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Numerical Study of the Breakdown of Surface Divergence Based Models for Interfacial Gas Transfer Velocity at Large Contamination Levels

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Abstract : The effect of various levels of contamination on the interfacial air–water gas transfer velocity is studied by Direct Numerical Simulation (DNS). The interfacial gas transfer is driven by isotropic turbulence, introduced at the bottom of the computational domain, diffusing upwards. The isotropic turbulence is generated in a separate, concurrently running the large-eddy simulation (LES). The flow fields in the main DNS and the LES are solved using fourth-order discretisations of convection and diffusion. To solve the transport of dissolved gases in water, a fifth-order-accurate WENO scheme is used for scalar convection combined with a fourth-order central discretisation for scalar diffusion. The damping effect of the surfactant contamination on the near surface (horizontal) velocities in the DNS is modelled using horizontal gradients of the surfactant concentration. An important parameter in this model, which corresponds to the level of contamination, is ReMa⁄We, where Re is the Reynolds number, Ma is the Marangoni number, and We is the Weber number. It was previously found that even small levels of contamination (ReMa⁄We small) lead to a significant drop in the interfacial gas transfer velocity KL. It is known that KL depends on both the Schmidt number Sc (ratio of the kinematic viscosity and the gas diffusivity in water) and the surface divergence β, i.e. K_L∝√(β⁄Sc). Previously it has been shown that this relation works well for surfaces with low to moderate contamination. However, it will break down for β close to zero. To study the validity of this dependence in the presence of surface contamination, simulations were carried out for ReMa⁄We=0,0.12,0.6,1.2,6,30 and Sc = 2, 4, 8, 16, 32. First, it will be shown that the scaling of KL with Sc remains valid also for larger ReMa⁄We. This is an important result that indicates that - for various levels of contamination - the numerical results obtained at low Schmidt numbers are also valid for significantly higher and more realistic Sc. Subsequently, it will be shown that - with increasing levels of ReMa⁄We - the dependency of KL on β begins to break down as the increased damping of near surface fluctuations results in an increased damping of β. Especially for large levels of contamination, this damping is so severe that KL is found to be underestimated significantly.

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