LES of droplet-laden non-isothermal channel flow

W R Michalek¹, R Liew², J G M Kuerten¹,³ and J C H Zeegers²

¹Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands
²Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands
³Faculty EEMCS, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands
E-mail: w.michalek@tue.nl

Abstract. In this paper subgrid models for LES of droplet-laden non-isothermal channel flow are tested and improved for three Reynolds numbers based on friction velocity, \(Re_\tau\) of 150, 395, and 950 with the aim to develop a simulation method for LES of a droplet-laden Ranque-Hilsch vortex tube. A new subgrid model combining the beneficial properties of the dynamic eddy-viscosity model and the approximate deconvolution model is proposed. Furthermore, the subgrid model in the droplet equations based on approximate deconvolution is found to perform well also in non-isothermal channel flow. At the highest Reynolds number in the test the dynamic model yields results with a similar accuracy as the approximate deconvolution model.

1. Introduction

The Ranque-Hilsch vortex tube (RHVT) is a well-known tool to achieve cooling in a device without moving parts. In an RHVT the incoming high pressure gas flow is separated into a hot and a cold stream. The final goal of the present research project is to investigate the possibilities of the RHVT as a tool to separate droplets from a gas flow at high pressure, \(e.g.\) for cleaning or drying of natural gas. Separation is possible thanks to the high swirl in the flow through the RHVT. Firstly, contaminated natural gas expands in the vortex chamber. This causes condensation of water vapor and subsequent rapid growth of the droplets. Secondly, flow with a high swirl number causes a large centrifugal force which transports droplets to the wall, where they can be separated. The present paper is a first step towards the modeling of the flow in an RHVT by means of large-eddy simulation (LES). To that end, suitable subgrid models for the droplets in the non-isothermal flow in the RHVT have to be developed.

2. Governing equations and numerical method

As a basis for the LES model, an Eulerian-Lagrangian approach will be used. This means that equations governing the carrier gas flow, in particular the Navier-Stokes equation, the continuity equation and a passive temperature equation and additionally equations for position, velocity and temperature for each droplet have to be solved. To achieve accurate results for LES good subgrid models in the fluid equations are needed. A well validated model in the droplet equations is also crucial, since in LES only filtered flow quantities are available, while the governing equations for the droplets require unfiltered carrier gas quantities. The subgrid
model in the droplet equation is needed to account for the effect of the unresolved and filtered scales in the fluid temperature and velocity on the droplets. To develop and validate such subgrid models, we considered the specific test case of non-isothermal droplet-laden channel flow at relatively low Reynolds numbers. This case allows us to check the LES results with results of direct numerical simulations (DNS).

The Navier-Stokes equation for incompressible flow (see equation 1) and a convection-diffusion equation for the passive temperature scalar (see equation 3) were solved in a channel geometry with periodic boundary conditions in streamwise and spanwise directions. The Navier-Stokes equation is solved in rotational form:

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \times \mathbf{\omega} + \nabla P = \nu \Delta \mathbf{u} + \mathbf{F}, \]

where \( \mathbf{u} \) is the velocity, \( \mathbf{\omega} = \nabla \times \mathbf{u} \) is the vorticity, \( \nu \) is the fluid kinematic viscosity, \( P = \frac{\rho_f}{\rho} + \frac{1}{2} \mathbf{u}^2 \) with \( p \) the fluctuating part of the pressure and \( \rho_f \) the fluid mass density. Then, \( \mathbf{F} \) is the driving force, constant in time and space. The continuity equation for the incompressible flow reads:

\[ \nabla \cdot \mathbf{u} = 0. \]

The temperature equation solved (Bird, Stewart & Lightfoot, 1960, p. 316) reads:

\[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = D \Delta T, \]

where \( T \) is the fluid temperature and \( D \) the thermal diffusivity.

The droplets were considered in a Lagrangian way. The equation of motion of droplet \( i \) with velocity \( \mathbf{v}_i \) (Maxey & Riley, 1983) reads:

\[ \frac{d\mathbf{x}_i(t)}{dt} = \mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}_i \frac{1 + 0.15Re_P^{0.687}}{\tau_p}, \]

where \( \mathbf{u}(\mathbf{x}_i, t) \) is the fluid velocity at position \( \mathbf{x}_i \) of droplet \( i \), \( \tau_d = \rho_d d_d^2/(18 \rho_f \nu) \) is the droplet relaxation time with \( d_d \) droplet diameter and \( \rho_d \) droplet mass density. Moreover, \( Re_p = d_d \mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}_i \nu \) is the droplet Reynolds number. The Lagrangian tracking of the droplets is performed by numerically integrating the equation:

\[ \frac{d\mathbf{x}_i(t)}{dt} = \mathbf{v}_i, \]

The temperature equation for droplet \( i \) with temperature \( T_{p,i} \) (Bird, Stewart & Lightfoot, 1960, p. 409) reads:

\[ \frac{dT_{p,i}}{dt} = \frac{T(\mathbf{x}_i, t) - T_{p,i}}{\tau_t}(1 + 0.3Re_p^{1/2}Pr_t^{1/3}), \]

where \( T(\mathbf{x}_i, t) \) is the fluid temperature at the droplet position, \( \tau_t = \tau_d Pr_f c_{pd}/c_{pf} \) the droplet thermal relaxation time with \( Pr \) the Prandtl number of the fluid and \( c_{pd} \) and \( c_{pf} \) the heat capacities of droplet and fluid.

We performed simulations at fixed values of the time-averaged Reynolds number based on friction velocity \( Re_f = \frac{u_f}{\nu} \), where \( u_f \) is friction velocity and \( H \) is half the channel height, equal to \( Re_f \) of 150, 395, and 950. However, in this paper we will focus on the two highest Reynolds numbers, since they are more relevant for the real application. Table 1 presents the corresponding values of Reynolds number based on bulk velocity, \( Re_b \) as well, along with the number of the points in streamwise, wall-normal and spanwise direction, and the size of the computational domain in the three directions. For every test case four sizes of the droplets were considered with 100,000 droplets for each size. The dimensionless sizes of the droplets and corresponding Stokes number are presented in table 2.
Table 1. Parameters of the numerical simulations performed.

| Case  | $Re_\tau$ | $Re_m$ | Grid          | Domain            |
|-------|-----------|--------|---------------|-------------------|
| DNS 150 | 150       | 2290   | $128 \times 129 \times 128$ | $4\pi \times 2 \times 2\pi$ |
| DYN 150 | 150       | 2420   | $32 \times 64 \times 32$    | $4\pi \times 2 \times 2\pi$ |
| ADM 150 | 150       | 2290   | $32 \times 64 \times 32$    | $4\pi \times 2 \times 2\pi$ |
| DNS 395 | 395       | 6940   | $256 \times 193 \times 192$ | $2\pi \times 2 \times \pi$  |
| DYN 395 | 395       | 7360   | $32 \times 49 \times 64$    | $2\pi \times 2 \times \pi$  |
| ADM 395 | 395       | 6940   | $32 \times 49 \times 64$    | $2\pi \times 2 \times \pi$  |
| DNS 950 | 950       | 18953  | $768 \times 385 \times 768$ | $2\pi \times 2 \times \pi$  |
| DYN 950 | 950       | 19390  | $96 \times 97 \times 128$   | $2\pi \times 2 \times \pi$  |
| ADM 950 | 950       | 18780  | $96 \times 97 \times 128$   | $2\pi \times 2 \times \pi$  |

Table 2. The ratio $d_d/H$ for the three simulations.

| $St$ = 0.2 | $St$ = 1.0 | $St$ = 5.0 | $St$ = 25 |
|------------|------------|------------|------------|
| $Re_\tau$ = 150 | $4.6 \times 10^{-4}$ | $1.0 \times 10^{-3}$ | $2.3 \times 10^{-3}$ | $5.1 \times 10^{-3}$ |
| $Re_\tau$ = 395 | $1.7 \times 10^{-4}$ | $3.9 \times 10^{-4}$ | $8.7 \times 10^{-4}$ | $1.9 \times 10^{-3}$ |
| $Re_\tau$ = 950 | $7.2 \times 10^{-5}$ | $1.6 \times 10^{-4}$ | $3.6 \times 10^{-4}$ | $8.1 \times 10^{-4}$ |

3. Model used in LES

Two LES subgrid models were considered: the dynamic eddy-viscosity model (DYN) (Germano, Piomelli, Moin & Cabot, 1991), (Lilly, 1992) and the approximate deconvolution model (ADM)

Figure 1. Profile of mean streamwise fluid velocity at $Re_\tau$=395.  
Figure 2. Profile of mean streamwise fluid velocity at $Re_\tau$=950.
(Stolz, Adams & Kleiser, 2001). We will first show some important results of fluid properties and turn to droplet results in the next section.

In figures 1 and 2 the profiles of the mean streamwise velocity of the fluid are presented for Reynolds numbers $Re_\tau=395$ (figure 1) and 950 (figure 2). Figures 3 and 4 present the root mean square (RMS) of the streamwise velocity of the fluid, whereas the profiles of the mean fluid temperature are shown on figures 5 and 6. These figures show that for the lower Reynolds number the velocity properties of the fluid are far better predicted by ADM, whereas for the mean fluid temperature the dynamic model agrees better with the DNS than the ADM. Therefore, a mixed model (MIX), in which ADM is applied to the Navier-Stokes equation and the dynamic eddy diffusivity model to the temperature equation, has been considered as well at the two lower Reynolds numbers. This mixed model gives the same results for the fluid velocity as ADM, but improves the temperature predictions with respect to ADM, as can be seen in figure 5. Also, the RMS of the temperature of this model is close to the DNS results (see figure 6).
7), because the under-prediction of the thermal diffusivity is significantly reduced, compared to $Re_τ=150$.

The LES results at the highest Reynolds number, $Re_τ=950$, are presented in figures 2, 4, 6, and 8. The difference between the results of the dynamic model and ADM is so small that we can conclude that the dynamic model is suitable for LES of the RHVT, where the Reynolds number is very high.

4. Subgrid model in droplet equations

In LES, droplet velocity and temperature fluctuations are generally under-predicted, especially when the droplet relaxation time is of the same order of magnitude as the Kolmogorov time. This under-prediction is caused by the filtering of the fluid velocity, which affects all scales of motion, but especially the smallest scales. In order to improve the prediction of the fluctuations of the droplet velocity and temperature, a subgrid model based on approximate deconvolution

![Figure 7](image1.png)  
**Figure 7.** RMS of the fluid temperature at $Re_τ=395$.

![Figure 8](image2.png)  
**Figure 8.** RMS of the fluid temperature at $Re_τ=950$.

![Figure 9](image3.png)  
**Figure 9.** RMS of the droplet streamwise velocity at $Re_τ=395$, $St = 5$.

![Figure 10](image4.png)  
**Figure 10.** RMS of the droplet streamwise velocity at $Re_τ=950$, $St = 5$. 
Figure 11. RMS of the droplet wall-normal velocity at $Re_\tau=395$, $St = 5$.

Figure 12. RMS of the droplet wall-normal velocity at $Re_\tau=950$, $St = 5$.

(Kuerten, 2006) has been applied to the equations for the droplet velocity and temperature.

Referring to the equations 4 and 6 the filtered value of the velocity $\overline{u}_i$ is replaced by the defiltered velocity $u^*_i$ and the filtered temperature $\overline{T}$ by the defiltered temperature $T^*$. The subgrid model in the droplet equation models the effect of the missing subgrid scales on a droplet. The defiltering depends on the subgrid model. In the dynamic eddy-viscosity model a filter appears explicitly only as a test filter. We assume that the primary filter has identical shape and adopt the top-hat filter with filter width $\Delta$ as the primary filter. In the ADM the defiltered velocity field $u^*_i$ is obtained by the operation:

$$u^*_i = Q_N \overline{u}_i = \sum_{k=0}^{N} (I - G)^k \overline{u}_i$$

where $G$ is the filter kernel, $N = 5$ and the filter is given by Stolz et al. (Stolz, Adams & Kleiser, 2001).

Figure 13. Mean droplet temperature at $Re_\tau=395$, $St = 5$.

Figure 14. Mean droplet temperature at $Re_\tau=950$, $St = 5$. 
Figures 9 and 10 show the RMS of the streamwise velocity components of the droplets. Figures 11 and 12 show the RMS of the wall-normal velocity components of the droplets. Again, for both quantities presented, the difference between the results of the two models vanishes when the Reynolds number become higher. Also the improvement of the results of the droplet velocity by using the subgrid model in the droplets equations is well visible (DYNw, ADMw).

Figures 13 and 14 show the profile of the mean temperature of the droplets. Figures 15 and 16 show the RMS of the temperature of the droplets. In these figures the benefit of using the mixed model at $Re_\tau=395$ is well visible. In the case of $Re_\tau=395$, the profile of the mean temperature (see figure 13) is improved by using the mixed model. Again for the two lower Reynolds numbers, the mixed model gives the best results for all quantities considered. For $Re_\tau=950$ the profile of the mean temperature of the droplets (see figure 14) and the RMS of the droplet temperature (see figure 16) predicted by the dynamic model are so close to the results of the DNS, that the dynamic model will be used in the LES of the RHVT.

5. Conclusions

Using the mixed model is beneficial for flows with $Re_\tau=395$, and for $Re_\tau=150$ as well. The mixed model yields results for fluid and droplet velocity with a similar quality as the ADM model, and temperature results with quality very close to the quality of the dynamic eddy-diffusivity model. For $Re_\tau=950$ the dynamic model performs so well that the accuracy of the results compared to the results of the DNS is sufficient. In the RHVT, the flow has a higher Reynolds number than in the test case. This is promising for the dynamic model, since this performs better at higher Reynolds numbers. For LES with Lagrangian droplet tracking the subgrid model in the droplet equation based on approximate deconvolution is recommended. The presented results show that this subgrid model substantially improves the results for droplet velocity and temperature RMS.

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