Large-eddy simulation of particle-driven gravity currents using the Relaxation-Term model

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Abstract. We present Large-Eddy Simulations (LES) of two laboratory-scale lock-exchange flows at Grashof numbers of up to $10^8$ and a Schmidt number of unity. The unresolved subgrid scales (SGS) are modeled with the Relaxation-Term (RT) approach. We compare the LES results with those of fully resolved Direct Numerical Simulations (DNS) to rate the quality of the approach. We find that reductions of the grid resolution by factors of about four in each spatial and in the temporal direction are feasible compared to marginally resolved DNS. This corresponds to a reduction of computer time by about two orders of magnitude.

1. Introduction

In LES, the small scales of fluid motion are removed from the solution by a spatial low-pass filter (primary filter), cf. Sagaut (2006). Only flow structures larger than the filter width are computed and the interaction with smaller scales has to be modeled. Ideally, the minimum grid resolution for a sufficiently accurate description of the large scales should be much lower in LES compared to fully resolved DNS. Therefore, the overall computational costs are expected to decrease considerably. However, the mathematical modeling of the non-resolved SGS poses a major challenge for LES as the quality of the LES solution depends essentially on the SGS model. Considerable research efforts have led to a variety of SGS models for incompressible flows, cf. the reviews by Lesieur & Métais (1996); Domaradzki & Adams (2002); Meneveau & Katz (2000), and the monographs by Pope (2000) and Sagaut (2006).

LES of so-called lock-exchange flows (cf. section 2), which constitute a classical example of particle-driven gravity currents, were performed by Alendal (1997) and Ooi et al. (2009), for instance. The LES approach is applied to the Navier–Stokes equations and to the transport equation of the particle concentration (assuming an Eulerian particle description, cf. section 2). Usually, Smagorinsky-type models are employed. In the present work, the performance of the so-called Relaxation-Term (RT) model (Schlatter et al., 2004) is investigated in more detail for the lock-exchange configuration. This model already demonstrated an excellent performance in LES of a variety of transitional and turbulent flows.

2. Configuration and governing equations

A sketch of the lock-exchange configuration (described in Cartesian coordinates $x_1, x_2, x_3$) is depicted in figure 1. The spatial domain is a fluid-filled 3-D rectangular box in which suspended
Figure 1. Lock-exchange configuration: Initially, a reservoir is filled with particle-laden fluid (black) while the remaining part of the channel contains lighter clear fluid. The heavier particle suspension propagates into the channel as soon as the separating lock is released.

Particles are initially located in a small section at one end of the channel (gravity acts in negative \( x_3 \) direction, \( \xi^g \)). Once the barrier between clear and particle-laden fluid is removed (at time \( t = 0 \)), the heavier particle-laden fluid propagates into the channel and forms a bottom-riding gravity current.

In still fluid, the particles are assumed to settle with the Stokes settling velocity \( U_s \) in direction \( \xi^g \). We consider only dilute suspensions for which only the advection and the diffusion of the particles is relevant and for which the Boussinesq approximation can be applied. With these assumptions, the nondimensional governing equations for LES read

\[
\begin{align}
\nabla \cdot u &= 0, \\
\frac{\partial u}{\partial t} + (u \cdot \nabla) u &= -\nabla p + \frac{1}{\sqrt{Gr}} \Delta u + c \xi^g + s^u, \\
\frac{\partial c}{\partial t} + (u + U_s \xi^g) \cdot \nabla c &= \frac{1}{\sqrt{Gr \cdot Sc}} \Delta c + s^c,
\end{align}
\]

where the particles are represented by a continuous concentration \( c \). Furthermore, \( u \) stands for the velocity of the carrier fluid, \( p \) for the pressure (normalized by the mean density), \( Gr \) denotes the Grashof number and \( Sc \) the Schmidt number of the particle suspension. The SGS terms for \( u \) and \( c \) are denoted as \( s^u \) and \( s^c \), respectively (note that \( s^u = s^c = 0 \) for fully resolved DNS). For more details on the origin of these equations, the corresponding boundary conditions and the definition of the nondimensional parameters, we refer to Necker et al. (2002) and Henniger (2011). At \( t = 0 \), the fluid is at rest and only the concentration interfaces are weakly disturbed in the spanwise direction, cf. Henniger (2011).

In this work, we examine two flows with Grashof numbers \( Gr = 5 \cdot 10^6 \) and \( Gr = 1 \cdot 10^8 \), respectively. The Schmidt number is set to \( Sc = 1 \) and the Stokes particle settling velocity to \( U_s = 0.02 \) in both simulations. We refer to Necker et al. (2002) for the motivation of these settings.

3. Energy budget in LES

In fully resolved DNS, the available energy, i.e. the sum of kinetic and potential energy integrated over the computational domain \( \Omega \), can be written as

\[
E^{\text{kin}}(t) + E^{\text{pot}}(t) = E^{\text{kin}}(t_0) + E^{\text{pot}}(t_0) + E^{\text{res}}(t), \quad t \geq t_0,
\]

where \( t_0 \) is a reference time, and the residual \( E^{\text{res}} \) gathers all energy contributions corresponding to physical effects which change \( E^{\text{kin}} + E^{\text{pot}} \) over time. In LES, a significant amount of kinetic energy is dissipated by the SGS term \( s^u \). The corresponding integral loss of energy is represented by

\[
E^{\text{kin,sgs}} = \int_{t_0}^{t} \int_{\Omega} u \cdot s^u \, dV \, dt^*.
\]
Similarly, the potential energy of the concentration changes by

\[ E_{\text{pot, sgs}} = - \int_{t_0}^{t} \int_{\Omega} x \cdot \xi_i s^c \, dV \, dt. \] (4)

In the present configuration, \( |E_{\text{pot, sgs}}| \) is usually much smaller than \( |E_{\text{kin, sgs}}| \). The available energy in a LES becomes

\[ E_{\text{LES}}(t) + E_{\text{pot}}(t) = E_{\text{LES}}(t_0) + E_{\text{pot}}(t_0) + E_{\text{kin, sgs}}(t) + E_{\text{pot, sgs}}(t) \]

\[ \lesssim E_{\text{LES}, \text{no-sgs}}(t) + E_{\text{pot, no-sgs}}(t), \] (5)

where the subscript ‘LES’ indicates that the quantities are computed from a LES rather than from a fully resolved DNS, and the superscript ‘no-sgs’ denotes that a LES is performed without a SGS model.

The inequality on the right-hand side of equation (5) is a consequence of the fact that the smallest (dissipative) flow scales are not resolved in a LES. Especially kinetic energy accumulates where the subscript ‘LES’ indicates that the quantities are computed from a LES rather than from a fully resolved DNS, and the superscript ‘no-sgs’ denotes that a LES is performed without a SGS model.

In the present configuration, \( u \) are sufficiently small (note that \( u \leq 75 \Delta x \) for our SGS model). As demonstrated later, the grid Péclet number

\[ Pe_{\Delta x} = \sqrt{Gr} \max \{|1, Sc| \max \{|u_i|\Delta x_i\}, \ i \in \{1, 2, 3\}, \] (6)

turns out to be a good measure to anticipate if a simulation is a fully resolved DNS or a LES. For the present configuration and nondimensionalization, we can approximate \( \max \{|u_i|\Delta x_i\} \) by \( \max \{\Delta x_i\} \) to obtain a sufficiently good a-priori estimate of \( Pe_{\Delta x} \).

### 4. Numerical approach and Relaxation-Term (RT) SGS model

In order to minimize spatial differentiation errors in LES, we employ compact finite differences in space. They are central and tenth-order accurate in the interior of the domain and at least fourth-order accurate at the boundaries. For the reference DNS, standard sixth-order finite differences in the interior are sufficiently accurate. The grids are moderately stretched in the vertical direction and equidistant in the others. In time, we use a three-step third-order Runge–Kutta integration scheme with \( \Delta t \approx 0.75 \Delta t_{\text{max}} \) (\( \Delta t_{\text{max}} \) is the marginally stable time step size with respect to the stability domain of the integration scheme). The numerical approach is described by Henniger et al. (2010) and Henniger (2011) in detail.

For the SGS terms, we use the Relaxation-Term (RT) model proposed by Schlatter et al. (2004). In discrete form (indicated by bold letters), it reads

\[ s = -\chi F_{hp} a, \quad \chi \geq 0, \quad a = u, c \] (7)

where \( \chi \) is a relaxation factor and \( F_{hp} \) a high-pass filter of the form

\[ F_{hp} = (I - F_{lp}^{M_{lp}})M_{hp} \] (8)
Table 1. Spatial resolutions $N_1 \times N_2 \times N_3$, relaxation factors $\chi$ and estimates of the corresponding grid Péclet numbers (6) for the lock-exchange flows with $Gr = 5 \cdot 10^6$ and $Gr = 1 \cdot 10^8$. For $Pe_{\Delta x} \lesssim 50$, the differences to the reference solutions as well as the SGS terms $s^u$ and $s^c$ vanish for ‘typical’ relaxation factors $\chi$, i.e. such LES are considered as fully resolved DNS (cf. section 5.2).

| $Gr = 5 \cdot 10^6$ | $Gr = 1 \cdot 10^8$ | $Pe_{\Delta x}$ ($\approx$) symbol |
|---------------------|---------------------|-------------------------------|
| $N_1 \times N_2 \times N_3$ | $N_1 \times N_2 \times N_3$ | $\chi$ |
| 1537 $\times$ 257 $\times$ 193 | n/a | 137 |
| 769 $\times$ 129 $\times$ 97 | n/a | 50 |
| 385 $\times$ 65 $\times$ 49 | 40 | 500 |
| 193 $\times$ 33 $\times$ 25 | 40 | 1000 |
| 97 $\times$ 17 $\times$ 13 | 30 | 4000 |
| 49 $\times$ 9 $\times$ 7 | 20 | 800 |
| n/a | 129 $\times$ 25 $\times$ 17 | 60 |
| n/a | 65 $\times$ 13 $\times$ 9 | 40 |
| n/a | 49 $\times$ 9 $\times$ 7 | 20 |

with $F_{lp}$ as a low-pass filter and the matrix exponents $M_{lp}$ and $M_{hp}$. For the specific design of $F_{lp}$ we refer to Stolz (2001) and Henniger (2011). Note that both filters are typically symmetric and positive (semi-)definite, i.e. $-\chi a^T F_{hp} a = a^T s \leq 0$.

For a given relaxation factor $\chi$, the spectral properties of the high-pass filter $F_{hp}$ determine how the different modes of a quantity $a$ are damped by the RT model (7). The relaxation factor $\chi \geq 0$ modulates the total amount of energy dissipation for a given high-pass filter $F_{hp}$. Therefore, $\chi$ is limited by a lower threshold below which the solution blows up due to lacking energy dissipation.

5. Results

5.1. General remarks and parameter settings

We study the convergence of the LES results towards those of the corresponding fully resolved DNS by varying simultaneously the numbers of grid points by factors of about two in all spatial directions and in time. The resolutions of the various simulations are listed in table 1 along with the a-priori estimates of the corresponding grid Péclet numbers $Pe_{\Delta x}$.

Generally, accurate LES are able to reproduce the results of fully resolved DNS at a sufficiently small error. Because it is a major objective to apply the LES approach also, and especially, to flow problems for which such reference results are not available, the approach must be reliable as well. Therefore, we have to require that appropriate parameter settings for the SGS model are known beforehand for a given configuration.

To check if the RT model (7) meets these two criteria, accuracy and reliability, and to identify suitable parameter settings for the model, we performed a large number (on the order of hundreds) of numerical experiments of transitional/turbulent channel and lock-exchange flows. The parameters were varied separately for $s^u$ and $s^c$; however, we found that using the same filter $F_{lp}$ and the same values of $\chi$, $M_{lp}$ and $M_{hp}$ for $s^u$ and $s^c$ leads to qualitatively good results (note that this observation may apply only to the present flows with Schmidt numbers $Sc$ on the order of one, but not for much larger or smaller $Sc$, cf. Hickel et al., 2007). The best results were obtained with $M_{lp} = 1$, $M_{hp} = 6$ and the same filter $F_{lp}$ as used by Schlatter et al. (2004) and Stolz (2001).
as this was the main optimization goal for the selection of the relaxation factors $\chi$, cf. the next paragraph. The front speeds of the lock-exchange flows, is depicted in figure 3. Generally, the total energies $E_{\text{LES}}$ of test simulations until a suitable value for $\chi$ is found. On the other hand, the results are not very sensitive with respect to increases of $\chi$ cannot be anticipated beforehand; however, we can formulate at least a rule of thumb for this parameter: the best optimization goal for the choice of $\chi$ is to maintain the total energy

$$E_{\text{LES}}^{\text{tot}}(t) = E_{\text{LES}}^{\text{pot}}(t) + E_{\text{LES}}^{\text{kin}}(t) - E_{\text{LES}}^{\text{sett}}(t) - E_{\text{LES}}^{\text{visc}}(t) \approx E_{\text{LES}}^{\text{tot}}(t = 0)$$

as closely as possible, cf. equation (5). This implies that $E_{\text{LES}}^{\text{tot}}(t) \approx E_{\text{LES}}^{\text{tot}}(0)$ is preserved as well. For the present flows, the energy $E_{\text{LES}}^{\text{res}}$ can be well approximated by $E_{\text{LES}}^{\text{res}} \approx E_{\text{LES}}^{\text{sett}} + E_{\text{LES}}^{\text{visc}}$ with

$$E_{\text{LES}}^{\text{sett}} = - \int_{t_0}^t \int_{\Omega} c \, U^s \, dV \, dt^* \quad \text{and} \quad E_{\text{LES}}^{\text{visc}} = \frac{1}{\sqrt{\text{Gr}}} \int_{t_0}^t \int_{\Omega} u \cdot \Delta u \, dV \, dt^*$$

as the loss of potential energy due to Stokes particle settling and the amount of dissipated energy due to fluid viscosity, respectively. Sufficiently good values of $\chi$ are quite well conserved over time $E_{\text{LES}}^{\text{tot}}$ as closely as possible, cf. equation (5). This implies that $E_{\text{LES}}^{\text{tot}}(t) \approx E_{\text{LES}}^{\text{tot}}(0)$ is preserved as well. For the present flows, the energy $E_{\text{LES}}^{\text{res}}$ can be well approximated by $E_{\text{LES}}^{\text{res}} \approx E_{\text{LES}}^{\text{sett}} + E_{\text{LES}}^{\text{visc}}$ with

$$E_{\text{LES}}^{\text{sett}} = - \int_{t_0}^t \int_{\Omega} c \, U^s \, dV \, dt^* \quad \text{and} \quad E_{\text{LES}}^{\text{visc}} = \frac{1}{\sqrt{\text{Gr}}} \int_{t_0}^t \int_{\Omega} u \cdot \Delta u \, dV \, dt^*$$

as the loss of potential energy due to Stokes particle settling and the amount of dissipated energy due to fluid viscosity, respectively. Sufficiently good values of $\chi$ cannot be anticipated beforehand; however, we can formulate at least a rule of thumb for this parameter: the best results are obtained with relaxation factors $\chi$ close to the lower stability constraint (note that this is a preliminary and empirical finding from the numerical experiments). The values of $\chi$ used in this work are listed in table 1. Typically, the individual adjustment requires a number of test simulations until a suitable value for $\chi$ is found. On the other hand, the results are not very sensitive with respect to increases of $\chi$ by a value of up to about ten nondimensional units.

5.2. Integral quantities

We first investigate the evolution of the total masses of suspended particles, $m(t)$, for the two test cases. As depicted in figure 2, the total masses differ significantly from the solution of fully resolved DNS beyond $Pe_{\Delta x} \approx 200$ for $Gr = 5 \cdot 10^6$ and $Pe_{\Delta x} \approx 800$ for $Gr = 1 \cdot 10^8$. Generally, the total masses tend to decrease more slowly over time for increasingly coarse grids. Note that the initial amounts, $m(t = 0)$, decrease as well which is attributed to the specific boundary conditions for the concentration, cf. Necker et al. (2002). Also the energy budgets are affected, cf. the next paragraph. The front speeds of the lock-exchange flows, $x_1^f$, decrease for coarser grids, as shown in the same plots. The differences become significant beyond $Pe_{\Delta x} \approx 400$ for $Gr = 5 \cdot 10^6$ and $Pe_{\Delta x} \approx 1 \cdot 10^8$.

The evolution of the energies $E_{\text{LES}}^{\text{pot}}$, $E_{\text{LES}}^{\text{kin}}$, $E_{\text{LES}}^{\text{sett}}$, $E_{\text{LES}}^{\text{visc}}$, $E_{\text{LES}}^{\text{tot}}$, $E_{\text{LES}}^{\text{kin,sgs}}$ in equations (9) & (10) is depicted in figure 3. Generally, the total energies $E_{\text{LES}}^{\text{tot}}$ are quite well conserved over time as this was the main optimization goal for the selection of the relaxation factors $\chi$. However,
Figure 3. Temporal evolution of different energy contributions (the line types are specified in table 1). Left: $Gr = 5 \cdot 10^6$; right: $Gr = 1 \cdot 10^8$.

the accuracy with which $E_{\text{tot}}^{\text{LES}}$ is maintained suffers from the grid coarsening, also because the discretization errors come more into play at lower resolutions.

The observations made for $m$ and $x_{1f}$ are also reflected by the developments of the potential energies $E_{\text{pot}}^{\text{LES}}$ and of the kinetic energies $E_{\text{kin}}^{\text{LES}}$, respectively, as they are tightly connected to each other. More precisely, the potential energies tend to be larger than in the reference DNS, whereas the kinetic energies are smaller for most of the time, i.e. the conversion of the former into the latter is more and more hampered for increasingly coarse grids. The differences to the results of fully resolved DNS become significant beyond $Pe_{\Delta x} \approx 400$ for $Gr = 5 \cdot 10^6$ and $Pe_{\Delta x} \approx 800$ for $Gr = 1 \cdot 10^8$. Only the losses of potential energy due to Stokes particle settling, $E_{\text{sett}}^{\text{LES}}$, are quite close to the reference solutions in all LES.

Because only the largest flow structures contain notable amounts of energy, all energy contributions should ideally be close to the corresponding results of fully resolved DNS, except for the energy losses due to viscous dissipation, $E_{\text{visc}}^{\text{LES}}$. Therefore, the differences between $E_{\text{visc}}^{\text{LES}}$ and the reference energies $E_{\text{visc}}$ of the respective fully resolved DNS have to be compensated by the SGS model, i.e. $E_{\text{visc}}^{\text{LES}} + E_{\text{kin,sgs}}^{\text{LES}}$ should approximate $E_{\text{visc}}$ as closely as possible. This is well
satisfied up to $Pe_{\Delta x} \approx 200$ for both configurations, as demonstrated in figure 3. When we plot these two contributions relatively to each other (figure 4), we find that $|E_{\text{kin, sgs}}|$ exceeds $|E_{\text{visc, LES}}|$ beyond $Pe_{\Delta x} \approx 400$.

For increasingly coarse grids, the viscous and diffusive terms in the momentum and concentration transport equation, respectively, become more and more negligible such that the SGS model has to take over almost all energy dissipation and concentration diffusion. Obviously, such simulations are controlled mostly by the SGS parameters, whereas the influence of the Grashof and Schmidt number vanishes. This is well rendered by the simulations performed on the respective coarsest grids: they yield nearly identical results although the Grashof numbers of the two flows differ significantly.

As stated in section 3, we identify fully resolved simulations by proving that $|E_{\text{kin, sgs}}|$ and $|E_{\text{LES}} + E_{\text{pot, LES}} - E_{\text{kin}} - E_{\text{pot}}|$ are sufficiently small. We find from figures 3 & 5 that the magnitudes of $E_{\text{kin, sgs}}$ and $E_{\text{LES}} + E_{\text{pot, LES}} - E_{\text{kin}} - E_{\text{pot}}$ are negligible below $Pe_{\Delta x} \approx 50$, i.e. this is the boundary between fully resolved DNS and LES corresponding to our definition.

5.3. Flow details

To assess the LES results more qualitatively, we visualize isopycnal surfaces ($c = 0.5$) of the various LES for three representative times $t = 8, 12, 16$ (depicted in figures 6 & 7). The results for $Pe_{\Delta x} \approx 100$ are not shown as they are very close to those of the reference DNS with $Pe_{\Delta x} \lesssim 50$. 

Figure 4. Temporal evolution of $E_{\text{kin, sgs}}/E_{\text{visc, LES}}$ with $E_{\text{kin, sgs}}$ as the energy dissipated by the SGS model and $E_{\text{visc, LES}}$ as the energy dissipated by the fluid viscosity (the line types are specified in table 1). Left: $Gr = 5 \cdot 10^6$; right: $Gr = 1 \cdot 10^8$ (note that the coarsest resolution exceeds the upper limit of the diagram).

Figure 5. Temporal evolution of the energy differences $E_{\text{LES}} + E_{\text{pot, LES}} - E_{\text{kin}} - E_{\text{pot}}$ (the line types are specified in table 1). Left: $Gr = 5 \cdot 10^6$; right: $Gr = 1 \cdot 10^8$. 

Generally, the initial formations of the lobe-and-cleft instability (cf. Necker et al., 2002) are rendered quite accurately for grid Péclet numbers up to $Pe_{\Delta x} \approx 200$ in both configurations. For increasingly coarse grids, the fronts appear to be more unstable than in the reference DNS which is indicated by an earlier formation of sharp clefts. Beyond $Pe_{\Delta x} \approx 200$ for $Gr = 5 \cdot 10^6$ and $Pe_{\Delta x} \approx 400$ for $Gr = 1 \cdot 10^8$, the grids are not fine enough to resolve the lobe-and-cleft instability anymore, such that also the spanwise spacings of these structures are incorrect. On the coarsest grids, the flows remain almost two-dimensional. Similarly, the secondary instabilities of the Kelvin–Helmholtz vortices behind the current heads are qualitatively acceptable for grid Péclet numbers up to $Pe_{\Delta x} \approx 200 \ldots 400$. Beyond this resolution quality, the gaps between current heads and ‘proximate wakes’ are not present anymore (cf. the snapshots at $t = 12$).

As mentioned before, we assume that the boundary between fully resolved DNS and LES is located at about $Pe_{\Delta x} \approx 50$. For this number, the concentration interfaces at the current heads are resolved with about three grid points for $Gr = 5 \cdot 10^6$ and six grid points for $Gr = 1 \cdot 10^8$. Correspondingly, the interfaces can be resolved only up to $Pe_{\Delta x} \approx 150$ and $Pe_{\Delta x} \approx 300$, respectively. This indicates, together with the previous qualitative findings, that the resolution of this interface may be crucial for acceptably good predictions of such flows.

6. Summary and conclusions

We found that LES using the RT model yield accurate results for grid resolutions that are coarser by a factor of about four in each spatial (and thus also in the temporal) direction compared to just sufficiently resolved DNS. In this context, ‘just sufficiently resolved’ means that the grid resolutions are just fine enough to resolve also the dissipative scales (but not much finer). This is indicated by a vanishing energy dissipation due to the SGS model, $E^{\text{kin,sgs}}$, and a vanishing difference between the available energies of DNS and LES, $E_{\text{LES}}^{\text{kin}} + E_{\text{LES}}^{\text{pot}} - E_{\text{kin}} - E_{\text{pot}}$.

Regarding the reliability of the results, we observed that the low-pass filter $F_{\text{lp}}$ as well as the
| $Pe_{\Delta x}$ | $t = 8$ | $t = 12$ | $t = 16$ |
|----------------|--------|--------|--------|
| $\approx 50$  | ![Image](image1.png) | ![Image](image2.png) | ![Image](image3.png) |
| $\approx 200$ | ![Image](image4.png) | ![Image](image5.png) | ![Image](image6.png) |
| $\approx 400$ | ![Image](image7.png) | ![Image](image8.png) | ![Image](image9.png) |
| $\approx 800$ | ![Image](image10.png) | ![Image](image11.png) | ![Image](image12.png) |
| $\approx 1600$| ![Image](image13.png) | ![Image](image14.png) | ![Image](image15.png) |
| $\approx 3200$| ![Image](image16.png) | ![Image](image17.png) | ![Image](image18.png) |
| $\approx 4800$| ![Image](image19.png) | ![Image](image20.png) | ![Image](image21.png) |

**Figure 7.** Isopycnal layer ($c = 0.5$) of the particle concentration at time $t = 8, 12, 16$ for $Gr = 1 \cdot 10^8$ and different resolutions, cf. table 1.

values of the model parameters $M_{lp}$ and $M_{hp}$ can be chosen more or less uniquely. However, the relaxation factor $\chi$ had to be adjusted individually. Generally, its value is constrained by a lower stability limit below which the dissipation of (kinetic) energy is not sufficient to yield physical solutions. We found empirically that the best results are obtained for $\chi$ close to this lower constraint. Moreover, our results appeared to be not very sensitive to an increase of $\chi$ by up to about ten. For the present flows, the optimal values for $\chi$ varied in a range of $\chi \approx 20 \ldots 60$ which indicates that an individual adjustment of $\chi$ to a given simulation setup is necessary. In practice, however, the lower stability constraint for the value of the relaxation factor $\chi$ is usually not known beforehand, as it depends strongly on the specific flow configuration, grid resolution and Grashof/Reynolds number (and possibly also on the Schmidt number). Therefore, we need to determine it iteratively by running several LES of a given configuration. A possible remedy for this problem might be an appropriate dynamic procedure which computes $\chi$ automatically.
All essential large-scale flow features (including the lobe-and-cleft structures) of the lock-exchange flows were well rendered for grid Péclet numbers up to \( \text{Pe}_{\Delta x} \approx 200 \). The various integral quantities matched the reference results quite well even for somewhat larger grid Péclet numbers. However, the SGS dissipation still played a lesser role than the viscous dissipation in the aforementioned grid Péclet number regime. This reflects the fact that only rather small portions of the full wavenumber spectra were actually cut off by the primary grid filter.

An important aspect concerns the front speed of the lock-exchange flows: when we decreased the grid resolutions, we observed significant decreases of the propagation velocity, independent of the particular parameter values for the SGS model. Generally, the spatial resolutions corresponding to \( \text{Pe}_{\Delta x} \approx 200 \) were just able to resolve the concentration interfaces at the heads of the lock-exchange flows. This observation indicates that it might be mandatory to resolve these interfaces for a sufficiently accurate representation of the lobe-and-cleft instability, the break-up of the Kelvin–Helmoltz vortices and for a correct prediction of the front velocity.

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