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DIRECT SIMULATION OF SCALAR TRANSFER ACROSS WAVY GAS-LIQUID INTERFACES

Valerio DE ANGELES and Sanjoy BANERJEE

Department of Chemical Engineering
University of California, Santa Barbara, CA 93106

ABSTRACT

Direct numerical simulation techniques (DNS) have been developed for investigations of transport processes between turbulent gas and liquid streams separated by a wavy interface. The results indicate qualitative similarity between turbulence structures, in the vicinity of a continuous interface, to those in wall turbulence—if the shear rates correspond. There are detailed differences, however, primarily on the liquid side. The liquid-side tangential velocity fluctuations peak right at the interface, whereas on the gas side they peak a small distance away—much like in wall turbulence. The interfacial shear stress pattern correlates with gas-side sweeps and ejections, whereas it does not correlate with liquid-side structures. Heat and mass transfer mechanisms are primarily controlled by the sweeps on each side. Simple parameterizations of the scalar transfer velocity are developed based on these mechanisms and compare well with experiments and DNS. Capillary waves appear to have little effect on scalar transfer.

INTRODUCTION AND NUMERICAL METHOD

Prediction of scalar transfer rates between immiscible, turbulent streams is still poorly understood but is of central importance to many industrial and environmental processes, e.g., gas, moisture and heat transfer between the ocean and the atmosphere is crucial in determining long-term climate. The lack of understanding and, hence, of reliable quantitative estimates of interphase exchange rates is related to the complex nature of the interface. The interface moves and deforms, forming waves with a substantial range of length scales, some of which may break, forming spray and entraining bubbles, making measurements and simulations difficult.

Early theories for scalar transfer postulated that laminar films existed on both sides of the interface [1], but this gave the wrong dependency on molecular diffusivity compared to experiments [2], leading to the postulate that the interfacial surface was periodically renewed on each side by turbulent eddies [3]. The parameter that must be determined, then, is the surface renewal rate. Various hypotheses have been advanced for this [4]—all without an experimental basis, until recently.

In this paper we shall be concerned with scalar transfer rates between immisible fluid streams where turbulence is generated by the shear in the interfacial region itself, rather than in regions far from the interface.. Rashidi and Banerjee [5] and Komori et al [6] have shown by experiments that the interfacial region is somewhat similar to that in wall turbulence, giving rise to streaks and bursts at sufficiently high shear rates. However, little quantitative information is available about the details of the phenomena and their effect on interphase scalar transfer. It is the purpose of this paper to contribute to a better understanding of such problems using direct numerical simulation (DNS).

It is not clear at the outset that DNS can elucidate the interphase scalar transfer problem because only flows at relatively low Reynolds numbers can be fully resolved. However, the scales over which concentration changes occur normal to the interface are 0 (1 mm) on the gas side and 0(10μm) on the liquid side. Therefore, resolving regions containing several capillary waves of 0(1 cm) should be sufficient, and such regions can be handled by DNS. The numerical method for the DNS cannot be described here, except cursorily, but details are available in [7,8]. Suffice it to say that a region of about 200 shear-based units is resolved on each side of the interface—continuity of velocity and stress being used to couple the phases. Each fluid domain is mapped into a rectangular parallelepiped at each time step and the Navier-Stokes equations solved in the computational domains by a pseudospectral method.

For the scalar transfer calculations the interfacial region must be more finely resolved than the velocity field, when the Schmidt number (Sc) >> 1. This is done by stretching (contracting) the collocation point spacing by a scaling proportional to appropriate powers of Sc on the gas and liquid sides. The simulations have been validated against the experiments by Rashidi and Banerjee, and Komori et al.

RESULTS

The Velocity Field. Gas-liquid flow with a flat interface, obtained by imposing high surface tension and gravitational forces, clarifies the effect of the boundary conditions on the turbulence structure in isolation from possible effects that might arise from interfacial waves. Because of the typical density differences on the two sides of the interface for gas-liquid flows, the gas sees the interface almost like a solid wall, due to the comparatively high inertia of the liquid (see intensities in Figure 1). The intensities in

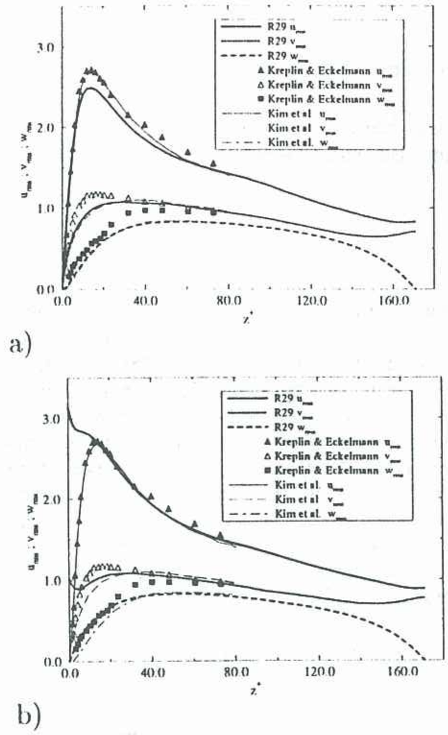
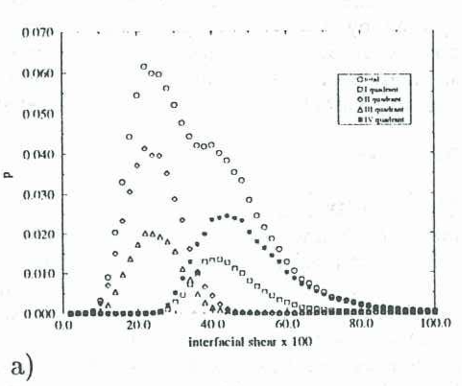
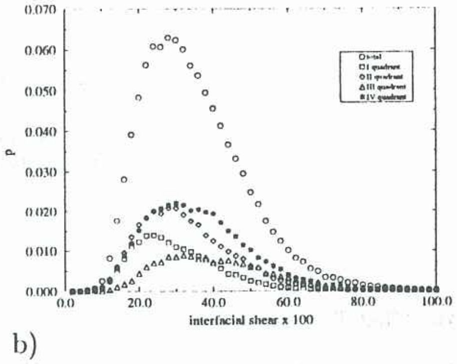


Figure 1: Turbulence intensities compared with Kreplin and Eckelmann's data and Kim and Moin's simulations (Phys Fluids 22, 1233, 1979; JFM 177, 133, 1987, respectively): a) gas; b) liquid.

the streamwise, spanwise and normal directions on the liquid side, however, peak at the interface (see Figure 1). The interface appears to behave like a slip surface to the liquid—albeit with a mean shear imposed. The turbulence structures on the two sides, however, still consist of quasi-streamwise vortices and streaks, confirming experimental observations [5]. However, sweeps and ejections associated with these quasi-streamwise vortices have different behavior (Fig. 2)—they correlate well with shear stress on the gas side, e.g., sweeps give rise to high shear stress regions at the interface. On the liquid side, this correlation is not observed.



a)



b)

Figure 2: The probability of strongly coherent events in various quadrants vs. the shear stress in the interfacial region over which they occur: a) gas; b) liquid.

When the interface is free to deform, waves form with the typical shapes shown in Figure 3. Interface-normal and spanwise velocity fluctuations increase on the liquid side. On the gas side, the main effect of waves is to increase fluctuations in the streamwise direction and decrease them in the spanwise direction. Deforming interfaces appear to exert less "blocking" than a rigid boundary on the interface-normal velocity fluctuations, reducing the redistribution of energy to the spanwise direction.

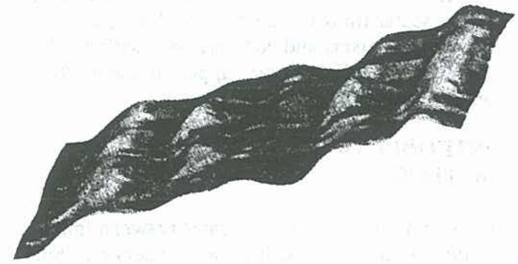
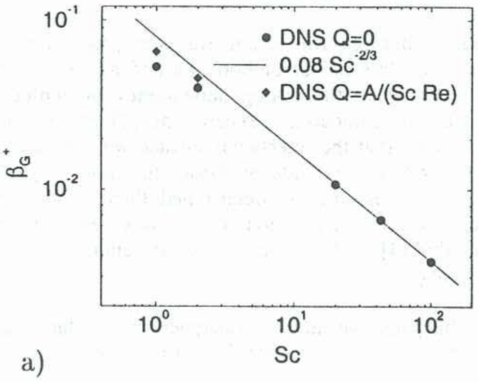


Figure 3: An instantaneous snapshot of the interface between the turbulent gas and liquid streams showing also the contours of shear stress.

__Scalar fluxes__. Simulations over an extensive range of Sc were done for gas-liquid flow with a flat interface and show that mass transfer velocity changes as the -1/2 and -2/3 power of Sc on the liquid and gas sides, respectively, as shown in Figure 4. Analysis of the



a)

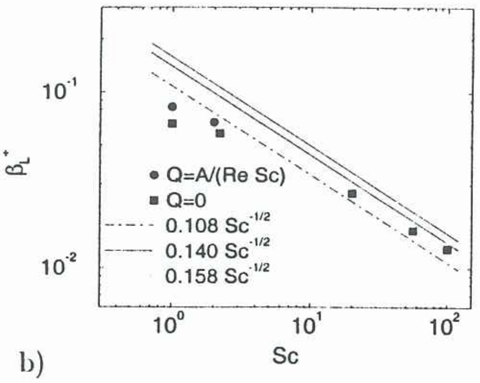


Figure 4: Nondimensionalized mass transfer velocity (β^+) versus Sc a) gas; b) liquid. Nondimensionalization by the friction velocity u*. Q is an artefact to correct for periodic bc's in the DNS. Q=0 is inaccurate at low Sc.

correlation of turbulence structures with mass transfer velocity shows that, on the liquid side, sweeps are important over the whole range of Sc analyzed. On the gas side, however, mass transfer velocity depends mainly on sweeps for low Schmidt numbers, but as Sc increases, ejections also become important. When the interface is allowed to freely deform, mass transfer velocity decreases on the gas side. On the liquid side, mass transfer velocity is virtually unchanged, as indicated by the results in Table 1.

Table 1: DNS values of nondimensional mass transfer velocity (β^+) for flat and wavy interfaces.

Interface Shape	Gas Sc=1	Gas Sc=2	Gas Sc=5	Liquid Sc=1	Liquid Sc=2	Liquid Sc=5
Flat	0.067	0.045	0.024	0.083	0.065	0.0405
Wavy	0.063	0.040	0.021	0.087	0.077	0.0434

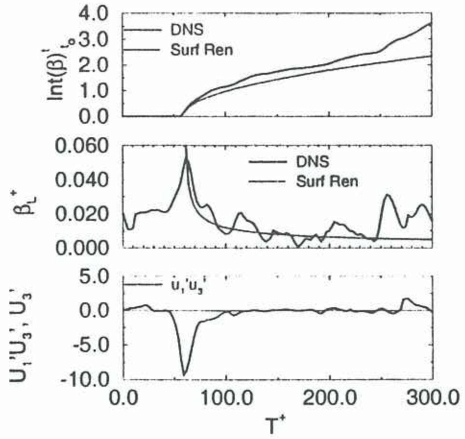


Figure 5: Comparison of the DNS-calculated mass transfer velocity on the liquid side with predictions of the surface renewal model, assuming renewal occurs when a sweep impinges on the interface (indicated by the peak in $u'_1 u'_3$).

<u>**Parameterizations.**</u> Based on these results, mass transfer relationships can be developed, without adjustable parameters. These are derived using sweeps/ejections to give the renewal rate. When the interface fluid is replenished by a sweep, a high concentration gradient is established, and the regions of the interface below the sweeps give the largest contribution to the overall mass flux. When this region is observed in a Lagrangian frame, moving with the interface velocity, the mass transfer decays like $(\mathrm{Time})^{-1/2}$, as shown in Figure 5. The mass transfer parameterizations are then [4]:

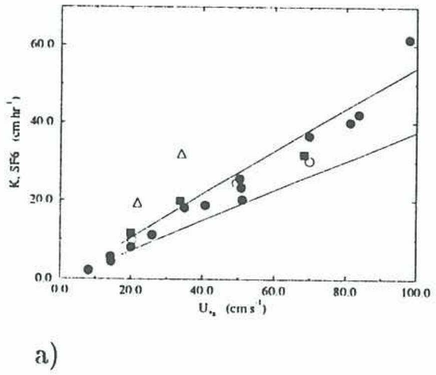
$$\overline{\beta}_l\,Sc^{0.5}/u_l^* = 0.108 \text{ to } 0.158 \qquad (1)$$

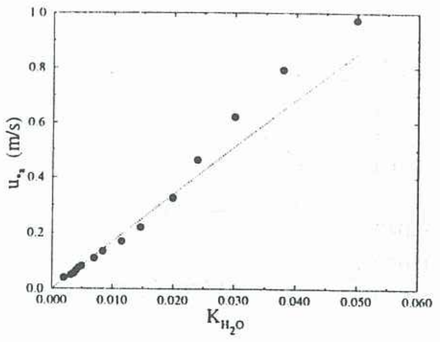
on the liquid side, where $\overline{\beta}_l$ is the mass transfer velocity and u_l^* is the friction velocity

$$\overline{\beta}_g\,Sc^{0.66}/u_g^* = 0.07 \text{ to } 0.09 \qquad (2)$$

on the gas side, where subscript g now denotes the gas side.

Equation 1 compares well with wind-wave tank data for SF_6 transfer rates [9] in Figure 6a. The lower bound of Equation (2) also compares well with the moisture transfer data [10] and the DNS results in Figure 6b. This indicates clearly that sweeps and, to a lesser extent, ejections formed in the near-interface regions dominate the scalar transfer process and that capillary waves play a secondary role.





b)

Figure 6. Comparison of a) equation (1) with liquid-side mass transfer velocity experiments using SF_6 desorption [9] and b) equation (2) with gas-side mass transfer velocity (moisture transfer) [10]. Both experiments conducted in large wind-wave tanks. The deviant points in a) are for breaking waves .

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