ESTIMATION OF FREE SURFACE MASS TRANSFER COEFFICIENTS USING EXPERIMENTAL DPIV VELOCITY DATA

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ABSTRACT

A Direct Numerical Simulation (DNS) of the scalar advection equation was used to compute the transfer coefficient for the passive scalar transfer across a shear-free gas-liquid interface. The liquid velocities used in the simulation were derived from a Digital Particle Image Velocimetry (DPIV) technique applied to an experimental channel flow. Essentially, this work combines two well proven tools, DPIV and DNS, to estimate the mass transfer coefficient across a boundary.

Specifically, two-dimensional DPIV experiments were used to provide streamwise and spanwise velocities at the free surface, from which were computed the vertical velocity gradient. These velocities, and their Taylor Series expansion normal to the interface, were used to solve the fully three-dimensional, time instantaneous concentration equation in the liquid, similar to the work in McCready et al. (1986), but not limited to two dimensions and with real velocity data.

For comparison, we also solved the scalar field equation using simulated velocities from an incompressible channel flow simulation, as outlined in Lam and Banerjee (1988). The main difference between the two velocity fields, DNS and DPIV, is that the DNS does not allow a wavy interface, but enforces a rigid, free-slip surface. The DPIV values are actually three dimensional velocities projected onto a flat surface.

The scalar transfer coefficient computed by the numerical simulation, using both the DPIV and rigid surface DNS velocity data, was comparable to experimental values obtained by Komori et. al. (1989). However, the transfer coefficient calculated using DPIV data was closer to Komori, with the DNS data predicting a consistently higher scalar transfer. It was observed that the R.M.S. of $\frac{\partial w}{\partial z}$ from the DNS were higher than those found in the DPIV data. It was hypothesized that the rigid surface in the DNS created a higher velocity gradient at the interface, thus leading to an enhancement of the scalar transfer.

BACKGROUND

Several models have been proposed to predict scalar transfer across an interface. Most models are based on the surface-renewal theory (Danckwerts 1951), and use various length and velocity scales of the interfacial turbulence to predict the size and residence time of the renewing eddies. For a review of the various models, see Banerjee (1990).

McCready et al. (1986) numerically solved a two-dimensional (spanwise and normal) concentration equation , and assumed that the velocity components consisted of a single sinusoidal frequency in space and random in time. They found that the mass transfer coefficient depends on the Schmidt number to the -0.5 power, and is related to mean square value of the velocity gradient normal to the interface.

Komori et al. (1989) has done experimental work measuring the absorption of CO_2 into channel flows. Using tracer dyes, he correlated bursting events at the wall to the renewal upwellings at the free surface, and made the conclusion that these 'ejections' were responsible for most of the scalar transfer at the interface. His simultaneous measurements of the transfer of CO_2 across the interface, and the resulting mass transfer coefficients, provided the benchmark experimental results for the current study.

Komori et al. (1992) has also numerically investigated scalar transfer in a fully three-dimensional DNS, and tracked the concentration of CO_2 on the liquid side. Their simulation used a freely deforming free surface, in comparison to many DNS that use rigid free-slip surfaces (Lam and Banerjee 1988). Their results qualitatively reproduced their experimental values, in the mean and turbulent intensities, and in the scalar transfer coefficient. They also reported that the scalar flux was enhanced by bursts from the wall, and that the flux was correlated by the R.M.S. spanwise vorticity. However, the numerical resolution in Komori et al. was quite modest (40 nodes in surface normal direction), especially considering that the Schmidt number for CO_2 transfer is of the order of 600. This resolution was not able to capture the thin scalar boundary layer near the interface.

NUMERICAL PROCEDURES

In this paper, we improve upon McCready et al.ś model (1986) by replacing his simplified velocity signal by the velocities obtained from a DPIV measurement in a channel flow. The velocities are linearly interpolated from the free surface, and the resulting three-dimensional velocity field is used to solve the concentration advection equation for a passive scalar. The scalar equation is solved in a thin region underneath the interface, so as to capture the scalar boundary layer.

The equation governing the evolution of a passive scalar (e.g. heat, mass) in the liquid layer is given by,

$$\frac{\partial C}{\partial t} + \nabla \cdot (\vec{u}C) = \frac{1}{Pe}\nabla^2 C \tag{1}$$

$$Pe = ScRe = \frac{\nu}{D}\frac{D}{u_* h} \tag{2}$$

where C is the concentration of the gas dissolved in the liquid, $\vec{u}$ is the liquid velocity, ν is the liquid kinematic viscosity and D is the diffusivity of the scalar in the liquid. The non-dimensional groups appearing in the equation are the Schmidt number and the Reynolds number. For slightly soluble gases, such as CO_2, the Schmidt number is large, on the $O(600)$, which for turbulent flows, produces a large Peclet number. For large Peclet number, convection dominates over diffusion, except in a thin boundary layer at the interface. In the bulk, the fluid is well mixed by the turbulence, and we can assume that the scalar has a constant value, valid up to the edge of the boundary layer, where the scalar rapidly increases to take on the interfacial value. If we rescale this equation by the concentration boundary layer thickness δ, then the transformed equation becomes,

$$\begin{aligned}\frac{\partial C}{\partial t} + \frac{\partial (uC)}{\partial x} + \frac{\partial (vC)}{\partial y} + \frac{h}{\delta}\frac{\partial (wC)}{\partial \eta} &= \\ \frac{1}{Pe}\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{h^2}{\delta^2}\frac{\partial^2 C}{\partial \eta^2}\right)\end{aligned} \tag{3}$$

where the variable η runs from -1 to +1 across the thin boundary layer. The equation was solved using a pseudospectral Direct Numerical Simulation (DNS) that has been shown to accurately simulate turbulent channel flows (Lam and Banerjee 1988). The non-dimensional boundary conditions were,

$$C(\eta = -1) = 1 \quad \text{(free surface)} \tag{4}$$

$$C(\eta = +1) = 0 \quad \text{(boundary edge)} \tag{5}$$

The velocities used in solving equation (3) for the scalar were derived from two sources: Two dimensional DPIV measurements from the surface of a channel flow; and numerically simulated velocities from a fully three-dimensional turbulent channel flow. The two-dimensional DPIV data were obtained from a series of photographs taken of silvered microballoons floating on the surface of an experimental channel flow (Kumar et al. 1998). From these pictures (and with the continuity equation), the surface parallel velocities and the normal velocity gradient were computed. This data was incorporated into the three-dimensional simulation by expanding the velocities in the interface-normal direction by a first-order Taylor Series, similar to what McCready assumed,

$$u = \alpha(x,y,t) = \bar{U}(x,y,t)|_{z=0} \tag{6}$$

$$v = \gamma(x,y,t) = \bar{V}(x,y,t)|_{z=0} \tag{7}$$

$$w = \psi(x,y,t)z = \frac{\partial w}{\partial z}(x,y,t)|_{z=0}z \tag{8}$$

where the z-coordinate measures the distance from the interface. Since the velocities change between successive photographs, we linearly interpolated the velocity for simulation times between those of the photographs. This is necessary due to the Courant limit of the simulation; the time step for stability is much less than the time step between photographs.

The velocities from the DNS were computed using a pseudo-spectral code, similar to that described in Lam and Banerjee (1988) or Kim et al. (1987). The velocities were then spectrally interpolated onto the scalar grid points in the boundary layer. Also, for the finer scalar time steps, the velocities were assumed to be constant in time, i.e. the velocity was used at the previous time step and not interpolated between time steps.

Once the simulated concentration fields reached statistical steady-state, the average diffusive flux at the interface was recorded, and the following coefficient was calculated,

$$\beta^+ = \frac{flux}{u_*(C_b - C_o)} \tag{9}$$

which is the mass transfer coefficient normalized by the friction velocity. The parameter C_o is the interfacial concentration of the scalar, and C_b is the bulk concentration of the scalar, defined as,

$$C_b = \frac{\int_0^{2h} dz\bar{U}\bar{C}}{\int_0^{2h} dz\bar{U}} \tag{10}$$

RESULTS

The scalar transfer coefficient using the DNS velocity data was computed at one Reynolds number, but for a variety of Schmidt numbers, as shown in Table 1. The Reynolds number, Re_*, is based on the liquid half depth, h and the friction velocity, u_*. Plotting the transfer coefficients as a function of Schmidt number reveals the -0.5 scaling, as shown in Figure 1.

The simulations using the DPIV velocity data are summarized in Table 2. The Reynolds number for the flow was 80 (2800 using the mean velocity and liquid depth); however, the liquid depth was varied from 1.5 cm.

The values for β^+ using DNS and DPIV velocity data are given in their respective tables mentioned above. The values for $\beta^+ Sc^{0.5}$ were computed for each run, and compared to the value determined by a similar experiment of Komori et al. (1989). These values are shown in Table 3. In Komori's experiments, the values of β^+ were measured using CO_2, which has a much higher Schmidt number than those used in the simulations. The comparison is made by looking at the value of $\beta^+ Sc^{1/2}$, since Komori's experiments were run using CO_2, which has a much higher Schmidt number than those used in the simulations.

The value from the DPIV data compares favorably to the value measured by Komori. However, the coefficient derived from the 'pure DNS' simulation was roughly triple that of Komori. Part of the reason for this overprediction is the higher values of $\frac{\partial w}{\partial z}$ seen at the interface, which are compared in Table 4. It is hypothesized that the rigid surface imposed in the simulation were responsible for the enhancement of $\frac{\partial w}{\partial z}$

CONCLUSIONS

Velocity data computed from the free surface using a DPIV technique was coupled to a DNS of the concentration field in a channel flow. The resulting mass transfer coefficients were similar to those found in experiments. Using simulated velocities in the DNS led to coefficients roughly triple that found in the experiment, an event caused by the larger $\langle \frac{\partial w}{\partial z} \rangle$ values, an event attributed to the rigid free-slip surface imposed in the velocity simulation.

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TABLE 1: PARAMETERS GOVERNING FULL DNS SCALAR SIMULATIONS

Run Id.	Re_*	Sc	β^+	$\beta^+ Sc^{0.5}$
1	85	4	0.0343	0.0687
2	85	10	0.0226	0.0716
3	85	20	0.0169	0.0757
4	85	56	0.0106	0.0794
5	85	100	0.0078	0.0778

TABLE 2: PARAMETERS GOVERNING DPIV SCALAR SIMULATIONS

Run Id.	u_*[cm/s]	2 h[cm]	Re_*	Re_{av}	Sc	β^+	$\beta^+ Sc^{0.5}$
1	1.169	1.50	80	2800	20	0.0.0068	0.0.0305
2	1.169	1.50	80	2800	56	0.0.0037	0.0.0278

TABLE 3: COMPARISON OF DNS, DPIV AND EXPERIMENTAL DATA

Source	2 h [cm]	Re_*	$\beta^+ Sc^{0.5}$
Komori	1.1	82	0.0273
DPIV	1.5	80	0.0292
DNS		85	0.0761

TABLE 4: COMPARISON OF DNS AND DPIV VALUES OF $\frac{\partial w}{\partial z}$

Source	$\frac{\partial w}{\partial z}$
DPIV (h=0.75cm)	1.039
DPIV (h=1.5cm)	0.478
DNS	2.221

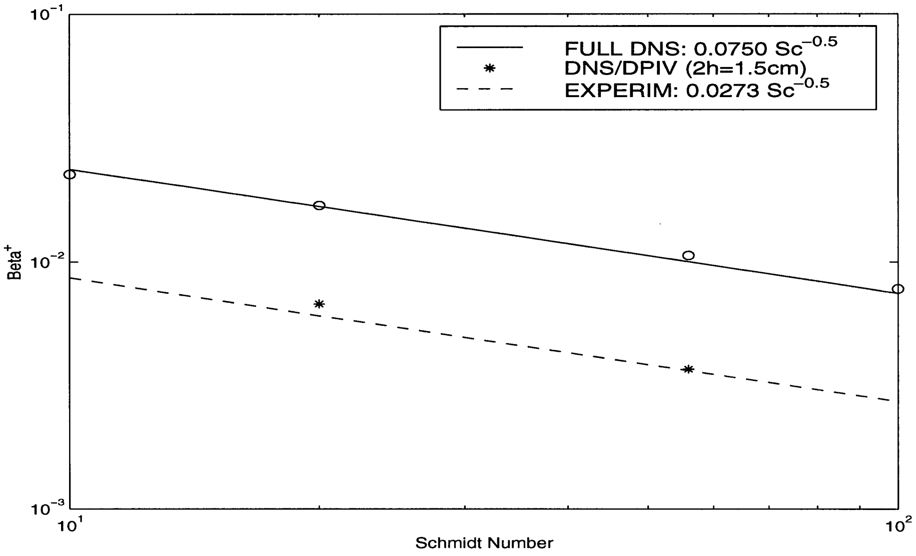

Figure 1: Comparison of Scalar Transfer Coefficients