Dynamically Consistent Computation of Exchange Processes at the Air-Sea Interface

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Summary

- Dynamically consistent framework for exchange processes—must account for surface waves
- Balance of mass, energy, momentum, etc.
- Coordinate systems: Eulerian; Lagrangian; more general coordinates
- Perturbation expansions
- Interpretation of observations from moving platforms
- Effects of wave breaking
- Coupled model systems
- Conclusions
An *dynamically consistent framework* for modelling atmosphere–ocean exchange processes *must take surface waves into account*: 

- *implicitly*, via, for example, a Charnock-type relation between air–sea momentum flux and wind speed, and empirically-based exchange coefficients for heat and mass, or

- *explicitly*, using, e.g., a spectral wave prediction model and analytical or numerical models for the interaction between the wave field and the atmospheric and oceanic surface boundary layers (e.g. Jenkins 1989 Dt. Hydrogr. Z., 1992 JPO)
Modelling *and observing* processes occurring in the vicinity of the sea surface is challenging, due to the presence of the moving interface.

*Momentum* may be transferred across the interface by fluctuating pressure forces, whereas *heat* and *mass* transfer is restricted by the presence of thin *laminar boundary layers*.

*Wave breaking* can disrupt the laminar boundary layers and enhance heat and mass transport across the interface (e.g. Melville, Veron, White 2002 JFM; Sullivan, McWilliams, Melville 2004 JFM).
Coordinate systems

There are advantages to using *curvilinear coordinate systems* which follow the water surface:

- We may resolve vertical variations at small distances from the surface
  - useful for computing *heat, gas, and particle exchange* through the water surface, and *ice* formation.

- *Time-independent curvilinear coordinates* (e.g. Longuet-Higgins 1953: Can be used with surface waves of fixed form.

- *Lagrangian coordinates* (e.g. M. S. Chang 1969; J. E. Weber 1983; Jenkins JPO 1986, 1987): Coordinate transformation may distort unacceptably for long times ($t$).
Generalized Lagrangian mean (GLM) formulation (Andrews & McIntyre JFM 1978ab): Not quite surface following, coordinate transformation becomes singular at critical levels.

‘Sigma’-coordinates: Vertical coordinate displacements only (G. Mellor 2003 JPO)—may be insufficiently general.

General, time-dependent curvilinear coordinates (Jenkins 1992 JPO): Includes Eulerian (Cartesian) and the other coordinate systems mentioned above, as special cases.
Example of a coordinate system, above and below a wave surface.

In this particular case we have \( x = (y_1 - ae^{-k|y_3|} \sin(ky_1 - \omega t), y_2, ae^{-k|y_3|} \cos(ky_1 - \omega t)) \). Above the interface, the coordinate system is isomorphic: below the interface \( J = 1 + O(\epsilon^2) \).
The use of a general coordinate system may also be valuable when interpreting time-dependent or time-averaged gas concentration measurements from sensors which are at moving locations.
General, time-dependent coordinates

In a Cartesian coordinate system $\mathbf{x} = (x_1, x_2, x_3)$:

(1) $\rho^x \left[ u^x_{j,t} + u^x_l u^x_{j,l} + \Phi^x_{,j} + 2(\Omega \times \mathbf{u}^x)_j \right] - \tau^x_{j,l,l} = 0,$

(2) $\rho^x_{,t} + u^x_l \rho^x_{,l} + \rho^x u^x_{l,l} = 0,$

(3) $C^x_{,t} + u^x_l C^x_{,l} + C^x u^x_{l,l} + F^x_{l,l} = 0,$

where $\rho$ is the fluid density, $C$ is tracer concentration, $F_l$ is tracer flux, $\mathbf{u} = (u_1, u_2, u_3)$ is the velocity, $\Omega$ is the rotational angular velocity vector, $\Phi$ is a force (e.g. gravitational) potential and the tensor $\tau_{j,l}$ incorporates both pressure and shear stress. Repeated indices are summed from 1 to 3.
In curvilinear coordinates, \( y = (y_1, y_2, y_3) \) with Jacobian \( J = \det[x^y_{j,l}] \), cofactors \( K_{jl} \), we may write

\[
\begin{align*}
(4) & \quad P_{j,t} - T_{jl,l} = S_j, \\
(5) & \quad (\rho^y J)_{,t} + [K_{ml} \rho^y (u^y_m - x^y_{m,t})]_l = 0, \\
(6) & \quad (C^y J)_{,t} + [K_{ml} C^y (u^y_m - x^y_{m,t})]_l + K_{ml} F^y_{m,l} = 0,
\end{align*}
\]

where \( P_j = \rho^y J u^y_j \) is the ‘concentration of \( x_j \)-momentum in \( y \)-space’, \( T_{jl} = \left[ \tau^y_{jm} - \rho^y u^y_j \left( u^y_m - x^y_{m,t} \right) \right] \), \( K_{ml} \) is minus the flux of \( x_j \)-momentum across \( y_l \)-surfaces, and \( S_j = -\rho^y \Phi^y_{,l} K_{jl} - 2\rho^y J (\Omega \times u^y)_j \) is a source function representing the potential and Coriolis forces.
Perturbation expansion

- Coordinate transformation $x^y = y + \xi$

- Quasilinear approximation: compute fluxes to second order in wave slope $\epsilon$. For any variable $\phi$:

\[
\phi \approx \phi^{(0)} + \Re \sum_k \phi^{(1)}_k \exp[k_j y_j - \omega(k) t] + \phi^{(2)}.
\]

- Momentum transferred from atmosphere to waves during wind-wave generation

- Contributions from different second-order terms, see subsequent slide
In water column, momentum transferred from waves to current:

- in surface/under-ice/bottom boundary layers
- in water column, at a rate dependent on $\frac{\partial \nu_E}{\partial y_3}$, where $\nu_E$ is eddy viscosity

Gas and particle/droplet/bubble flux should be computable within the same formalism.
Computed vertical profile of the various contributions to the downward momentum flux over wind waves, calculated by the quasi-linear eddy-viscosity-based model of Jenkins (1992 J. Phys. Oceanogr.). 1, $\tau_{13}/\rho$; 2, $p\zeta_1/\rho$; 3, $-\sigma_{11}\zeta_1/\rho$; 4, $\tau_{13}\xi_1/\rho$; 5, $u\zeta_t$; 6, $-u'w'$; 7, $Uu'\zeta_1$. Notation: $c$ is the vertical curvilinear coordinate, with $c = 0$ being the water surface; $\xi$ and $\zeta$ are the horizontal and vertical coordinate displacements; $U$ is the mean horizontal velocity; $u$ and $v$ are the horizontal and vertical velocity components; $\sigma_{jl} = \tau_{jl} + p\delta_{jl}$ is the traceless stress tensor; over-bars and primes denote mean and fluctuating values with respect to the curvilinear coordinate system.
Observations from moving platforms

The use of time-dependent curvilinear coordinates and moving reference frames is useful and important for interpretation of measurements of gas/chemical species as well as for modelling.

Even when wave- and motion-induced fluctuations are sufficiently small so that perturbation theory may be applied, it is probable that averaging procedures may result in a bias which is of second order in the wave slope \((ak)\).
Effect of wave breaking

Time-dependent modelling of wave breaking (e.g. Grilli, Guyenne, Dias, (Int. J. Numer. Meth. Fluids 2001) has become very sophisticated. However, a great deal of insight can also be obtained from simpler models, such as the stationary breaking-crest solution of Jenkins (1994 JFM) illustrated in the next slide. This model predicts that the geometrical scale (length of overturning loop) \( \approx 8 g^{-1/3} \Psi^{2/3} \), where \( \Psi \) is the flux of fluid in the jet. The physical length scale is very variable (loop major axis typically \( \approx 10^{-2} - 10^{-1} \lambda \), where \( \lambda \) is the wavelength.

Sullivan et al. (JFM 2004) used a parameterized impulse forcing from breaking wave crests to drive a large-eddy simulation for the water column.
Effect of wave breaking

Stationary-flow approximation for breaking-wave crest (see Jenkins 1994 *J. Fluid Mech.*), with a schematic turbulent plume. The streamlines are in the reference frame moving with the wave crest.
Spray and bubbles

- The most extreme way of disrupting the laminar boundary layer
- Diffusive transfer most effective across the surface of small droplets/bubbles, however:
- More mass in larger droplets/bubbles.
- Spray/spume from ‘tearing of wave crests’, however:
- Jets of breaking waves eject water horizontally, one method of an apparent drag reduction effect from spray (see recent paper by V. K. Makin in BLM and presentation by Vladimir Kudryavtsev)
- Overpressure in bubbles which are carried to depth may cause supersaturation in water column (e.g. $O_2$, Thorpe 1984; Farmer et al. 1993 *Nature*)
Spray and bubbles

- Enhancement of evaporation due to spray

  \[ \frac{c}{c_0} \propto \left( \frac{z}{z_0} \right) \frac{w_t}{\kappa u_*} \]

- Monin–Obukhov theory for effect of stability of water column due to the presence of droplets/bubbles?

- Size distributions: characteristic large/small bubble sizes determined by balance between forces:
  - Turbulent shear \( u_* \), \( u_* \left( \frac{\rho_a}{\rho_w} \right) \)
  - Gravity \( g \)
  - Surface tension \( \gamma / \rho_w \)
  - Viscosity \( \nu_w \)
Outline of coupled model system

- Turbulence closure models (e.g. Burchard, Applied Turbulence Modelling in Marine Waters, 2002) in atmospheric and oceanic boundary layers, modified by wave-induced mean variables. Curvilinear surface-following coordinates may be employed.

- Movement/diffusion of particles, water droplets, and gas bubbles (Thorpe 1984 JPO), depending on intensity of turbulence etc.

- Computation or parameterization of Langmuir circulations, depending on the horizontal spatial scale chosen. (‘Langmuir turbulence’, driven by spatially-varying wave-induced current, Craik & Leibovich 1976 ff.)
Interfacial boundary conditions:

- Dynamic effects of surface films of molecular and greater thickness (e.g. Jenkins & Jacobs 1997 *Phys. Fluids*), sea ice formation, etc.

- Parameterize the effect of wave breaking in disrupting surface layer, turbulence generation, generation of spray, air bubbles, etc., but ensure conservation of e.g. momentum when taking the whole system into account.
Conclusion

Since gas flux through the sea surface is controlled by processes which have a much smaller vertical scale than the height of surface waves, there are advantages in applying a model framework in time-dependent curvilinear coordinates.

Spatial and temporal averaging is possible with respect to such coordinates: however, it is important to be aware of inherent second-order bias effects.

The application of spectral wave models has been shown to be valuable in gas transfer studies: however, it is important to have a good representation of the high-frequency tail of the wave spectrum, in order to represent microbreaking etc.
Conclusion

Awareness of the dynamical consequences of using such time-dependent coordinates is also valuable in interpreting the results of observations from moving (and stationary) instruments located near the water surface, since coordinate-dependent biases of averaged measurements may occur. Where possible, time-dependent measurements should consider the phase of surface waves.