equation for the surface elevation η . The force balance at the free surface determines three stress conditions imposed upon the contiguous bulk-flow stress field. The local normal and tangential components of the surface traction force are balanced by the corresponding wind stresses. Projecting these stress conditions onto the direction normal to the free surface and the two directions tangential to the surface and parallel to the x and y axes, yields the dynamic boundary conditions at the free surface as

$$\hat{\mathbf{n}} \cdot \mathbf{T} \cdot \hat{\mathbf{n}}^\top + \sigma \kappa = \tau_n^s \quad (4)$$

$$\hat{\mathbf{i}}_x \cdot \mathbf{T} \cdot \hat{\mathbf{n}}^\top = \tau_{t_x}^s + (\hat{\mathbf{i}}_x \cdot \hat{\mathbf{i}}_y) \tau_{t_y}^s \quad \text{and} \quad \hat{\mathbf{i}}_y \cdot \mathbf{T} \cdot \hat{\mathbf{n}}^\top = (\hat{\mathbf{i}}_y \cdot \hat{\mathbf{i}}_x) \tau_{t_x}^s + \tau_{t_y}^s \quad (5)$$

Here

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} \quad (6)$$

is the stress tensor,

$$\mathbf{D} = \frac{1}{2} [\nabla \mathbf{v} + (\nabla \mathbf{v})^\top] \quad (7)$$

is the symmetric part of the velocity gradient tensor, $\mu = \rho\nu$ is the dynamic viscosity,

$$\hat{\mathbf{n}} = \frac{\nabla \mathcal{F}}{\|\nabla \mathcal{F}\|} \quad (8)$$

is the unit normal vector,

$$\hat{\mathbf{i}}_x = \frac{(\hat{\mathbf{n}} \times \hat{\mathbf{j}})}{\|\hat{\mathbf{n}} \times \hat{\mathbf{j}}\|} \quad \text{and} \quad \hat{\mathbf{i}}_y = \frac{(\hat{\mathbf{n}} \times \hat{\mathbf{i}})}{\|\hat{\mathbf{n}} \times \hat{\mathbf{i}}\|} \quad (9)$$

are the unit tangential vectors, σ is the surface tension, $\kappa = \nabla \cdot \hat{\mathbf{n}}$ is the curvature of the surface, $\tau_n^s = \tau_n^s \hat{\mathbf{n}}$ is the normal wind stress, and $\tau_t^s = \tau_{t_x}^s \hat{\mathbf{i}}_x + \tau_{t_y}^s \hat{\mathbf{i}}_y$ is the tangential wind stress, respectively.

2.2. Coordinate Transformation

[9] Considering only the situation in which the surface elevation function $\eta(x, y, t)$ is of single value, the time-dependent physical domain can be mapped to a rectangular computational domain by the transformation:

$$\tau = t, \quad \xi = x, \quad \psi = y, \quad \zeta = \frac{z+h}{h}, \quad (10)$$

where $\bar{h} = h + \eta(\xi, \psi, \tau)$ and ζ ranges from 0 to 1. The temporal differential operators with respect to t is related to the new variables by

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} - \frac{\eta_\tau \zeta}{\bar{h}} \frac{\partial}{\partial \zeta}. \quad (11)$$

The spatial differential and the Laplacian operators, after the coordinate transformation, become

$$\begin{aligned} \nabla &= \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k} \\ &= \left(\frac{\partial}{\partial \xi} - \frac{\eta_\xi \zeta}{\bar{h}} \frac{\partial}{\partial \zeta} \right) \hat{e}_\xi + \left(\frac{\partial}{\partial \psi} - \frac{\eta_\psi \zeta}{\bar{h}} \frac{\partial}{\partial \zeta} \right) \hat{e}_\psi + \left(\frac{1}{\bar{h}} \frac{\partial}{\partial \zeta} \right) \hat{e}_\zeta \end{aligned} \quad (12)$$

$$\begin{aligned} \nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\ &= \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \psi^2} + \frac{\left[1 + (\eta_\xi^2 + \eta_\psi^2) \zeta^2 \right]}{\bar{h}^2} \frac{\partial^2}{\partial \zeta^2} \\ &\quad - \frac{2\eta_\xi \zeta}{\bar{h}} \frac{\partial^2}{\partial \xi \partial \zeta} - \frac{2\eta_\psi \zeta}{\bar{h}} \frac{\partial^2}{\partial \psi \partial \zeta} \\ &\quad + \left[2(\eta_\xi^2 + \eta_\psi^2) - \bar{h}(\eta_{\xi\xi} + \eta_{\psi\psi}) \right] \frac{\zeta}{\bar{h}^2} \frac{\partial}{\partial \zeta}. \end{aligned} \quad (13)$$

Note that these transformed operators are now time dependent.

[10] Substituting the transformed operators (11)–(13) into the governing equations (1) and (2) yields the transformed solenoidal constraint as

$$\frac{\partial u}{\partial \xi} - \frac{\eta_\xi \zeta}{\bar{h}} \frac{\partial u}{\partial \zeta} + \frac{\partial v}{\partial \psi} - \frac{\eta_\psi \zeta}{\bar{h}} \frac{\partial v}{\partial \zeta} + \frac{1}{\bar{h}} \frac{\partial w}{\partial \zeta} = 0, \quad (14)$$

and the transformed momentum equation in the computational domain becomes

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial \tau} &= -\frac{1}{\rho} \nabla p + \frac{\zeta \eta_\tau}{\bar{h}} \frac{\partial \mathbf{v}}{\partial \zeta} + \nabla \cdot (\boldsymbol{\nu} \mathbf{v}) + \nu \nabla^2 \mathbf{v} \\ &\equiv -\frac{1}{\rho} \nabla p + \mathbf{R}(\eta, \mathbf{v}), \end{aligned} \quad (15)$$

where the new gradient and Laplacian operators are defined as in (12) and (13), respectively.

[11] The transformed kinematical free-surface boundary condition, which is now satisfied at $\zeta = 1$, remains the same form as (3),

$$\frac{\partial \eta}{\partial \tau} = \left[w - u\eta_\xi - v\eta_\psi \right]_{\zeta=1}. \quad (16)$$

[12] As will be described in the numerical implementation of the model (section 3), the normal-stress condition (4) serves as a Dirichlet condition for the solution of the pressure field; accordingly, the transformed normal-stress condition at $\zeta = 1$ is expressed as

$$\begin{aligned} (p)_{\zeta=1} &= \rho g \eta + \sigma \kappa - \tau_n^s + \frac{2\mu}{\bar{N}} \left[-\left(1 + \eta_\psi^2 \right) \frac{\partial u}{\partial \xi} - \left(1 + \eta_\xi^2 \right) \frac{\partial v}{\partial \psi} \right. \\ &\quad \left. + \eta_\xi \eta_\psi \left(\frac{\partial u}{\partial \psi} + \frac{\partial v}{\partial \xi} \right) - \eta_\xi \frac{\partial w}{\partial \xi} - \eta_\psi \frac{\partial w}{\partial \psi} \right]_{\zeta=1}, \end{aligned} \quad (17)$$

where $\bar{N} = 1 + \eta_\xi^2 + \eta_\psi^2$. The tangential-stress conditions (5) are employed as Neumann conditions for temporal integration of the horizontal momentum equations [see, e.g., Tsai and Yue, 1996]. Expanding the two transformed tangential-stress conditions and solving for the normal derivatives of the horizontal velocities, $(\partial u / \partial \zeta)_{\zeta=1}$ and $(\partial v / \partial \zeta)_{\zeta=1}$, result in

$$\begin{aligned} \left(\frac{\partial u}{\partial \zeta} \right)_{\zeta=1} &= \frac{\bar{h}}{\bar{N}^2} \left[\frac{1}{\mu} \left(1 + \eta_\xi^2 \right)^{-1/2} \bar{N}^{3/2} \tau_{t_\xi}^s \right. \\ &\quad \left. + \eta_\psi \left(1 - \eta_\xi^2 + \eta_\psi^2 \right) \left(\frac{\partial u}{\partial \psi} + \frac{\partial v}{\partial \xi} \right) \right. \\ &\quad \left. + \eta_\xi \left(1 + \eta_\xi^2 - \eta_\psi^2 \right) \frac{\partial v}{\partial \psi} + 2\eta_\xi \eta_\psi \frac{\partial w}{\partial \psi} \right. \\ &\quad \left. - \left(1 - \eta_\xi^2 + \eta_\psi^2 \right) \frac{\partial w}{\partial \xi} + \eta_\xi \left(3 + \eta_\xi^2 + 3\eta_\psi^2 \right) \frac{\partial u}{\partial \xi} \right]_{\zeta=1} \end{aligned} \quad (18)$$

$$\begin{aligned} \left(\frac{\partial v}{\partial \zeta} \right)_{\zeta=1} &= \frac{\bar{h}}{\bar{N}^2} \left[\frac{1}{\mu} \left(1 + \eta_\psi^2 \right)^{-1/2} \bar{N}^{3/2} \tau_{t_\psi}^s \right. \\ &\quad \left. + \eta_\xi \left(1 + \eta_\xi^2 - \eta_\psi^2 \right) \left(\frac{\partial u}{\partial \psi} + \frac{\partial v}{\partial \xi} \right) \right. \\ &\quad \left. + \eta_\psi \left(1 - \eta_\xi^2 + \eta_\psi^2 \right) \frac{\partial u}{\partial \xi} + 2\eta_\xi \eta_\psi \frac{\partial w}{\partial \xi} \right. \\ &\quad \left. - \left(1 + \eta_\xi^2 - \eta_\psi^2 \right) \frac{\partial w}{\partial \psi} + \eta_\psi \left(3 + 3\eta_\xi^2 + \eta_\psi^2 \right) \frac{\partial v}{\partial \psi} \right]_{\zeta=1} \end{aligned} \quad (19)$$

2.3. Conservation of Energy

[13] The accuracy in numerical integration of the momentum equation subject to the boundary conditions can be checked by monitoring the energy conservation. The energy equation is derived from the vector product of the velocity with the momentum equation and integrating over the whole fluid domain $\mathcal{V}$. Upon utilizing the divergence theorem in conjunction with the free-surface boundary conditions, the energy equation can be further simplified and expressed as

$$\begin{aligned} \frac{D}{Dt} \int \int_{\mathcal{V}} \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} dV + \frac{1}{2} \rho g \int \int_{S_0} \frac{\partial (\eta^2)}{\partial t} dS_0 + \sigma \int \int_{S_0} \frac{\partial \eta}{\partial t} \kappa dS_0 \\ + \rho \nu \int \int_{\mathcal{V}} \nabla \mathbf{v} \cdot [\nabla \mathbf{v} + (\nabla \mathbf{v})^\top] dV \\ = \int \int_{S_0} \frac{\partial \eta}{\partial t} \tau_n^s dS_0 + \int \int_{S_f} \mathbf{v} \cdot \boldsymbol{\tau}_t^s dS_f, \end{aligned} \quad (20)$$

where S_f is the free surface and S_0 is the mean surface, $z = 0$. The first and second terms on the left-hand side ($\equiv dE_k/dt$ and dE_η/dt) represent the rates of change in the kinetic energy and the potential energy due to free-surface motions, respectively. The third term ($\equiv dE_\sigma/dt$) stands for the rate of work done by the surface tension. The fourth term ($\equiv dE_\nu/dt$) denotes the rate of energy dissipation caused by viscosity. The two terms on the right-hand side ($\equiv dE_{\tau_n^s}/dt$

and dE_{τ_s}/dt) represent the power inputs by the exerted normal and tangential surface stresses, respectively.

3. Numerical Implementation

3.1. Spatial Discretization

[14] The transformed Navier-Stokes equation (15) subject to the solenoidal constraint (14) and the three dynamic free-surface boundary conditions (17)–(19) are integrated numerically in time for the velocity field $\mathbf{v}$. The free-surface deformation η is tracked by integrating the kinematical free-surface boundary condition (16). The computational domain is closed in the horizontal directions by imposing periodic conditions, and in the vertical direction by the free surface ($\zeta = 1$) and the free-slip boundary on the bottom ($\zeta = 0$).

[15] The flow variables u , v and p are arranged on the discrete grid system (ξ_i, ψ_j, ζ_k) with the vertical coordinate spans from $\zeta = 0$ to 1, while w on the vertically staggered grids $(\xi_i, \psi_j, \zeta_{k+1/2})$, where $\zeta_{k+1/2} = (\zeta_k + \zeta_{k+1})/2$. A stretched vertical discretization system is employed such that the numerical grids cluster when approaching the upper boundary so as to allow proper resolution of the boundary layer adjacent to the water surface. Both the continuity and Navier-Stokes equations are satisfied on the discrete grids where u , v and p are assigned. In the equations and boundary conditions, the spatial-differential operators with respect to ξ and ψ are approximated by the pseudo-spectral method, and the operators with respect to ζ are approximated by the second-order finite-difference scheme.

[16] For the nonlinear terms in the governing equations and the boundary conditions, such as the convective terms and those attributed to algebraic mapping, aliasing errors can arise from local multiplication of the values at the discrete grids followed by the pseudo-spectral scheme to evaluate the derivative. Such aliasing errors become severe in the present model when the surface steepness is large. Employing truncation rules to formally exclude the possibility of aliasing is therefore inevitable.

[17] The choice of the numerical schemes depends on the physical processes of interest. In this work, the focus is on the interaction between the surface waves and the underlying turbulent boundary layer. For such a purpose, the model is required to have the computational capabilities in terms of accuracy and efficiency to resolve the processes of various spatial scales, including the surface gravity waves, the capillary ripples, the laminar sublayer, and the shear turbulence. The combined use of the pseudo-spectral method in the cyclic horizontal domain, and the finite-difference scheme with stretched grids in the vertical direction becomes a natural choice for numerical approximation of the spatial derivatives. In particular, the pseudo-spectral approximation of the horizontal derivatives converts the solution of the three-dimensional pressure Poisson equation into a one-dimensional ordinary differential equation in the spectral space. This drastically reduces the computational burden in solving for the nonhydrostatic pressure. Such a mixed numerical method using both the finite-difference and the pseudo-spectral schemes has been widely used in various examples of numerical simulation of turbulent boundary layer, such as turbulent channel flow [e.g., *Moin and Kim*, 1982] and planetary boundary layer [e.g., *Moeng*, 1984].

3.2. Temporal Integration

[18] Low-storage Runge-Kutta scheme [Williamson, 1980] is adopted for temporal integration of the Navier-Stokes equation as well as the kinematical free-surface boundary condition. The discretized form of the transformed momentum equation (15), after employing the low-storage Runge-Kutta scheme of m th-order, can be expressed as

$$(\mathbf{v})_{n+} = (\mathbf{v})_{n-} + b_{n+}(\mathbf{Q})_{n+}, \quad (21)$$

$$(\mathbf{v})_{n+\frac{j}{m}} = (\mathbf{v})_{n+\frac{j-1}{m}} + b_j(\mathbf{Q})_{n+\frac{j}{m}}, \quad (22)$$

$$(\mathbf{Q})_{n+\frac{j}{m}} = a_j(\mathbf{Q})_{n+\frac{j-1}{m}} + \Delta t \left[-(\nabla p)_{n+\frac{j-1}{m}} + (\mathbf{R})_{n+\frac{j-1}{m}} \right], \quad (23)$$

where $j = 1$ to m represents the interval step in the m th-order Runge-Kutta integration, $(\mathbf{v})_n$ and $(\mathbf{v})_{n+1}$ are the velocities at the discrete times $\tau = n\Delta\tau$ and $(n+1)\Delta\tau$, respectively, and a_j and b_j are constant coefficients. Note that the coefficients a_j and b_j are not unique. For second-order scheme, the possible combinations of the coefficients are $(a_1, b_1, a_2, b_2) = (0, 2/3, -5/9, 3/4)$, $(0, 1/2, -1/2, 1)$ and $(0, 1, -1, 1/2)$. A more complete list of the coefficients for second-, third- and fourth-order schemes are given by Williamson [1980]. The low-storage Runge-Kutta scheme is also applied for temporal integration of (16).

3.3. Solution of Pressure Poisson Equation

[19] For each interval step at $\tau = (n + \frac{j-1}{m})\Delta\tau$ in the Runge-Kutta time integration (21, 22), the pressure field is first solved before updating toward the next time interval at $\tau = (n + \frac{j}{m})\Delta\tau$ for the new velocities. A Poisson equation for the pressure field $(p)_{n+\frac{j}{m}}$ is obtained by taking the divergence of the temporal-discretized Navier-Stokes equation (equations (21) and (22)) and applying the solenoidal constraint (14) to the velocity field at the new time interval, i.e., $(\nabla \cdot \mathbf{v})_{n+\frac{j}{m}} = 0$. (For simplicity of the expression, the subscript $n + \frac{j}{m}$ is replaced with the subscript $+$, and the subscript $n + \frac{j-1}{m}$ is eliminated in the following equations.)

The resulting Poisson equation is

$$\begin{aligned} \mathcal{L}p &= \frac{\partial^2 p}{\partial \xi^2} + \frac{\partial^2 p}{\partial \psi^2} + \frac{1}{h^2} \frac{\partial^2 p}{\partial \zeta^2} \\ &= \epsilon(p, \eta, \eta^+) + \frac{1}{\Delta\tau} \frac{1}{b} \nabla^+ \cdot \mathbf{v} + \frac{a}{\Delta\tau} \nabla^+ \cdot \mathbf{Q} + \nabla^+ \cdot \mathbf{R} \\ &\equiv \epsilon(p, \eta, \eta^+) + S(v, \eta, \eta^+), \end{aligned} \quad (24)$$

where the operator $\mathcal{L} \equiv (\partial^2/\partial \xi^2) + (\partial^2/\partial \psi^2) + 1/h^2(\partial^2/\partial \zeta^2)$, and ϵ includes the terms in the Poisson equation with nonconstant coefficients,

$$\begin{aligned} \epsilon(p, \eta, \eta^+) &= \left(\frac{1}{h^2} - \frac{1}{h h^+} \right) \frac{\partial^2 p}{\partial \zeta^2} + \zeta \left[\frac{\partial}{\partial \xi} \left(\frac{\eta_\xi}{h} \frac{\partial p}{\partial \zeta} \right) + \frac{\partial}{\partial \psi} \left(\frac{\eta_\psi}{h} \frac{\partial p}{\partial \zeta} \right) \right] \\ &\quad + \frac{\zeta}{h^+} \left(\eta_\xi^+ \frac{\partial^2 p}{\partial \xi \partial \psi} + \eta_\psi^+ \frac{\partial^2 p}{\partial \psi \partial \xi} \right) \\ &\quad - \frac{(\eta_\xi \eta_\xi^+ + \eta_\psi \eta_\psi^+)}{h h^+} \zeta \frac{\partial}{\partial \zeta} \left(\zeta \frac{\partial p}{\partial \zeta} \right), \end{aligned} \quad (25)$$

and S is the source term. Solution of the pressure Poisson equation can also be considered as finding the inversion $\mathcal{L}^{-1}$ such that

$$f(p) = p - \mathcal{L}^{-1}[\epsilon(p, \eta, \eta^+) + S(v, \eta, \eta^+)] = 0. \quad (26)$$

For the case of vanishing ϵ , such as that in the works of *Moeng* [1984] and *Tsai* [1998], the mixed scheme of pseudo-spectral and finite-difference methods results in a tridiagonal system of equations for the discrete Fourier coefficients of the pressure field. To retain the efficiency of tridiagonal matrix inversion, solution of the pressure Poisson equation (24) would require iterations. A direct approach is the fixed-point iteration [e.g., *Sullivan et al.*, 2000],

$$\mathcal{L}p^{(m)} = \epsilon(p^{(m-1)}, \eta, \eta^+) + S(v, \eta, \eta^+), \quad (27)$$

where the subscript m denotes the iteration level. Starting from a previous estimate of the pressure at iteration $m - 1$, the pressure Poisson equation for $p^{(m)}$ is solved by the same method as in the work by *Tsai* [1998] and *Tsai et al.* [2005].

[20] The number of iterations, however, increases as the steepness of the free-surface deformation grows. Furthermore, the fixed-point iteration (27) might diverge in rare cases. To accelerate the convergence of iteration, secant modification of Newton's formula [*Zhang*, 1997] is employed after every two fixed-point iterations,

$$\begin{aligned} p^{(m)} &= p^{(m-2)} - \frac{p^{(m-2)} - p^{(m-1)}}{\frac{f(p^{(m-2)}) - f(p^{(m-1)})}{p^{(m-2)} - p^{(m-1)}}} \\ &= p^{(m-2)} - \frac{[p^{(m-2)} - p^{(m-1)}][p^{(m-2)} - p^{(m-3)}]}{2p^{(m-2)} - p^{(m-1)} - p^{(m-3)}}, \end{aligned} \quad (28)$$

in which $p^{(m-2)}$ and $p^{(m-1)}$ are used as the two initial guesses in the quasi Newton's formula. The chosen mixed scheme guarantees converged iterations for all the simulations considered in this work (see sections 4 and 5) and also gives the optimal convergence rate.

[21] The accuracy in solving the pressure Poisson equation also determines if the mass conservation constraint of the velocity field is being satisfied. We therefore use the maximal error norm of the solution, $\|\mathcal{L}p^{(m)} - \epsilon(p^{(m)}) - S\|_{L_\infty}$, as the convergence criterion for the iterative procedure, instead of the commonly used difference norm, $\|p^{(m)} - p^{(m-1)}\|_{L_2}$. For the simulations presented in the following two sections, the convergence criterion has been chosen to be 10^{-6} , which results in a maximum velocity divergence of 10^{-9} and requires less than 10 iterations.

3.4. Treatment of Free-Surface Boundary Conditions

[22] At the time intervals of the temporal integration, the free-surface velocity $(v)_{\zeta=1}$ and the deformation η are known prior to solving for the pressure field. As such, the transformed normal-stress condition (17) can be considered as the Dirichlet condition on the upper boundary $\zeta = 1$ for the Poisson equation. For the convenience of numerical implementation, the discretized pressure p and the horizontal velocities, u and v , are distributed at the grid points on the free-surface boundary; and the vertical velocity w is stag-

gered half grid from the boundary. The present staggered-grid system differs from the traditional grid arrangement for no-slip boundary [e.g., *Moin and Kim*, 1982; *Moeng*, 1984], in which the vertical velocities are arranged on the boundary, instead.

[23] In contrast to the normal-stress condition, the tangential-stress conditions do not provide evolution equations; rather they describe the surface-normal momentum flux across the boundary. Accordingly, the tangential-stress surface conditions are satisfied implicitly in integrating the horizontal momentum equations at the free surface [*Tsai and Yue*, 1996]. The tangential-stress conditions are employed to solve for the vertical derivatives of the horizontal velocities, $(\partial u / \partial \zeta)_{\zeta=1}$ and $(\partial v / \partial \zeta)_{\zeta=1}$, as described in (18) and (19). The convection and diffusion terms in the ξ and ψ components of the transformed Navier-Stokes equation (15) at $\zeta = 1$ involve evaluation of the vertical derivatives, such as $\partial^2 u / \partial \zeta^2$ and $\partial(uv) / \partial \zeta$. Adopting central-difference schemes to compute these terms requires horizontal velocities at the fictitious grids above the free surface, which can be evaluated readily from (18) and (19). Similarly, the vertical velocity w arranged at the fictitious grids staggered above the free surface can also be determined from the solenoidal condition at the free surface.

4. Validation Studies

[24] All the governing differential equations and the boundary conditions are nonlinear; in particular, the nonlinear boundary conditions are satisfied on an unknown free surface. Validation of the developed model by direct comparison of the computational results with the known analytical solutions, therefore, is only possible for the limiting cases of vanishing viscosity or small-amplitude approximation. We first validate the accuracy and convergence of the model by simulating a two-dimensional progressive gravity wave on a water surface, and comparing the results with numerical solutions of the same wave but propagating in an inviscid fluid using both series expansion [*Fenton*, 1988] and boundary integral method [*Tsai and Yue*, 1993]. The effectiveness of the numerical implementation on satisfying the nonlinear free-surface boundary conditions is then demonstrated by simulating a two-dimensional gravity-capillary wave, and comparing with the weakly nonlinear solution of *Fedorov and Melville* [1998].

4.1. Two-Dimensional Gravity Wave

[25] We consider the periodic, progressive gravity waves with wavelength $\lambda = 10$ cm. (We have also tested other wavelengths. The conclusions, however, are identical to the case of $\lambda = 10$ cm.) By choosing the characteristic length and velocity as $L = 1/k = \lambda/(2\pi)$ and $U = (g/k)^{1/2}$, the Froude number is fixed as $Fr = U/(gL)^{1/2} = 1$ and the Reynolds number is $Re = UL/\nu \approx 6286$. The simulation is initiated by using a surface profile and the corresponding velocity distribution from the Stokes solution of a steady gravity wave [*Fenton*, 1988] with a prescribed steepness ak . As a comparison, numerical simulation using a mixed-Eulerian-Lagrangian scheme and a boundary integral formulation [*Tsai and Yue*, 1993] is also conducted for the nonlinear free-surface flow under inviscid approximation. Note that both the steady Stokes solution [*Fenton*, 1988] and the

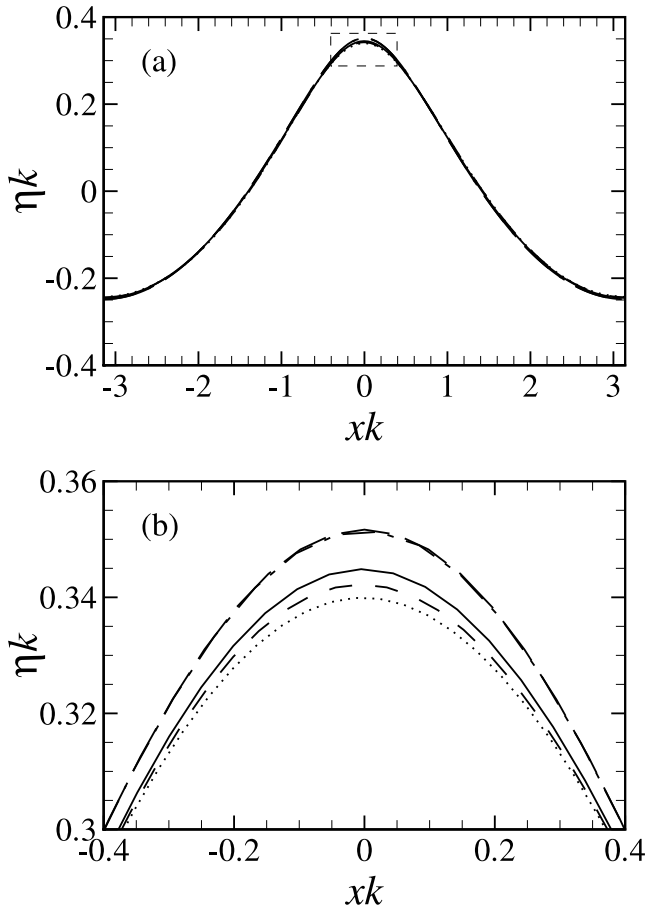


Figure 1. (a) Surface profiles of a two-dimensional progressive gravity wave after six wave periods computed by the present model using grid resolutions of $(N_x, N_z) = (128, 128)$ (solid line), $(32, 64)$ (dashed line) and $(24, 48)$ (dotted lines), by the boundary-integral method [Tsai and Yue, 1993] (dash-dotted line), and from the steady Stokes solution [Fenton, 1988] (long-dashed line). (b) The enlargement of the crest region indicated by the rectangle in Figure 1a.

simulation based on boundary integral method [Tsai and Yue, 1993] solve the Laplace equation subject to the inviscid dynamic free-surface boundary condition (Bernoulli equation). The present model, whereas, directly integrates the primitive Navier-Stokes equation subject to the solenoidal constraint and the stress-balance boundary conditions for the velocity field.

[26] The validation computations are conducted using three sets of grid resolution, $(N_x, N_z) = (24, 48)$, $(32, 64)$ and $(128, 128)$, where N_x and N_z are numbers of grids in the x and z directions, respectively; and for steepness $ak = 0.3$. For a gravity surface wave, the balance between the gravity and the inertia dominates the dynamics, and the effect of viscosity is minimal and confined within the thin boundary layer beneath the water surface. The surface profiles after six wave periods from the start of the simulation are shown in Figure 1. Despite the differences in the mathematical formulations and the numerical methods, the computation results from the present model, the inviscid boundary-integral simulation [Tsai and Yue, 1993] and the Stokes

solution [Fenton, 1988] are visually indistinguishable (Figure 1a). The differences in the surface profiles can only be seen in a zoomed window as shown in Figure 1b where the crest region is enlarged (about 8 times enlargement). The two solutions based on potential flow formulation are virtually identical. The crest elevations from the present simulations of viscous flow are slightly lower than that from computations of inviscid wave; this might be attributed to the effect of viscosity. The close comparison thus indicates the accuracy of the developed model in solving the field equations and in implementing the nonlinear free-surface boundary conditions. Also, the result of the low-resolution calculation, $(N_x, N_z) = (24, 48)$, deviates very little from that of the high-resolution simulation, $(N_x, N_z) = (128, 128)$, indicative of the accuracy and convergence of the present numerical scheme.

[27] The accuracy of the simulations can also be asserted by monitoring the global constraints, including the properties of mass and energy conservations. Figure 2 depicts the evolutions of three mass-conservation properties for the grid resolution of $(N_x, N_z) = (24, 48)$. At the end of the simulation, the mean free surface is conserved to be within the machine precision, $k^3 \int \eta dx dy < 10^{-16}$; while the error norm of the velocity divergence, $(gk)^{-1/2} \|\nabla \cdot \mathbf{v}\|_{L_2}$, is less than 10^{-10} , and the maximal velocity divergence, $(gk)^{-1/2} \|\nabla \cdot \mathbf{v}\|_{L_\infty}$, is less than 10^{-8} . Note that the error properties of velocity divergence depend on the value of convergence criterion used in iterative solution of the Poisson equation. We have used 10^{-6} as the criterion in all the calculations.

[28] In order to monitor the energy conservation, energy equation (20) is integrated in time with the simulation. For the case of the pure gravity wave without surface forcing, the terms E_σ , E_{τ_n} and E_{τ_t} vanish. The evolutions of the relative errors of the energy conservation, $[E_k(t) + E_\eta(t) + E_\nu(t)]/[E_k(0) + E_\eta(0) + E_\nu(0)]$ are plotted in Figure 3a for the three grid resolutions considered. The error decreases

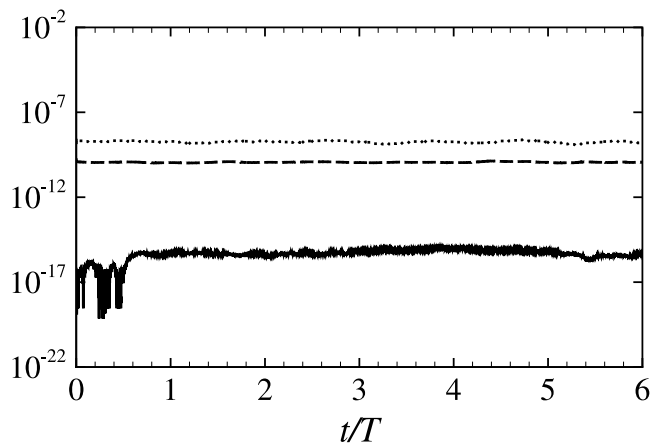


Figure 2. Evolutions of the properties of the mean free surface $k^3 \int \eta(x, y, t) dx dy$ (solid lines), the error norm of velocity divergence $(gk)^{-1/2} \|\nabla \cdot \mathbf{v}\|_{L_2}$ (dashed lines), and the maximal velocity divergence $(gk)^{-1/2} \|\nabla \cdot \mathbf{v}\|_{L_\infty}$ (dotted lines) for the validate simulation of a two-dimensional progressive gravity wave. The grid resolution is $(N_x, N_z) = (24, 48)$. The time t is normalized by the period T of the steady Stokes solution [Fenton, 1988].

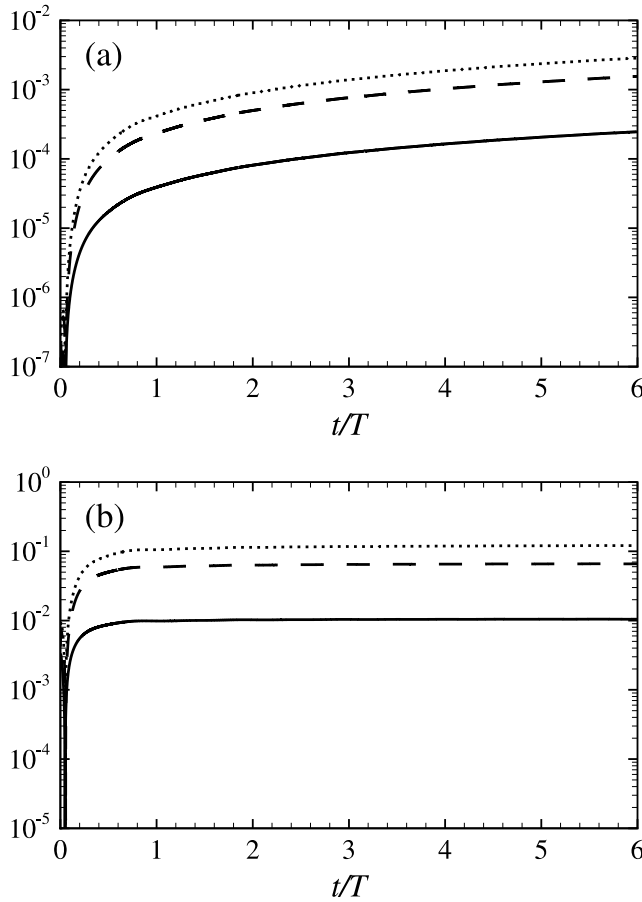


Figure 3. Evolutions of the relative errors of energy conservation for the validation simulation of a two-dimensional progressive gravity wave using the grid resolutions of $(N_x, N_z) = (24, 48)$ (dotted line), $(32, 64)$ (dashed line), and $(128, 128)$ (solid line). (a) Energy error normalized by the initial energy $[E_k(t) + E_\eta(t) + E_\nu(t)]'_0 / [E_k(0) + E_\eta(0) + E_\nu(0)]$. (b) Energy error relative to the energy lost by viscous dissipation $-[E_k(t) + E_\eta(t) + E_\nu(t)]'_0 / E_\nu(t)$. The time t is nondimensionalized by the period T of the steady Stokes solution [Fenton, 1988].

with finer grid resolution. Within a very short initial spinup period the energy errors increase significantly. After that the energy error becomes steady asymptotically. For the high-resolution computation, $(N_x, N_z) = (128, 128)$, the energy lost after six wave periods is only about 0.01% of the initial total energy; and the rate of relative energy lost owing to numerical dissipation and errors, $[E_k(t) + E_\eta(t) + E_\nu(t)]'_0 / E_\nu(t)$, remains to be about 1% of the viscous dissipation as shown in Figure 3b.

4.2. Two-Dimensional Gravity-Capillary Wave

[29] Since the surface boundary conditions are satisfied exactly on the free-surface boundary, the present model therefore is competent of simulating the strongly nonlinear surface processes, such as the capillary ripples rising on gravity waves. To demonstrate the effectiveness of the model in resolving the parasitic capillaries, gravity-capillary waves forced by a surface pressure are simulated and the results are compared with the weakly nonlinear (second-

order) solutions of *Fedorov and Melville* [1998]. Following the formulation of the analytical solution, a pressure distribution, which balances the viscous dissipation and achieves a steady weakly nonlinear solution, is applied on the water surface as

$$\tau_n^s(x, t) = p_0 \rho c_0^2 \cos(kx - \Theta - ct), \quad (29)$$

where p_0 is a nondimensional parameter which specifies the amplitude of the pressure forcing, $c_0 = (g/k + \sigma k)^{1/2}$ is the phase velocity of a linear gravity-capillary wave, $c = c_0[1 + (p_0/ak)\cos\Theta]^{1/2}$ is the weakly nonlinear phase velocity, and Θ is the phase shift of the maximum of the pressure forcing with respect to the crest of the gravity wave. Two possible solutions of Θ (Class 1 and Class 2, named Θ_1 and Θ_2) have been determined by *Fedorov and Melville* [1998], which give

$$\Theta_1 \approx -\pi + \frac{4\nu k}{c_0} \frac{ak}{p_0} \quad \text{and} \quad \Theta_2 \approx -\frac{4\nu k}{c_0} \frac{ak}{p_0}. \quad (30)$$

Such a shift is necessary for the pressure forcing to transfer energy into the wave to balance viscous dissipation. The physical properties of the two classes of waves, however, are only slightly different as long as the pressure forcing remains relatively small [Fedorov and Melville, 1998].

[30] The gravity-capillary wave simulation is made for the Class 1 wave with wavelength $\lambda = 5$ cm and initial steepness $ak = 0.28$. The value of the forcing amplitude is chosen as $p_0 = 0.0069$. The simulation is initiated with the surface profile and velocity field of a third-order weakly nonlinear Stokes gravity wave without any prescribed parasitic capillary waves. The surface tension and the pressure forcing are imposed spontaneously on the free surface at the start of the simulation. The computations are conducted using a grid resolution of $(N_x, N_z) = (128, 128)$. The global properties of mass and energy conservation resemble those of Figures 2 and 3 using the same grid resolution.

[31] The simulated results of the surface elevations η and slopes η_x are shown in Figure 4 at various representative time intervals. For comparison, pure gravity wave with no surface tension is also computed and the results are also presented. To better reveal the surface variation, the frame of reference is moved with the linear phase speed c_0 . As shown in Figure 4 (dotted lines), the initial surface elevation/slope of the pure gravity wave is symmetric/antisymmetric with respect to the crest. As time proceeds, the surface profile of the gravity-capillary wave becomes asymmetric and the crest shifts toward downstream; while that of the gravity wave remains symmetric. Accompanying the formation of the asymmetric surface profile, short-wavelength capillaries begin to generate from the crest and propagate downstream along the forward face of the dominant gravity wave. The generation and propagation of the capillaries continue; the leading waves of the capillary train even travel across the trough and reach the backward face of the next cyclic wave.

[32] For the present fully nonlinear computation, there exists no steady state for the posed initial condition and the surface forcing. Comparison with the weakly nonlinear, steady solution of *Fedorov and Melville* [1998] therefore

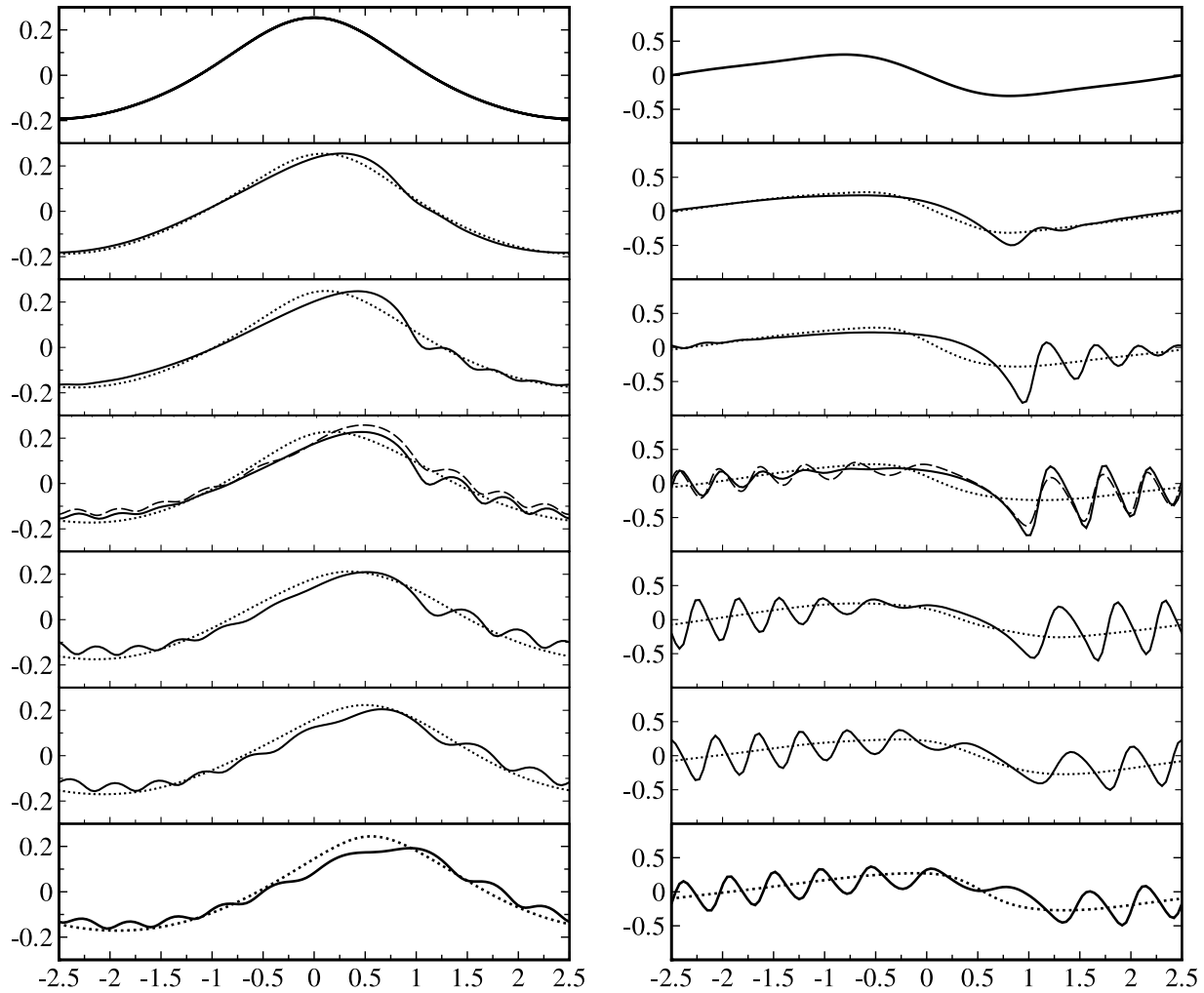


Figure 4. (left) Surface elevations and (right) slopes of gravity-capillary waves (solid lines) and gravity waves with no surface tension (dotted lines) from the present fully nonlinear simulation. From the top to the bottom, the simulation results are instantaneous profiles at the time intervals $t = nT_0/2$, where n is integer ranging from 0 to 6 and $T_0 = (gk + \sigma k^3)^{1/2}$ is the time period of the linear wave. The dashed lines in the plots for $t = 1.5T_0$ are the weakly nonlinear solutions of *Fedorov and Melville* [1998].

is made by choosing an instantaneous wave profile with a steepness similar to that of the steady wave. This is shown in Figure 4 at the time interval $t = 1.5T_0$, where $T_0 = (gk + \sigma k^3)^{1/2}$ is the period of a linear gravity-capillary wave. The weakly nonlinear solution is the case of $ak = 0.25$ in Figure 4 of *Fedorov and Melville* [1998]. Note that the viscous dissipation in the weakly nonlinear solution is confined to within the thin boundary layer, and is weaker than that of a real flow. Although the simulated wave is initiated with a greater steepness, the amplitude decays as the parasitic capillaries develop. At the time when the fully nonlinear wave evolves to a steepness close to that of the steady weakly nonlinear wave, the two results share qualitatively identical surface profiles with the same number of parasitic capillaries riding on the dominant gravity wave.

[33] Evolutions of the individual terms in the energy balance equation (20) for both the gravity-capillary and the gravity waves are shown in Figure 5. (The multiperiod undulation in the work done by the surface pressure forcing,

$E_{\tau_{sn}}^{\tau_s}$, is attributed to the deviation of the nonlinear phase velocity from the linear velocity c_0 of the surface forcing. As a consequence, the variations of other energy budget terms also exhibit such an undulation.) The viscous dissipation for a pure gravity wave is weak, and the kinetic and potential components dominate the balance of energy budget as shown in Figure 5b. However, for the gravity-capillary wave with parasitic capillaries developed, the viscous dissipation increases drastically, which is then reflected in the enhanced decay of both kinetic and potential energies. The e -folding dissipation rate of the gravity-capillary wave is estimated to be about 17 times that of a linear gravity wave, $\beta/\beta_0 \approx 17$. This is close to the laboratory measurement obtained by *Zhang* [2002].

5. Applications

[34] The simulated examples in the above validation study are two-dimensional flows. To further demonstrate

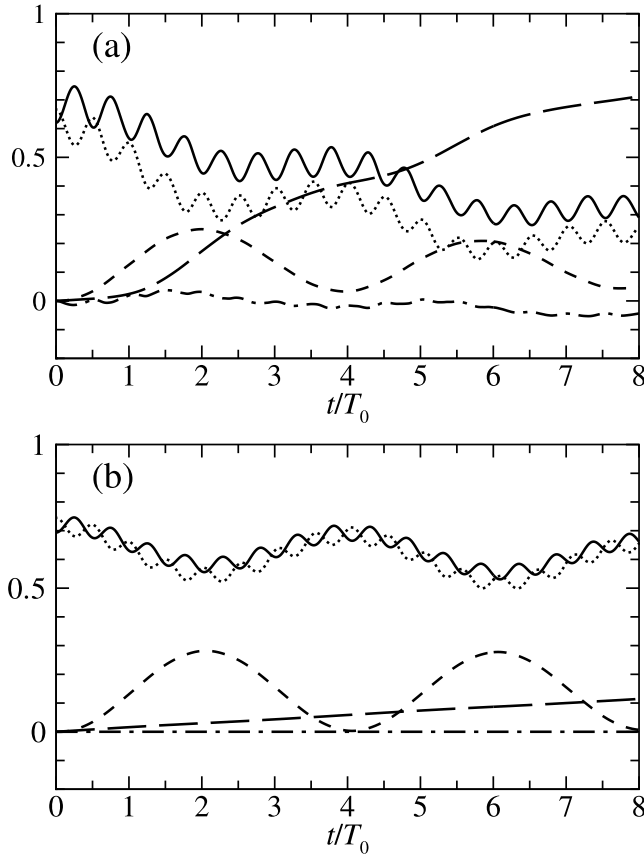


Figure 5. Evolutions of various terms in the energy budget equation (20) for (a) the gravity-capillary wave and (b) the gravity wave: the kinetic energy E_k (solid line), the potential energy E_η (dotted line), the work done by the surface tension E_σ (dash-dotted line), the work done by the surface normal forcing $E_{\tau_n}^s$ (dashed line), and the energy dissipation by viscosity $-E_\nu$ (long-dashed line). The time t is nondimensionalized by the period of the linear wave $T_0 = (gk + \sigma k^3)^{1/2}$.

the potential capabilities of the developed model for studying the small-scale processes on the dynamic ocean surfaces, three examples of three-dimensional flows are presented in this section. The first example considers short-crested gravity-capillary waves that exhibit characteristic rhombic patterns. The second application simulates the development into a crescent (or horseshoe) pattern of a steep gravity wave. It is worth noting that there exist other numerical methods, which employ boundary integral formulations, for the simulations of fully nonlinear three-dimensional free-surface flows [e.g., *Fructus et al.* 2005a; *Xue et al.* 2001]. The dominant dynamics of the nonlinear surface-wave motions are the focuses in these methods; and the underlying flows are considered to be inviscid and irrotational. In addition to resolving accurately the nonlinear dynamics of surface waves, the present model also emphasizes simulating the interaction between the surface waves and the turbulent flows underneath. The first two applications, therefore, aim to highlight the model capability of resolving the nonlinear surface-wave processes. In the third application, turbulent shear flow beneath a wind-driven wavy water surface is considered. This example will demonstrate

the types of flows amenable to simulation using the present model.

5.1. Short-Crested Gravity-Capillary Wave

[35] It has been observed from laboratory experiments of wind-wave generation that even during the initial stages of the developing process the water surface can exhibit three-dimensional wave patterns and the underneath flow field undergoes three-dimensional evolution [*Caulliez and Collard*, 1999; *Ebuchi et al.*, 1987; *Veron and Melville*, 2001]. The three-dimensional wave field is composed of oblique gravity waves with parasitic capillary waves appearing on the front faces of the dominant gravity waves. In the experiment of *Caulliez and Collard* [1999], steep three-dimensional waves exhibiting rhombic patterns emerge from a random short gravity-capillary wave field. The wave motions are formed by two predominant symmetric oblique waves with wavelength falling into a very specific range of $\lambda \approx 4 \sim 10$ cm, and propagating at angles $\varphi \approx \pm 30^\circ$ to the wind direction. *Caulliez and Collard* [1999] postulated that the formation of such well-pronounced wave patterns of definite scales at the early stage of wind-wave generation is attributed to resonant triad interaction of gravity-capillary waves.

[36] To demonstrate the appearance of such characteristic rhombic patterns and the subsequent development of the parasitic capillaries, the simulation is initiated with a weakly nonlinear short-crested wave field [*Hsu et al.*, 1979], which results from superposition of two oblique traveling periodic waves with the same wavelength λ and amplitude. The wave field is symmetric doubly periodic in both x and y directions with the corresponding wavelengths $\lambda/\cos \varphi$ and $\lambda/\sin \varphi$, where 2φ is the angle between the propagation directions of the two waves. From the characteristic length scales (4 to 10 cm) and oblique propagation angle (30°) observed by *Caulliez and Collard* [1999], a canonical problem with wavelength $\lambda = 7.5$ cm, steepness $ak = 0.35$ and propagation angle $\varphi = 30^\circ$ is posed for the simulation. Accordingly, the length and width of the computational domain are 8.66 cm and 15 cm, respectively; and the depth is 8 cm. The simulation is carried out with 128^3 grid points. In the vertical direction near the upper surface, the stretched grid distribution allows sufficient resolution of the viscous layer.

[37] The three-dimensional wave pattern and the distributions of the longitudinal and transverse surface slopes at the early and developed stages are depicted in Figure 6. To better reveal the wave pattern, the doubly periodic domain is repeated twice in both x and y directions. At the early stage of the evolution, the surface elevation exhibits rhombic patterns due to two gravity waves propagating obliquely to the wind (Figures 6a and 6b); but the wave begins to show sign of nonlinearity, as in the two-dimensional gravity-capillary wave considered in the previous section, with the longitudinal surface profile becoming asymmetric and tilting slightly toward the downstream face. As time proceeds, parasitic capillary waves develop on the front faces of the two obliquely propagating dominant gravity waves (Figures 6c and 6d) as observed in the experiments of *Caulliez and Collard* [1999] and *Veron and Melville* [2001]. The two groups of parasitic capillary waves, which reside on and propagate with the oblique steep waves, cross

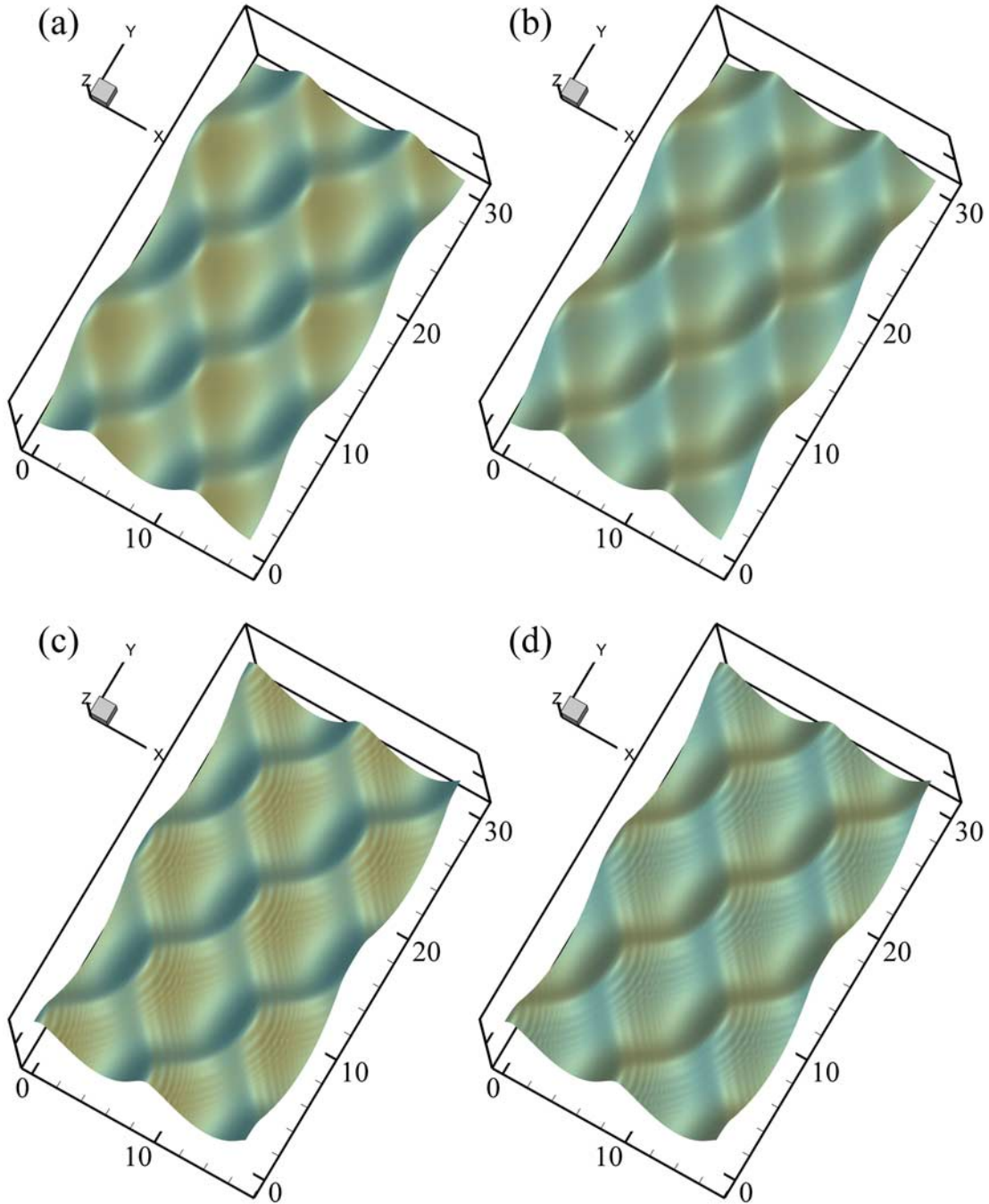


Figure 6. Three-dimensional surface patterns of short-crested gravity-capillary waves at two representative time intervals: (a, b) $t = 0.5T_0$ and (c, d) $2T_0$, where $T_0 = (gk + \sigma k^3)^{1/2}$ is the linear period. The color maps superimposed on the surface characterize the distributions of the longitudinal surface slope η_x (Figures 6a and 6c) and the transverse slope η_y (Figures 6b and 6d), with the blue/yellow color represents the positive/negative slope. The periodic domain is repeated twice in both the x and y directions.

each other and result in further nonlinear interaction between the two packets.

5.2. Development Into Crescent Pattern of a Steep Gravity Wave

[38] Three-dimensional gravity waves exhibiting crescent (or horseshoe) surface patterns have been observed exper-

imentally by Su [1982] and Su *et al.* [1982], and more recently by Caulliez and Collard [1999] and Collard and Caulliez [1999]. Stability analysis [McLean, 1982] indicates that the formation of these patterns is attributed to two-dimensional instabilities of one-dimensional wavetrains. Recent numerical simulations [Fructus *et al.*, 2005a, 2005b; Xue *et al.*, 2001] confirm the instability mechanism

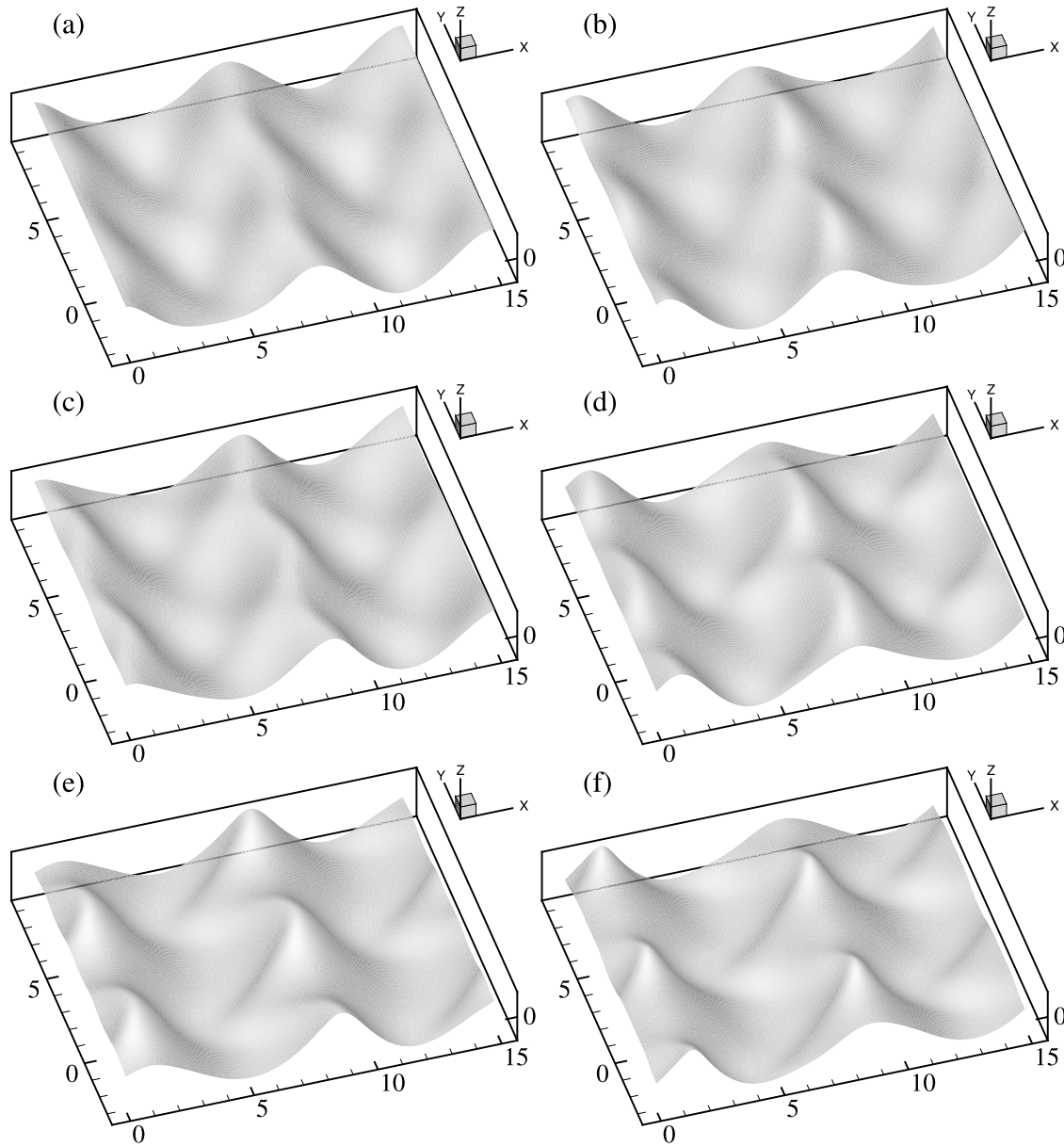


Figure 7. Three-dimensional prospective surface profiles showing the modulation of a steep gravity-wave train to form the crescent-shaped pattern at the time intervals $t = nT_0$, where $n = 0$ to 5 and $T_0 = (gk)^{1/2}$ is the linear period of the corresponding gravity wave. For clarity the periodic domain is twice in the y direction.

that an initial uniform wavetrain of large amplitude subject to three-dimensional perturbations is unstable and will evolve into a series of crescent-shaped wave groups as observed in the experiments.

[39] Following the simulations of *Fructus et al.* [2005a] and *Xue et al.* [2001], we consider the emergence of crescent wave pattern from a three-dimensional perturbation corresponding to the unstable modes obtained from linear stability analysis of *McLean* [1982]. Specifically, a perturbed surface deformation of the form,

$$\eta'(x, y, t) = \frac{1}{2} a_\epsilon [\sin(k_x x + k_y y - \omega t) + \sin(k_x x - k_y y - \omega t)],$$

(31)

and the corresponding perturbed velocity field are added to the plane gravity wave of wave number k and surface amplitude a , where a_ϵ is the perturbation amplitude, the longitudinal and transverse perturbation wave numbers $k_x = (1 + p)k$ and $k_y = qk$. For the present simulation, the values of p and q are chosen as 0.5 and 1.23 , which corresponds to the most unstable perturbation of the subharmonic class II instability in the analysis of *McLean* [1982]. The initial plane gravity wave field is prescribed from numerical solution of the exact Stokes wave of *Fenton* [1988] with steepness $ak = 0.25$ and wavelength $\lambda = 7.5$ cm. The initial amplitude of the perturbed wave is 20% that of the plane gravity wave, $a_\epsilon/a = 0.2$. For the perturbed wave number $(p, q) = (0.5, 1.23)$, the sizes of the computation

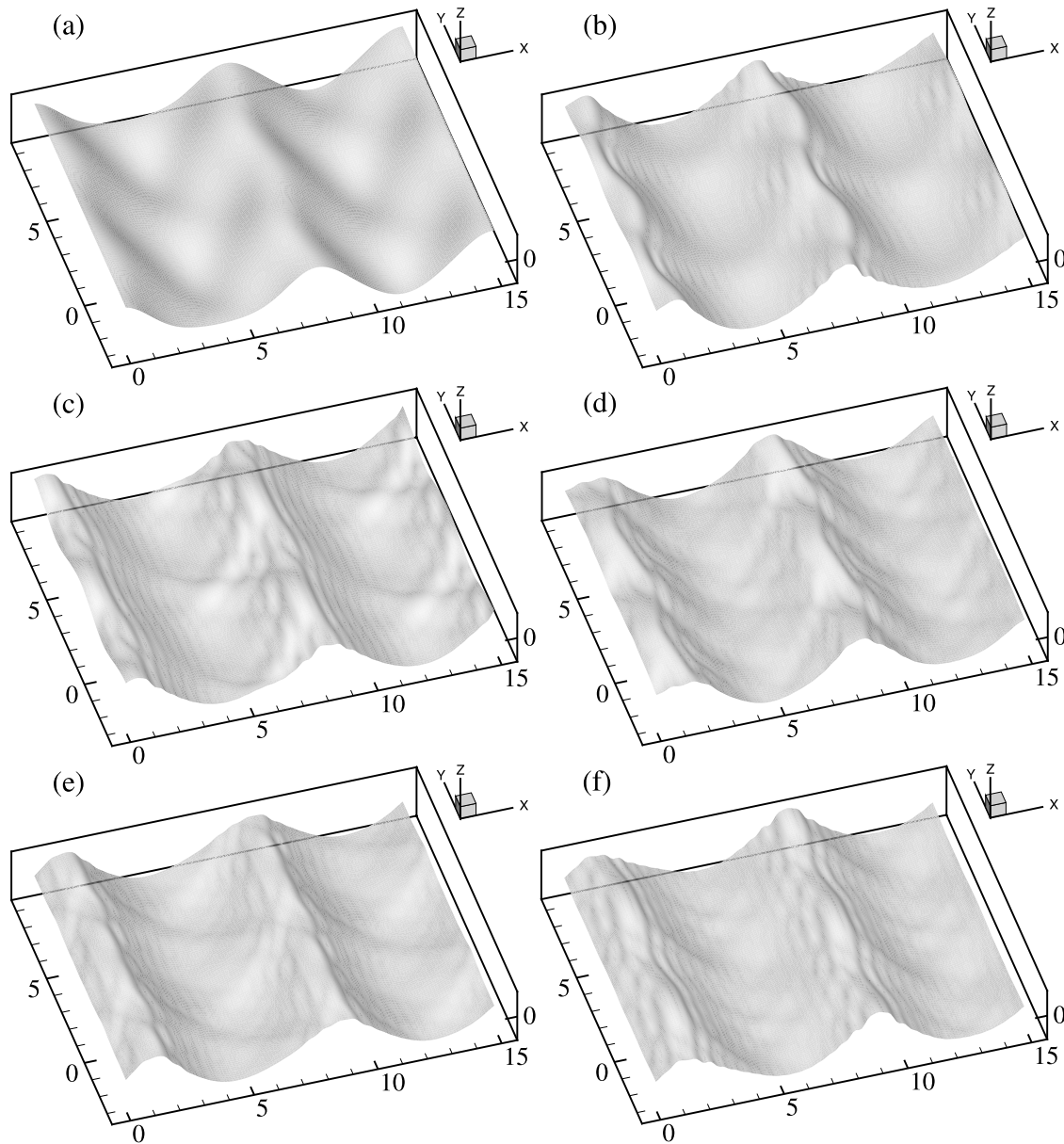


Figure 8. Three-dimensional prospective surface profiles showing the nonlinear evolution of a gravity–capillary wave train and the generation of parasitic capillaries at the time intervals $t = nT_0$, where $n = 0$ to 5 and $T_0 = (gk + \sigma k^3)^{1/2}$ is the linear period of the corresponding gravity wave. For clarity the periodic domain is repeated twice in the y direction.

domain are $\lambda/p = 15$ cm and $\lambda/q \approx 6.1$ cm, respectively, in the longitudinal (x) and transverse (y) directions; the lower boundary is located at $z = -6$ cm. The number of grids used for the computation is $(N_x, N_y, N_z) = (128, 64, 128)$.

[40] Instantaneous prospective surface profiles at representative time intervals of the nonlinear evolution are shown in Figure 7. For clarity of illustration, the domain is repeated two wavelengths in the y directions. Shortly after the start of the simulation, the perturbed disturbance grows and the staggered row-shift surface structure begins to form (Figures 8b and 8c). As the evolution continues, the crescent-shaped patterns are well formed (Figures 8e and 8f). The forward fronts of the crescents have sharper crest angles than the trough edges where two crescents meet. The

nonlinear features of these crescent-shaped patterns are identical to those that have been observed in the computations by *Xue et al.* [2001] and *Fructus et al.* [2005a]. These results also demonstrate the capability of the present model in simulating the nonlinear interaction processes of surface gravity waves.

[41] With the developed model, which can resolve the surface waves down to the capillary scale, the effect of capillary waves in the formation of the crescent waves can be simulated readily. Such an issue has not yet been studied. The corresponding surface profiles of Figure 7 but with surface tension included in the free-surface boundary condition are depicted in Figure 8. Similar to the case without surface tension, at the early stage of the evolution, clear

three-dimensional surface patterns have been developed from the initial perturbation (Figure 8b). Accompanying the growth of the staggered row-shift undulation of the dominant gravity wave, capillary waves also generate from the crests and propagate downstream. The effect of these parasitic capillary waves on the development of the unstable perturbation is still not appreciable at this early stage. The impact, however, becomes significant as the evolution proceeds, as shown from Figures 8c–8f. The growth of the unstable three-dimensional waves is apparently moderated. The formation of the crescent-shaped wave patterns is not as discernible as that of the pure gravity wave. Such a distinct feature in impeding the continuous growth of the instability seems also attributed to the enhanced dissipation due to the parasitic capillaries.

5.3. Turbulent Shear Flow Beneath a Wind-Driven Wavy Water Surface

[42] Breaking of very short gravity waves without air entrainment, which is termed “micro-breaking” by *Banner and Phillips* [1974], occurs ubiquitously over the oceans. It is found that the occurrence of microbreaking is far more widespread than that of whitecaps caused by spilling breakers in open oceans [*Banner and Peregrine*, 1993]. This also suggests significant impacts of microscale wave breaking on the fluxes of gas and heat across the air-sea interface [e.g., *Csanady*, 1990; *Zappa et al.*, 2001]. Moreover, microscale breaking waves also govern to a large extent the reflection and the backscattering of electromagnetic waves in active microwave remote sensing of the oceans [e.g., *Banner and Fooks*, 1985; *Rozenberg et al.*, 1999]. In contrast to the visible manifestation of whitecapping, micro-breaking is more difficult to detect owing to the lack of air entrainment. A popular approach in recent years to identify and quantify microscale wave breaking is to infer the event from infrared imagery of water surface [e.g., *Jessup et al.*, 1997]. The accuracy of the technique thus relies on relating quantitatively the small-scale surface signatures to the underlying turbulence processes.

[43] The surface deformation of a microbreaking wavelet is characterized by a bore-like crest accompanied by parasitic capillary waves distributed along the forward face [e.g., *Ebuchi et al.*, 1987; *Jessup et al.*, 1997]. The typical wavelength is within $O(0.1 \sim 1)$ m and the amplitude is a few centimeters. The underlying flow structures were investigated in detail in laboratory flumes by *Okuda* [1982] and *Ebuchi et al.* [1987]. In the measurement by *Okuda* [1982], flow separation with distinct vorticity near the crest was identified. In addition to the parasitic capillary waves trapped on the forward face of the dominant wave, *Ebuchi et al.* [1987] also observed streamwise streaky structures on the windward face.

[44] No numerical simulations of the flow processes have yet been performed ever since the observation of *Ebuchi et al.* [1987]. We postulate that the fine structures on the wind-wave surface observed by *Ebuchi et al.* [1987] might be induced by the interaction between the surface gravity waves and the sheared turbulent flow underneath. We therefore pose the simulation by considering a three-dimensional turbulent shear flow beneath surface waves, and driven by pressure forcing and shear stress. For the posed model flow, the distribution of the surface-normal pressure

forcing is specified by (29). Following the measurement of *Banner and Peirson* [1998], the streamwise tangential shear stress is modeled as

$$\tau_{tx}^s(x, t) = \tau_0[1 + \cos(kx - \Theta_t - ct)], \quad (32)$$

where τ_0 is the mean tangential shear stress and Θ_t is the phase shift of the maximum tangential stress with respect to the wave crest.

[45] To initiate the simulation, the flow field is posed by superposition of a two-dimensional nonlinear Stokes wave $\mathbf{v}_w$, a two-dimensional mean shear profile U and a three-dimensional fluctuating velocity field $\mathbf{v}'$,

$$\mathbf{v}(x, y, z) = \mathbf{v}_w(x, z) + U(x, z) + \mathbf{v}'(x, y, z), \quad (33)$$

where the shear velocity profile is given as

$$U(x, z) = \left[\frac{\tau_{tx}^s(x, 0)}{2\tau_0} \right] U_0 \exp\left(\frac{2\tau_0}{\rho\nu U_0} z \right), \quad (34)$$

U_0 is the initial mean surface velocity at $z = \eta$. The initial fluctuating velocity field $\mathbf{v}'$ is imposed as that in *Tsai et al.* [2005], which is homogeneous in both streamwise and spanwise directions. Thus the only flow structure of the initial velocity field is the two-dimensional wavy motion in the x - z plane associated with the gravity wave. We consider an initial gravity wave with a wavelength $\lambda = 7.5$ cm and steepness $ak = 0.25$. Both the width and the depth of the computational domain are chosen to be the same as the wavelength. The simulation is carried out with 128^3 grid points. The initial mean shear profile is chosen such that the surface velocity $U_0 = 10$ cm/s, the mean tangential shear stress $\tau_0 = 2$ dyn/cm² and the phase shift from the crest $\Theta_t = -50^\circ$. For the surface-normal pressure distribution (29), Class 1 forcing (30) is considered and the pressure parameter $p_0 = 0.00078$, which results in a normal-stress amplitude of $\|\tau_n^s\| = 0.963$ dyn/cm².

[46] Despite the idealizations inherent in conducting the simulation, the computed flow exhibits the major surface features, qualitatively identical to those observed in the experiment of *Ebuchi et al.* [1987]. To demonstrate the characteristic structures on the water surface, instantaneous contour distributions of the free-surface deformation (η) and the streamwise and spanwise surface slopes (η_x , η_y) are shown in Figure 9, and the turbulent fluctuating velocities (u' , v' , w') in Figure 10 at two representative time intervals. The turbulent fluctuating velocity $\mathbf{v}'$ is defined as

$$\mathbf{v}'(x, y, z) = \mathbf{v}(x, y, z) - \frac{1}{\lambda_y} \int_0^{\lambda_y} \mathbf{v}(x, \tilde{y}, z) d\tilde{y}. \quad (35)$$

[47] As depicted in the early stage of surface distributions (Figures 9a, 9c, and 9e), the initial water surface is prescribed by only a gravity wave deformation without any other fine structures. As the flow evolves (Figures 9b, 9d, and 9f), the distribution patterns of surface slopes clearly demonstrate the generation of parasitic capillary waves on the forward face of the predominant gravity wave as observed by *Ebuchi et al.* [1987] and *Veron and Melville* [2001] in wind-wave flumes. The capillary ripples extend

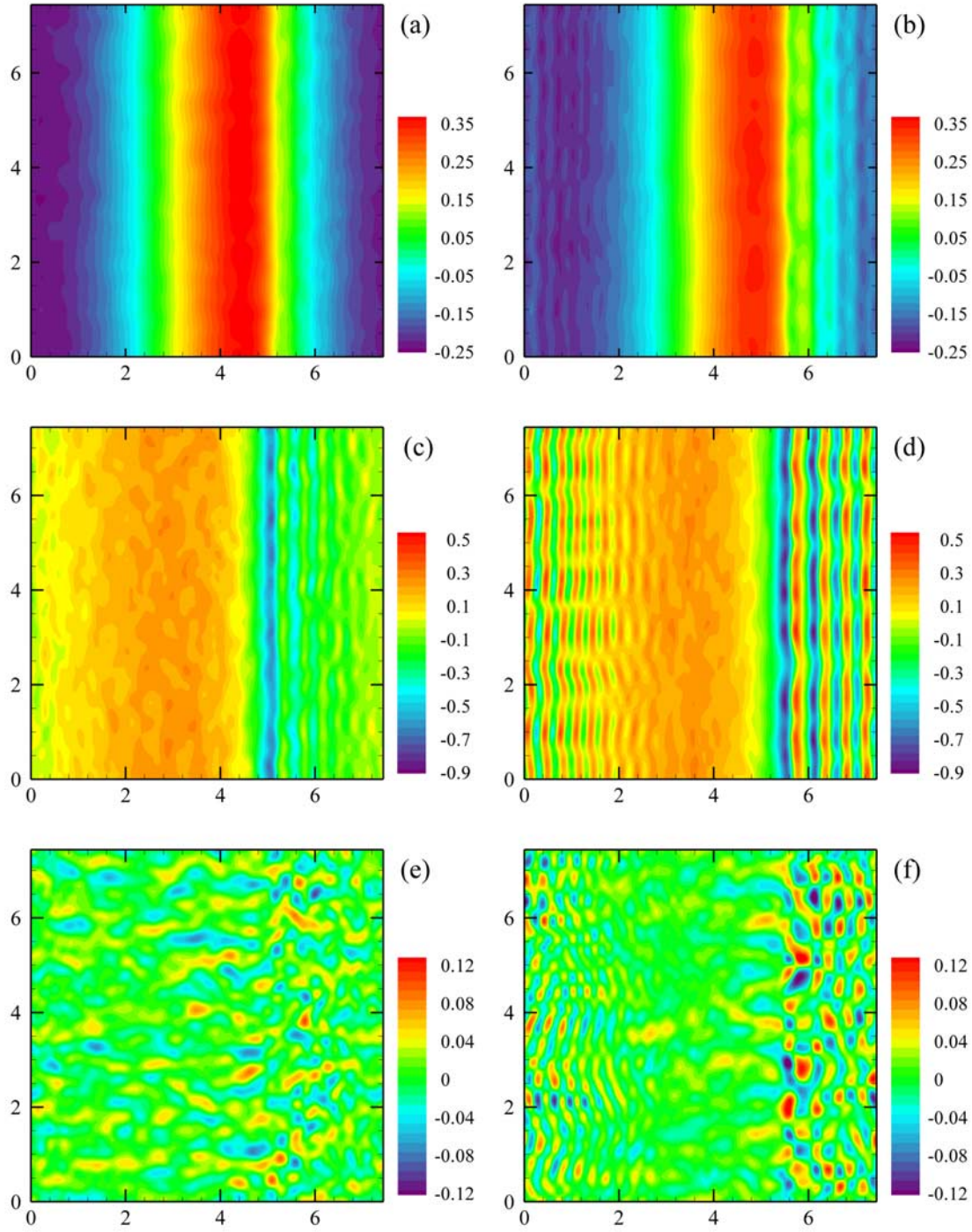


Figure 9. Representative contour distributions of the (a, b) surface elevation, (c, d) along-wind surface slope, and (e, f) cross-wind surface slope at $t = T_0$ (Figures 9a, 9c, and 9e) and $2T_0$ (Figures 9b, 9d, and 9f), where $T_0 = (gk + \sigma k^3)^{1/2}$ is the time period of the linear wave. The flow travels from left to right.

from the crest toward the trough of the gravity wave. The crest/trough lines of the parasitic ripples are more or less parallel to that of the dominant gravity wave but exhibit spanwise undulation.

[48] Accompanying the formation of the parasitic capillaries, elongated streaky structures also become apparent on the fluctuating velocity distributions (Figure 10). On the

backward face near the crest of the dominant gravity wave, both the along- and cross-wind fluctuating velocities exhibit streaky structures. The major streaks are arranged with somewhat equal transverse spacing. The average interval is about 0.625 cm, which is close to the observation of *Ebuchi et al.* [1987]. These surface fine structures are further illustrated by depicting in Figure 11 the three-

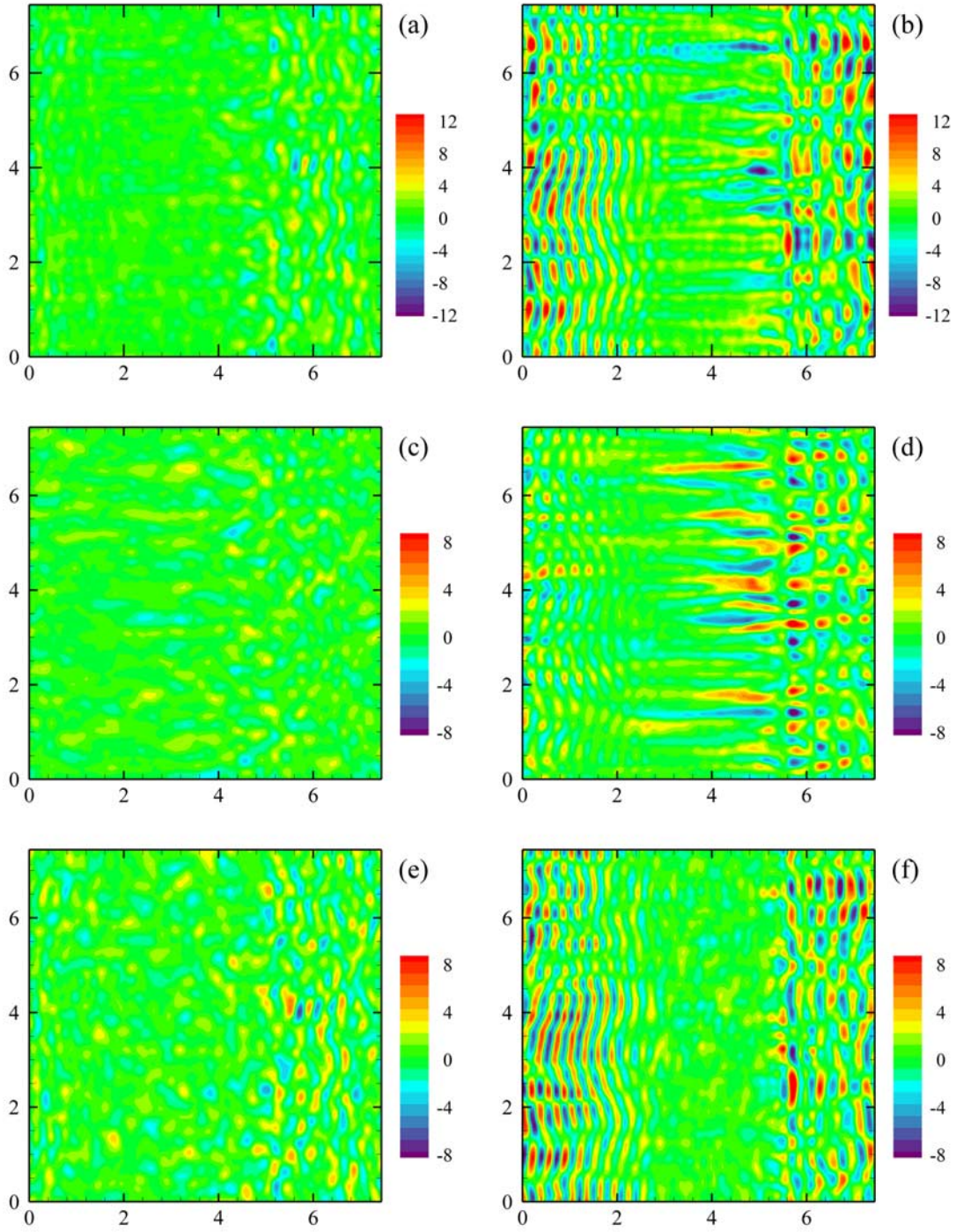


Figure 10. Representative contour distributions of the (a, b) surface turbulent streamwise velocity, (c, d) spanwise velocity, and (e, f) vertical velocity at $t = T_0$ (Figures 10a, 10c, and 10e) and $2T_0$ (Figures 10b, 10d, and 10f), where $T_0 = (gk + \sigma k^3)^{1/2}$ is the time period of the linear wave. The flow travels from left to right.

dimensional prospective surface profiles with the turbulent crosswind velocity distribution superimposed. The two pictures viewing from the front and back of the wave clearly resemble that observed by *Ebuchi et al.* [1987, Figure 11].

[49] In the region where parasitic capillary waves exist (forward face from the crest), the streamwise velocity

streaks are annihilated. Instead, the fluctuating velocity distributions exhibit two-dimensional oscillatory patterns. For the streamwise and vertical components, the patterns resemble a chessboard. The positive and negative extreme velocity regions are arranged alternately in both streamwise and spanwise directions of the chessboard patterns; with the streamwise wavelength identical to that of the parasitic

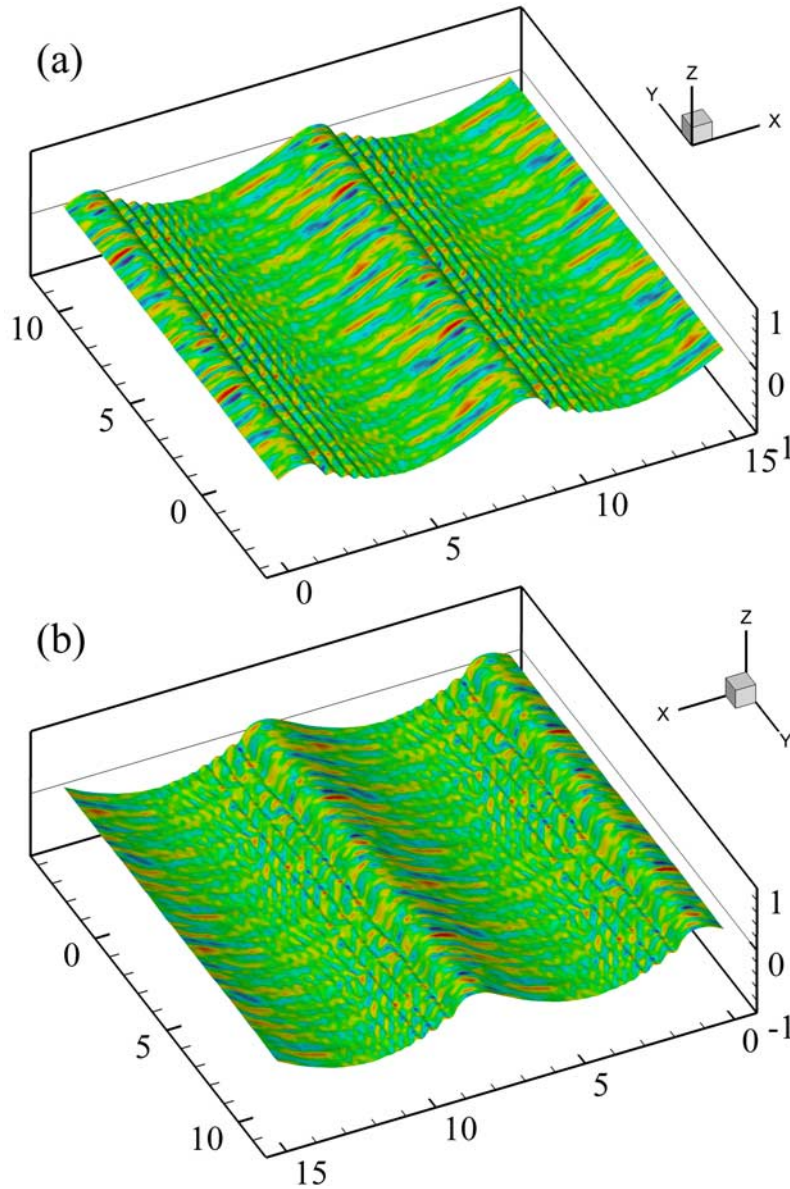


Figure 11. Three-dimensional prospective surface profile, viewing from (a) the back and (b) the front of a wind-driven surface wave showing the parasitic capillary waves on the forward face and the streaky velocity structures on the backward face. The color map superimposed on the surface is the contour distribution of the cross-wind turbulent velocity $v'(x, y, z)$ with the red/blue color representing the positive/negative value. For clarity the periodic domain is repeated twice in both the x and y directions.

capillaries, and the spanwise spacing close to that of the velocity streaks. These surface structures imply strong interactions between the streaky velocity field associated with the turbulent shear flow and the orbital velocities induced by the parasitic capillary waves. Further studies are needed to unravel the formation mechanisms of the parasitic capillary waves and the streamwise surface streaks, as well as the interaction between the two.

[50] To further illustrate the corresponding vortical structures beneath the characteristic surface features of Figure 11, contour distributions of the spanwise turbulent vorticity ω'_y on representative vertical planes parallel to the wind direction are shown in Figure 12. Some of the vortical structures have been identified in previous experimental

studies, although the results exhibit spanwise variability as suggested by *Jessup et al.* [1997]. The typical vorticity distributions (Figure 12a) confirm the laboratory observations of *Okuda* [1982] and *Ebuchi et al.* [1987] that a high-vorticity region exists near the crest of the dominant gravity wave. The distributions reveal that such a vortical roller originates from the accompanying parasitic capillaries [Longuet-Higgins, 1992], which induce vortex shedding by the curvature effect. *Yoshikawa et al.* [1988] and *Komori et al.* [1993] reported evidences of downward bursts underneath micro breakers in their laboratory experiments of wind waves. Such events can also be deduced from the downward drafted and backward extended tails of the eddies beneath the crests as shown in Figures 12b and 12c. The present

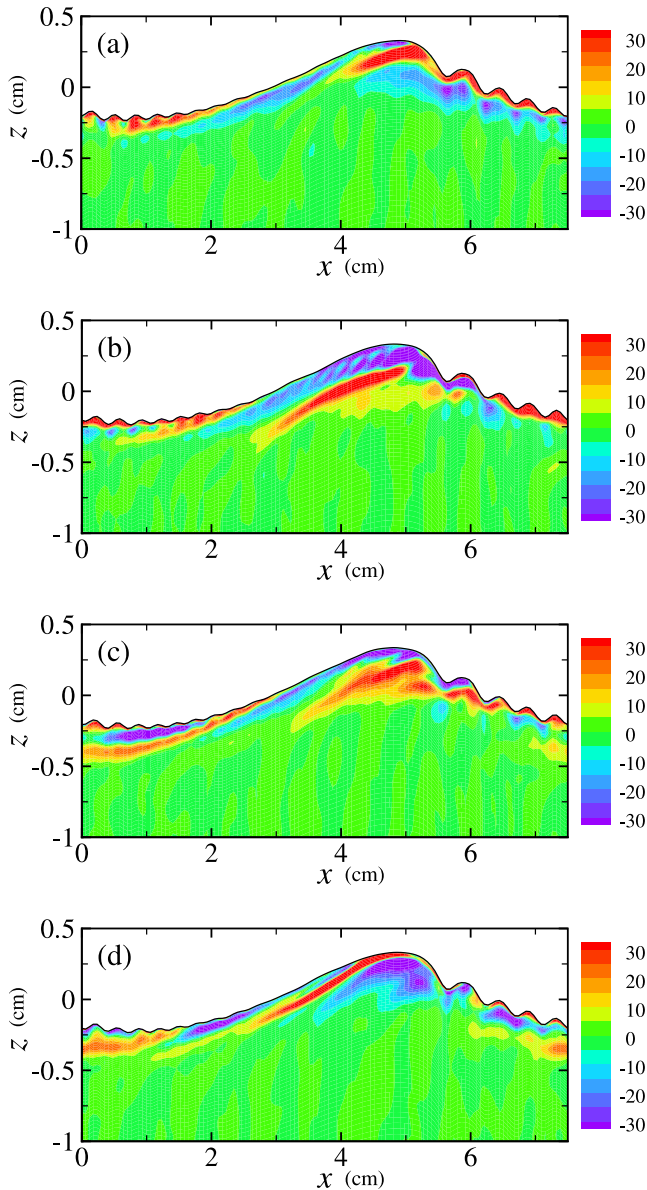


Figure 12. Contour distributions of the spanwise turbulent vorticity ω'_y , on representative vertical planes parallel to the wind direction, $y =$ (a) 0, (b) $0.24\lambda_y$, (c) $0.47\lambda_y$, and (d) $0.82\lambda_y$. The red/blue color represents the clockwise/counterclockwise vorticity. The flow travels from left to right.

numerical model should provide the detailed simulations necessary to unravel the generation mechanisms and evolution processes of these vortical structures.

[51] The characteristic vorticity distributions (Figures 12a–12c), which have been identified in the pervious experiments, however, are not the only structures observed in the present simulations. For instance, there also exist vortical structures with reverse rotations, as shown in Figure 12d. Again, the present simulation can be used for further investigations of these vortical flows.

6. Concluding Remarks

[52] We present a three-dimensional numerical model for process study of aqueous turbulent flow beneath a dynamic

ocean surface and driven by exerted surface forcing. The focuses are the transport processes within near-surface turbulent boundary layer where experimental measurements are impeded owing to the unsteady moving boundary, and also the nonlinear interactions between the surface waves and the underlying flow. In contrast to the previous models for similar purposes, the water surface of the present model is free to evolve, and the nonlinear free-surface boundary conditions are satisfied on the moving wavy surface exactly without employing any approximation or parameterization. The model is capable of resolving the surface processes with length scales down to that of capillary waves. The validity and the applicability of the developed model are demonstrated by simulating three distinctive three-dimensional surface processes which have been commonly observed in wind-wave flumes. In particular, the simulated examples highlight the potential impacts caused by the short-wavelength capillaries on the gravity dominant free-surface flows, and consequently reveal the necessity in incorporating such a microscale process in the parameterizations of transfer velocity. Another application of the developed model is to validate process modeling for the interaction between surface waves and the underlying turbulence [e.g., Ölmaz and Milgram, 1992; Teixeira and Belcher, 2002; Ardhuin and Jenkins, 2006].

[53] The total number of grids, which can be employed in a numerical simulation, is restricted by the practical limits of computer speed and memory. As a consequence, the maximum characteristic spatial scale of the flow, such as the wavelength, is also limited for the present direct numerical simulation (DNS) model employing no subgrid parameterizations. The maximum length scales of the flow processes that can be simulated by the present model cannot exceed $\mathcal{O}(1\text{ m})$; and the flow conditions (i.e., the range of Reynolds numbers) are limited to small-scale natural conditions [e.g., Gemmrich and Hasse, 1992] or laboratory settings such as those in the works of Caulliez and Collard [1999] and Jessup *et al.* [1997]. One possible extension of the DNS model to scale with the open-ocean conditions is to adopt the approach of large-eddy simulation (LES) [e.g., Sullivan *et al.*, 2004] and follow the development of large-wave simulation (LWS) of Dimas and Fialkowski [2000]. This, however, requires proper parameterizations of the subgrid-scale turbulence and the wave stresses. Such subgrid-scale parameterizations for free-surface turbulent flows are yet to be developed. (The LES/LWS model developed by Dimas and Fialkowski was two-dimensional.) The present three-dimensional DNS model can be adopted as a framework for future development of the LES/LWS model, in which only the long swells and large turbulent eddies are resolved. It can also readily be used to conduct a priori tests for the development of the subgrid-scale model.

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