Can turbophoresis be predicted by large-eddy simulation?

J. G. M. Kuerten[a)]
Department of Mechanical Engineering, J. M. Burgers Center, Technische Universiteit Eindhoven, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

A. W. Vreman[b)]
Vreman Research, Godfried Bomansstraat 46, 7552 NT Hengelo, The Netherlands

(Received 20 July 2004; accepted 15 September 2004; published online 23 November 2004)

Direct numerical simulation (DNS) and large-eddy simulation (LES) of particle-laden turbulent channel flow, in which the particles experience a drag force, are performed. In this flow turbophoresis leads to an accumulation of particles near the walls. It is shown that the turbophoresis in LES is reduced, in case the subgrid effects in the particle equations of motion are ignored. To alleviate this problem an inverse filtering model is proposed and incorporated into the particle equations. The model is shown to enhance the turbophoresis in actual LES, such that a good agreement with the DNS prediction is obtained. © *2005 American Institute of Physics*.
[DOI: 10.1063/1.1824151]

For many industrial and environmental applications the accurate prediction of particle transfer in an inhomogeneous turbulent flow is important. One of the mechanisms for transport of particles towards a wall is caused by the inhomogeneity of the turbulent velocity fluctuations and is called turbophoresis.[1,2] This phenomenon has been measured in, e.g., vertical turbulent pipe flow[3] and calculated by direct numerical simulation (DNS) in vertical turbulent pipe and channel flow.[4,5] In these numerical simulations the fluid is modeled as a continuous phase, while for each particle an equation of motion is imposed. The combined effect of drag force on a particle and inertia leads to turbophoresis.

Compared to DNS, large-eddy simulation (LES) is often able to produce acceptable results with less computational effort. However, most large-eddy simulations of particle-laden flows still use the filtered fluid velocity in the particle's equation of motion,[6] without incorporating a model for the difference between filtered and unfiltered velocities. In this Letter the effect of this disregard of the subgrid scales in the particle equations is studied by means of DNS and LES of particle-laden turbulent channel flow. Moreover, a method is proposed to improve the LES results by defiltering the fluid velocity used in the particle's equation of motion.[7] Armenio *et al.*[8] also studied the effects of the disregard of the subgrid velocity scales, but they focused on dispersion properties and did not consider the accumulation of particles in the near-wall regions.

Particle motion is governed by an equation for each individual particle. In this work we will only take nonlinear drag force into account, which has been justified by Armenio and Fiorotto.[9] Moreover, one-way coupling between the two phases is assumed, which is allowed because the present particle volume fraction is small (6×10^{-8}). Hence, the equation of motion for particle i with position $\mathbf{x}_i$ and velocity $\mathbf{v}_i$ reads

$$\frac{d\mathbf{v}_i}{dt}=\frac{\mathbf{u}(\mathbf{x}_i,t)-\mathbf{v}_i}{\tau_p}(1+0.15\,Re_p^{0.687}), \tag{1}$$

where $\mathbf{u}(\mathbf{x}_i,t)$ is the fluid velocity at the position of the particle. The particle relaxation time $\tau_p=\rho_p d_p^2/18\mu$, where d_p and ρ_p are the particle diameter and mass density, and μ is the fluid dynamic viscosity.

Large-eddy simulation solves the equations of motion for the filtered fluid velocity, in which the turbulent stress tensor is replaced by the subgrid model. The filtered fluid velocity is defined by $\overline{\mathbf{u}}(\mathbf{x})=\int G(\mathbf{x};\mathbf{y})\mathbf{u}(\mathbf{y})d^3y$, where $G(\mathbf{x};\mathbf{y})$ is a filter function. In the present paper we employ the top-hat filter. The description "top-hat" refers to the shape of the filter function in physical space.

If in an LES the particle equations (1) are solved with the filtered fluid velocity, three sources of error can be distinguished with respect to DNS. A *subgrid* error is introduced because particle equations (1) are solved with the filtered velocity. Second, a *modeling* error occurs because a real LES does not provide the exact filtered velocity to the particle equations, but only an approximation because of the limitations of the subgrid model. We also remark that the particle locations do in general not coincide with grid points and therefore interpolations are needed to obtain the fluid velocity at the particle locations. This introduces the *interpolation* error, since the LES is performed on a much coarser grid than the DNS. Since this error was found to be negligible for fourth-order interpolations,[10] we focus on the first two errors in this work.

We will present results of *a priori* and *a posteriori* LES particle simulations. Both types of simulations solve the particle equations of motion (1), albeit for different filtered fluid velocities. In the *a posteriori* case $\overline{\mathbf{u}}$ is provided by solving the Navier–Stokes equations closed with a subgrid model on a coarse grid. In the *a priori* case $\overline{\mathbf{u}}$ is provided by the explicit filtering of the DNS velocity on the fine grid and the subsequent restriction of this filtered signal from the fine DNS to the coarse LES grid. The effect of the subgrid error

a)Telephone: +31 40 247 2362. Fax: +31 40 247 5399. Electronic mail: j.g.m.kuerten@tue.nl
b)Telephone: +31 74 259 4591. Electronic mail: bert@vremanresearch.nl

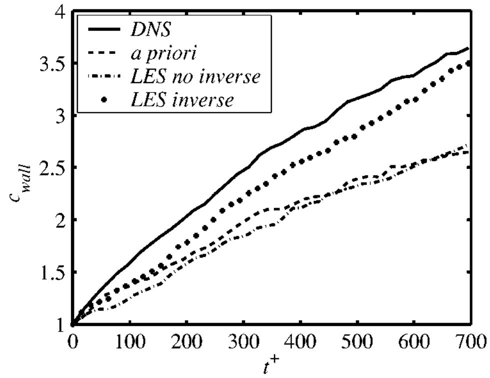

FIG. 1. Relative concentration of particles close to the wall as a function of time in wall units for $\tau_p^+=5.4$. The concentration is normalized by the initial concentration.

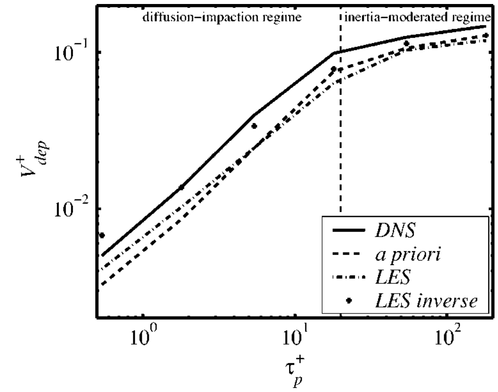

FIG. 3. Time-averaged particle deposition velocity as a function of particle relaxation time.

in the particle equation is defined as the difference between the DNS and the *a priori* LES results. The effects of the modeling error, which occur because the subgrid modeling in the fluid equation is not perfect, become visible in the differences between the *a priori* and *a posteriori* LES.

The simulation details of the DNS and LES of the particle-laden channel flows are described in the following. The Reynolds number based on the friction velocity and half the channel height H equals 180. All simulations start from a fully-developed turbulent flow with the particles homogeneously distributed over the domain. Six different particle relaxation times have been considered: in wall units $\tau_p^+=0.54$, 1.8, 5.4, 18, 54, and 180. One of the values considered, $\tau_p^+=5.4$, equals the Kolmogorov time based on the average dissipation rate. Values of τ_p^+ up to 20 fall within the diffusion-impaction regime;[2] where the particle deposition velocity increases with several orders of magnitude with particle relaxation time. Higher values of τ_p^+ are in the inertia-moderated regime where the particle deposition velocity is almost constant.

The numerical method uses a de-aliased Fourier–Galerkin approach in the periodic streamwise and spanwise directions, and a Chebyshev-collocation method in the wall-normal direction. Time integration is performed with a second-order accurate method. The computational domain has a size $2H$ in wall-normal, $4\pi H$ in streamwise, and $2\pi H$ in spanwise direction. In the DNS the number of Chebyshev points equals 129, whereas 128 Fourier modes are used in both periodic directions. The equations of motion for the particles are integrated in time by Heun's method. The fluid velocity at the particle position is found by fourth-order interpolation. If a particle reaches a wall, an absorbing boundary condition is used.

In the LES the grid is coarsened with a factor of 4 in the streamwise and normal directions and a factor of 2 in the spanwise direction. Thus the present grid ($\Delta x^+ \approx 71$, $\Delta z^+ \approx 17$) satisfies the requirements of a resolved LES (see for details Piomelli and Balaras[11]). As a subgrid model the dynamic Smagorinsky model is applied[12] using a three-dimensional top-hat test filter. The primary filter width Δ_i equals the LES grid size in each direction.

Figures 1–4 show results from DNS, *a priori* LES and *a posteriori* LES with and without inversion. The *a posteriori* results without inversion are standard large-eddy simulations neglecting the subgrid terms in the particle equations. The inversion technique, explained below, provides an adequate model for these terms, which is demonstrated by the *a posteriori* LES with inversion.

In Fig. 1 the concentration of particles closer to one of the walls than $H/20$ is plotted as a function of time and normalized by the initial concentration for $\tau_p^+=5.4$. The phe-

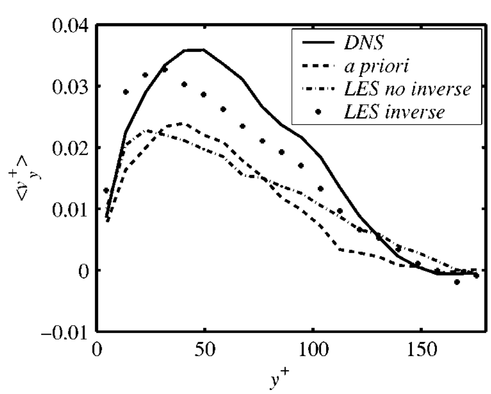

FIG. 2. Time-averaged wall-normal particle velocity as a function of the distance to the wall in wall units for $\tau_p^+=5.4$.

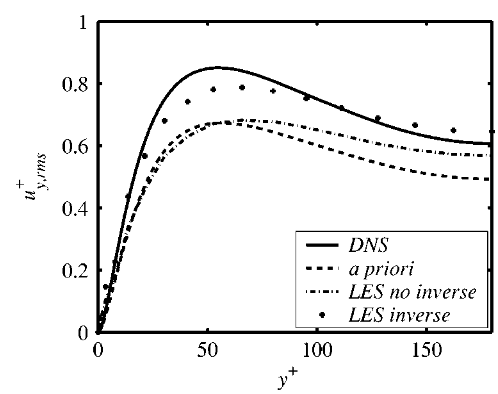

FIG. 4. Root-mean square of wall-normal fluid velocity fluctuations as a function of wall-normal coordinate.

nomenon of turbophoresis is evident from the DNS results. However, the turbophoresis turns out to be severely reduced in both the *a priori* and *a posteriori* LES without inversion. Figure 2, where the time-averaged wall-normal particle velocity component is shown, shows that the particle velocity is reduced over almost the whole height of the channel. Figure 3 confirms this finding for a wide range of particle relaxation times. In this figure the time-averaged particle deposition velocity $V_{dep}=V/ANdN_{dep}/dt$ is plotted as a function of τ_p^+ in wall units. Here, N is the number of particles, A the surface area of the walls, V the volume of the domain, and N_{dep} the concentration of deposited particles.[6] The DNS deposition velocities fall within the range of experimental data presented by Young and Leeming.[2] The *a priori* curve clearly illustrates that filtering the fluid velocity has a large impact on turbophoresis; especially in the diffusion impaction regime the increase in particle concentration is strongly reduced. For larger filter widths, not shown here, turbophoresis was found to decrease further.

The reduction of turbophoresis can be explained by the effect of the filtering on the turbulent velocity fluctuations. For small τ_p the turbophoretic force F on a particle is proportional to[2]

$$F \sim \frac{d}{dy}\langle u_y^2\rangle \approx \frac{d}{dy}\langle v_y^2\rangle. \tag{2}$$

The reduction of turbophoresis is thus related to the reduction of the wall-normal velocity fluctuations near the wall. Figure 4 indeed confirms the decrease of the turbulent velocity fluctuations in the wall-normal direction for the *a priori* LES case.

The results of the *a posteriori* LES without inversion in Figs. 1–3 are close to the *a priori* results. This indicates that the effect of the modeling error on turbophoresis is small in case the dynamic Smagorinsky model is applied. The secondary wall vortices, which were identified as the main reason for trapping of particles close to the wall by Marchioli and Soldati,[4] are still sufficiently resolved in the present LES solutions. A further indication of the quality of the LES results is the observation that the velocity fluctuations in the wall-normal direction correspond well with the *a priori* results (see Fig. 4).

Based on the magnitude of the subgrid error, which is the difference between the *a priori* LES and the DNS, it is concluded that LES is not able to predict turbophoresis accurately if the subgrid terms in the particle equations are neglected. However, it is possible to improve the LES results by retrieving part of the subgrid contributions to the fluid velocity by inverse filtering. Inverse filtering (or defiltering) frequently occurs in the literature of LES.[7,13–15] In all these cases defiltering is used to model the turbulent stress tensor. It has often been successful, but in practice a dissipation term remains necessary to control the extra fluctuations introduced by defiltering.

Filter inversion in LES never exactly recovers the unfiltered velocities. The first step in the LES-formalism is to transform the unfiltered velocities to filtered ones by defining a specific filter. The second step is to project the filtered velocities onto the LES grid. While the first step is formally invertible for some filters such as the top-hat filter used here, the second step never is. In the present LES the inversion is performed in Fourier space for the two periodic directions. In the wall-normal direction the inverse is approximated with a Taylor series up to second order in the filter width. Hence, for each velocity component a Fourier mode with wave numbers k_x and k_z in streamwise and spanwise direction is divided by

$$\frac{\sin(k_x\pi/N_x)\sin(k_z\pi/N_z)}{k_xk_z\pi^2/N_xN_z},$$

where N_x and N_z are the number of Fourier modes in streamwise and spanwise direction. The defiltering in the wall-normal direction is found by $f_j-\frac{1}{24}(f_{j+1}-2f_j+f_{j-1})$, where f_j denotes a Fourier mode of a velocity component in grid point y_j. At the walls the defiltered velocity is set equal to zero.

Inverse LES solves the particle equations of motion incorporating this defiltered fluid velocity, which leads to a substantially improved prediction of turbophoresis (see Figs. 1–3). According to Fig. 4, not only turbophoresis but also turbulent intensities correspond better with the DNS results if the defiltered LES velocity is used. Apparently, defiltering also improves the dispersion properties of particles in LES [compare Eq. (2)].

In particular in the diffusion-impaction regime (see Fig. 3), where the subgrid error is relatively large, inversion is necessary to obtain acceptable accuracy. In the inertia-moderated regime the inversion also improves the results, but the *a priori* results and the LES results without inversion are already quite good. This is in agreement with the common assumption that the motion of particles with large τ_p is mainly determined by the large eddies and is therefore relatively insensitive to the subgrid eddies (see Wang and Squires[6]).

Finally, the results of the particle velocity statistics are discussed in more detail. In Fig. 5 the particle velocity fluctuations in wall-normal direction are plotted as a function of the wall-normal coordinate for a small and a large value of τ_p. Results of DNS and inversely filtered LES are shown. We observe that the agreement between the DNS and the inverse

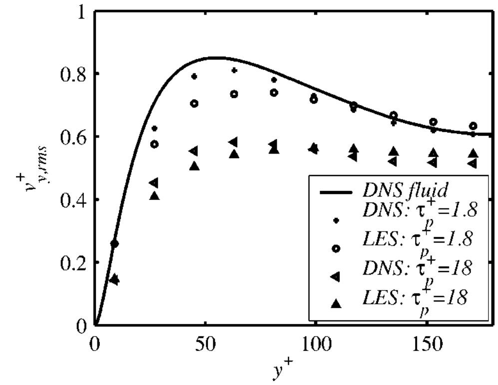

FIG. 5. Root-mean square of wall-normal particle velocity fluctuations as a function of wall-normal coordinate for DNS and inversely filtered LES. The wall-normal fluid velocity fluctuations of the DNS are included as the solid line.

LES results is quite good for both values of τ_p. It can be concluded that the LES not only predicts the turbulent fluid velocity fluctuations in an accurate way, but also the Lagrangian velocity correlation function. This will be clarified in the following. For times large compared to the particle relaxation time and neglecting Re_p, the solution of (1) is given by

$$\mathbf{v}(t) = \frac{1}{\tau_p}\int_{-\infty}^{t} \mathbf{u}[\mathbf{x}(\tau),\tau]e^{-(t-\tau)/\tau_p}d\tau. \tag{3}$$

This leads to a relation between the variance of the wall-normal particle velocity and a Lagrangian correlation function of the fluid velocity:

$$\langle v_y^2\rangle = \frac{1}{\tau_p}\int_{0}^{\infty} R_{yy}^L(\tau)e^{-\tau/\tau_p}d\tau. \tag{4}$$

Here $R_{yy}^L(\tau)=\langle u_y[\mathbf{x}(t),t]u_y[\mathbf{x}(t-\tau),t-\tau]\rangle$ is the Lagrangian correlation function of the wall-normal fluid velocity. Note that both $\langle v_y^2\rangle$ and R_{yy}^L depend on the wall-normal position. In general, the Lagrangian correlation time is large compared to the Kolmogorov time τ_K. Hence, if $\tau_p \leqslant \tau_K$, $R_{yy}^L(\tau)$ in (4) can be replaced by $R_{yy}^L(0)=\langle u_y^2\rangle$, which results in $\langle v_y^2\rangle=\langle u_y^2\rangle$. Figure 5 shows that for $\tau_p^+=1.8$ the particle velocity fluctuations are indeed close to the fluid velocity fluctuations, which were according to Fig. 4 well predicted by the inversely filtered LES. Figure 5 shows that the dynamic Smagorinsky model together with the defiltering operation also produces an accurate prediction of the variances of the fluid velocity for $\tau_p^+=18$. This observation combined with Eq. (4) indicates that the Lagrangian correlation function is also accurately predicted by the inversely filtered LES results.

In this Letter we have shown that turbophoresis cannot accurately be predicted by LES with the dynamic Smagorinsky subgrid model in the diffusion-impaction regime, if the filtered fluid velocity is used in the particle's equation of motion. However, defiltering of the fluid velocity in the LES substantially improves the results. This increases the possibility of accurate simulations of particle-laden turbulent flows by means of LES. Furthermore, we have shown that the particle velocity statistics of the defiltered LES results correspond well with the DNS. This indicates that the prediction of Lagrangian velocity correlation functions is also accurate.

This work was sponsored by the Stichting Nationale Computerfaciliteiten (National Computing Facilities Foundation, NCF) for the use of supercomputer facilities, with financial support from the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (Netherlands Organization for Scientific Research, NWO).

[1] M. W. Reeks, "The transport of discrete particles in inhomogeneous turbulence," J. Aerosol Sci. **14**, 729 (1983).
[2] J. Young and A. Leeming, "A theory of particle deposition in turbulent pipe flow," J. Fluid Mech. **340**, 129 (1997).
[3] B. Y. H. Liu and J. K. Agarwal, "Experimental observation of aerosol deposition in turbulent flow," J. Aerosol Sci. **5**, 145 (1974).
[4] C. Marchioli and A. Soldati, "Mechanisms for particle transfer and segregation in a turbulent boundary layer," J. Fluid Mech. **468**, 283 (2002).
[5] C. Marchioli, A. Giusti, M. V. Salvetti, and A. Soldati, "Direct numerical simulation of particle wall transfer and deposition in upward turbulent pipe flow," Int. J. Multiphase Flow **29**, 1017 (2003).
[6] Q. Wang and K. D. Squires, "Large eddy simulation of particle deposition in a vertical turbulent channel flow," Int. J. Multiphase Flow **22**, 667 (1996).
[7] J. G. M. Kuerten, B. J. Geurts, A. W. Vreman, and M. Germano, "Dynamic inverse modelling and its testing in LES of the mixing layer," Phys. Fluids **11**, 3778 (1999).
[8] V. Armenio, U. Piomelli, and V. Fiorotto, "Effect of the subgrid scales on particle motion," Phys. Fluids **11**, 3030 (1999).
[9] V. Armenio and V. Fiorotto, "The importance of the forces acting on particles in turbulent flows," Phys. Fluids **13**, 2437 (2001).
[10] J. G. M. Kuerten, "A priori testing of large-eddy simulation of particle-laden channel flow," in Proceedings of the Third International Symposium on Two-Phase Flow Modelling and Experimentation, Pisa, 2004.
[11] U. Piomelli and E. Balaras, "Wall-layer models for large-eddy simulations," Annu. Rev. Fluid Mech. **34**, 349 (2002).
[12] M. Germano, U. Piomelli, P. Moin, and W. H. Cabot, "A dynamic subgrid-scale eddy viscosity model," Phys. Fluids A **3**, 1760 (1991).
[13] M. Germano, "Differential filters for the large eddy numerical simulation of turbulent flows," Phys. Fluids **29**, 1755 (1986).
[14] B. J. Geurts, "Inverse modeling for large-eddy simulation," Phys. Fluids **9**, 3585 (1997).
[15] S. Stolz, N. A. Adams, and L. Kleiser, "An approximate deconvolution model for large-eddy simulation with application to incompressible wall-bounded flows," Phys. Fluids **13**, 997 (2001).