A new LES subgrid-scale approach for turbulence modulation by droplets

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Abstract

We present a new modeling approach for turbulence modulation by droplets on the subgrid-scale (SGS) level of Large-Eddy-Simulations (LES). Many SGS models exist for the effect of the gas phase SGS on the dispersed phase, but very few for the mechanisms vice versa, i.e. the modulation of turbulent intensity of the gas phase by droplets. The reasons are a lack of physical understanding and limited computational resources for extensive DNS studies. To address both problems a dimension-reduced and consequently less costly model, namely One-Dimensional-Turbulence (ODT), is used here to gather information about this specific flow phenomena. ODT is a stochastic tool simulating turbulent flows along a notional 1D line of sights. For modeling the turbulent advection instantaneous maps are applied to the line which represent the effect of individual eddies on property fields and the dispersed phase. After validating ODT for the case of a droplet-laden shear flow against DNS data, a concept is presented on how to gather turbulence modulation for several parameter ranges in a data base and how to make them accessible on the flight for LES. The three most significant parameters, unladen flow Reynolds number Re_L, droplet mass loading ϕ and droplet Stokes number St, are chosen to construct an efficient data base.

Keywords: Turbulence, Droplets, Multiphase Flow, One-Dimensional-Turbulence, ODT

Introduction

Precise capturing of the mixing process in the reaction zone of combustion simulations requires an accurate prediction of the turbulent quantities in this zone. Due to the unresolved scales in Large-Eddy-Simulations (LES) the effect of small droplets on the subgrid-scale gas flow structures are usually not taken into account. Especially the effect of droplets on the turbulence intensity can have a significant impact depending on several parameter. More generally speaking, the effect of particles on turbulence and turbulent structures is known as "turbulence modulation" and has been focus of many research studies since the early 1990s. Firstly done by Squires & Eaton [16] and extended by Boivin et al. [1], intensive investigations on homogeneous isotropic turbulence using a Direct-Numerical-Simulation (DNS) code have shown an overall attenuation of the turbulent kinetic energy and an increase of the energy dissipation rate induced by particles. Several groups continued the work on a variety of different flow phenomena [2, 4, 7, 20] and saw that the dispersed phase can also cause an augmentation of the turbulent kinetic energy and energy dissipation rate. The main contributor by controlling augmentation or attenuation of turbulent kinetic energy is the ratio of particle response time τ_p and the Kolmogorov time scale τ_η, which is called the Stokes number ($St = \tau_p/\tau_\eta$). Regarding now a LES cell in a spray application it is assumed to have homogeneous shear flow conditions driven by the velocities on the cell faces (illustrated in Fig. 1). The cell face velocities are interpolated between the velocities in each neighbor cell. The stationary turbulent variables of the gas phase in homogeneous shear turbulence only depend on the shear rate which is defined as the velocity difference over a distance. Including the information of the dispersed phase will be sufficient for defining the modulation of the turbulent intensity. Intensive investigations of the test case are aimed to develop a SGS model for turbulence modulation by droplets.

Gathering a data base for turbulence modulation using DNS, which can be accessed on the flight by LES, will be computationally very expensive even with access to a high-performance computational infrastructure. Thus, in this study an alternative, dimension-reduced approach is used, called One-Dimensional-Turbulence (ODT). ODT is a stochastic approach resolving the full range of length and time scales on an one-dimensional domain. After its first introduction [8] and extension [9] it has demonstrated to predict many topologically simple flows such as boundary layers and jets with large property gradients in one direction very well compared to DNS studies and experimental results. E.g. Schmidt et al. [14] and Sun et al. [18] extended the ODT model to predict dispersed-carrier phase interaction and Fistler et al. [5] introduced a new formulation of the dispersed-phase-eddy interaction. The two latter studies showed that ODT was capable to capture two-way coupling effects. Due to its cost-effective

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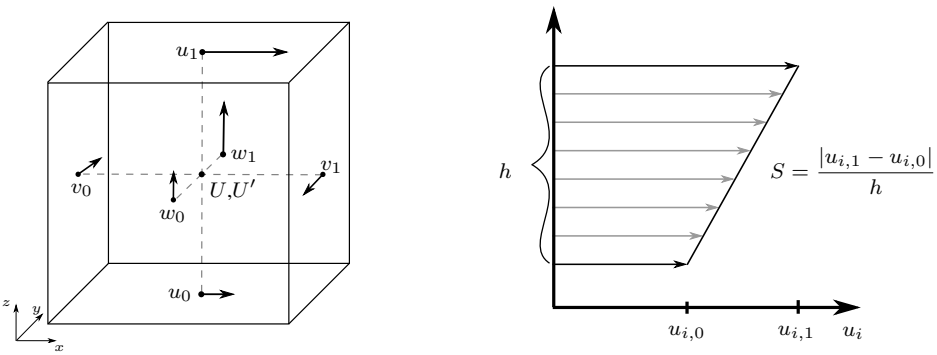

Figure 1: Illustration of the simplification considering the velocity field inside a LES cell as homogeneous shear turbulence driven by the velocities non-normal to the cell faces. The shear rate S is defined as the absolute velocity difference between $u_{i,0}$ and $u_{i,1}$ divided by the distance h between cell faces.

manner it is a promising tool to investigate turbulence modulation for a large range of variables. In this paper a new approach is presented which aims to develop an empirical one-equation SGS model based on the most dominant parameters, i.e. Stokes number St, unladen flow shear Reynolds number Re_L, and droplet mass loading ϕ.

Model Formulation

This section describes the concept of the ODT model, which is used in this study to simulate the carrier gas phase, and the Lagrangian model to track the dispersed phase. ODT is a stochastic model to simulate turbulent flows on a one-dimensional domain, which is oriented in the direction of the largest expected velocity gradients. In the presented case of homogeneous shear turbulence the domain is oriented along the velocity slope direction y. The streamwise direction is denoted as x and the spanwise direction as z.

One-Dimensional-Turbulence

The ODT implementation used in this study was described in detail in [10]. In the following we will give a brief summary of the fundamental ideas and formulations of ODT. The ODT is a numerical method to simulate realizations of turbulent flows using a stochastic model to capture the full range of the spatial and temporal turbulent cascade along a one-dimensional line. This line can be interpreted as a line of sight through a 3D flow phenomena. ODT solves the unsteady, one-dimensional transport equations for mass and momentum and models the advection effects of turbulence by remapping the profiles based on a stochastic process. In the so-called eddy events the fluid property profile is rearranged by implementing a triplet map in a manner consistent with turbulent scaling laws. The both main mechanisms, eddy event and diffusion equation, are performed consecutively.

The governing equations for mass and momentum are based on the Reynolds transport theorem in incompressible form and result in the continuity and diffusion equation, respectively. In discrete form for individual control volumes and with quantities in the cell center they are given as,

$$\frac{d}{dt}(\rho \Delta y A) = 0. \tag{1}$$

and

$$\frac{du_i}{dt} = -\frac{1}{\rho \Delta y A}(\tau_{i,e} - \tau_{i,w} + S_{p,i}). \tag{2}$$

Here, Δy is the cell length of the dynamically adaptive computational grid, u_i is the i^{th} fluid velocity component, ρ is the fluid density. To conserve the dimensionalty of mass and momentum the cell cross-section area A is set to 1m^2. This determination is important to ensure the droplet-number-density equal to DNS results. τ_i is the i^{th} viscous stress component evaluated on the east or west cell face and subscripted with e or w, respectively. $S_{p,i}$ represents the momentum exchange between dispersed and gas phase and ensures the two-way coupling.

In ODT simulations turbulence, which can be seen as a three-dimensional vortex stretching process, is modeled through eddy events. These result in remapping the flow quantity profiles over a sampled eddy region, which is

defined by a location y_0 and a size of the eddy l. This model consists of two key components, the mapping method, which is called triplet map, and a model to define the rate of eddy events [8]. The triplet map function compresses the original profile by a factor of three over the eddy region and three copies are filled in. To ensure continuity of the profile the second copy in the middle is inverted (see Fig. 2). A fluid at location $f(y)$ is mapped to location y and $f(y)$ is given as,

$$f(y) = y_0 + \begin{cases} 3(y-y_0) & \text{if } y_0 \leq y \leq y_0 + \frac{1}{3}l \\ 2l - 3(y-y_0) & \text{if } y_0 + \frac{1}{3}l \leq y \leq y_0 + \frac{2}{3}l \\ 3(y-y_0) - 2l & \text{if } y_0 + \frac{2}{3}l \leq y \leq y_0 + l \\ y - y_0 & \text{otherwise.} \end{cases} \tag{3}$$

The triplet map function conserves all quantities, increases scalar gradients and decreases length scales, what agrees with the behavior of canonical turbulent eddies [17]. An essential part of turbulence is the phenomena of return-to-isotropy, which requires on the ODT modeling side a re-distribution of turbulent kinetic energy among the velocity components. Additionally, momentum and energy exchange between gas and dispersed phase has to be ensured. This is achieved by introducing kernel transformations to the mapping function, which gives a profile transformation

$$u_i(y) \rightarrow u_i^{\mathrm{TM}}(y) + c_i K(y) + b_i J(y), \tag{4}$$

where u_i is the velocity in i^{th} direction before and u_i^{TM} after the mapping process. The Kernel $K(y)$ is defined as the fluid displacement profile under the triplet map and integrates to zero over the eddy region. $J(y)$ is the absolute of $K(y)$ and so it does not integrate to zero over the eddy region. Thus, it forces momentum change of the profiles if its kernel coefficient b_i is non-zero. c_i defines the kernel amplitude of $K(y)$. The effect of kernels on the mapped profiles is illustrated in Fig. 2. Due to momentum and kinetic energy conservation over the sampled eddy region it is required to meet the following equations:

$$A \int_{y_0}^{y_0+l} \rho u_i dy = A \int_{y_0}^{y_0+l} \rho(u_i^{\mathrm{TM}} + c_i K + b_i J) dy + S_{\mathrm{p},i}, \tag{5}$$

$$\frac{1}{2} A \int_{y_0}^{y_0+l} \rho u_i^2 dy = \frac{1}{2} A \int_{y_0}^{y_0+l} \rho(u_i^{\mathrm{TM}} + c_i K + b_i J)^2 dy - \Delta E_i + S_{\mathrm{pE},i}. \tag{6}$$

$S_{\mathrm{p},i}$ and $S_{\mathrm{pE},i}$ represent the sum of momentum and energy penalties caused by particles, respectively. $\triangle E_i$ stands for the above mentioned re-distribution of energy between velocity components. Under consideration of the measure preserving character of the mapping process itself, which means

$$\int_{y_0}^{y_0+l} \rho u_i dy = \int_{y_0}^{y_0+l} \rho u_i^{\mathrm{TM}} dy \qquad \text{and} \qquad \int_{y_0}^{y_0+l} \rho u_i^2 dy = \int_{y_0}^{y_0+l} \rho (u_i^{\mathrm{TM}})^2 dy, \tag{7}$$

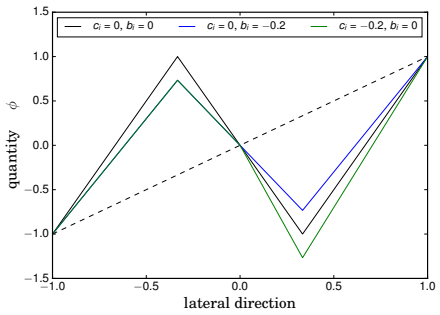

Figure 2: Illustration of a triplet map including kernel effects on a linear profile of a arbitrary quantity ϕ. (- -) original profile, (-) remapped profile.

and depending on the predefined energy distribution parameter α the determination of b_i and c_i defines the new profile.

Each eddy event (y_0, l) has a specific time scale $\tau_e(y_0, l)$ depending on its local fluid kinetic energy field E_{kin} and defined as

$$\frac{1}{\tau_e} = C\sqrt{\frac{2}{\rho l^3}(E_{kin} - Z\ E_{vp})}, \tag{8}$$

based on the scaling assumption of $E_{kin} \approx \frac{1}{2}\rho l^3/\tau_e^2$. Here, $E_{kin} = \frac{1}{2}\rho l \sum_i u_{i,k}^2$, where $u_{i,k} = \frac{1}{l^2}\int_{y_0}^{y_0+l} u(y)K(y)dy$.

The viscous penalty energy is given as $E_{\mathrm{vp}} = \frac{\mu^2}{2\rho l}$. C is the adjustable eddy rate parameter and scales the overall eddy event frequency. Z is the viscous penalty parameter, which suppresses unphysical small eddies. Also for large eddies an equivalent procedure exists with a parameter noted as Z_{LES}.

As a next step it is important to define the rate of eddy events λ, which is assumed to be depended on the eddy origin and length (y_0, l) and so on the current line state. This rate is modeled by using dimensional arguments, which are leading to

$$\lambda = \frac{1}{\tau_e l^2}. \tag{9}$$

The rate λ is the rate of eddies of length l in ODT-line and time scale τ_e. Its integral over both quantities defines the rate of all eddies Λ. With both rates we can construct an instantaneous joint probability density function (PDF) of eddy size and location, which is given as

$$P(y_0, l) = \frac{\lambda(y_0, l)}{\int\int \lambda(y_0, l) dy_0\, dl} = \frac{\lambda}{\Lambda}. \tag{10}$$

We assume that the occurrence of eddies of a certain size follows a Poisson process in time with a mean rate Λ, i.e. $P(\Delta t) = \Lambda exp(-\Lambda\Delta t)$. Technically this is solved by oversampling, i.e. generation of candidate eddies at a much higher rate than requested, and thinning of the Poisson process with an acceptance-rejection method. For details we refer to [10].

Dispersed phase

The target spray region for the SGS model is the post-secondary-break-up field, where the droplet sizes are small compared to the smallest gas flow structures and the non-slip velocities are small as well. Under these conditions the droplets are treated as spherical, point particles. Droplets are modeled in a Lagrangian way following Newton's second law of motion. The set of governing equations for each individual droplet are:

$$\begin{aligned} \frac{du_{d,i}}{dt} &= -\frac{u_{d,i} - u_{g,i}}{\tau_p} f + g_i, \\ \frac{dy_d}{dt} &= v_d. \end{aligned} \tag{11}$$

The subscripts d and g represent the droplet and the gas phase, respectively, and g_i is the i-th component of the gravity acceleration vector. The response time, $\tau_p = \rho_d d_d^2/18\mu$ based on Stokes flow, is given here with consideration of mass m_d and density ρ_d of the droplet phase and the fluid viscosity μ. The empirical correction factor f is defined as

$$f = 1 + 0.15 Re_p^{0.687}, \tag{12}$$

based on studies of Schiller and Naumann [13] for non-slip Reynolds numbers Re_p smaller than 200. The drag law (11) is solved by a first-order Euler method.

Due to the instantaneous character of eddy events it is required to model the droplet-eddy interaction. Schmidt et al. [14] developed the so-called instantaneous particle-eddy model (noted as *type-I*), which governs the lateral

displacement of particles due to an eddy event. It is defined as the only effect of droplet motion in ODT line-direction and so the relative velocity $v_d - v_g$ in this direction for the drag law (Eq. 11) is zero. This PEI model is used to capture droplet-eddy interaction for each particle which is located in the sampled eddy region.

The main model assumption is that the eddy time scale τ_e (Eq. 8) defines the time an eddy needs to create the remapped profile. That means the integration of the lateral motion of a droplet in Eq. 11 has to be corrected to account for a finite time a droplet needs to cross an eddy. Therefore, the analytical solution for the drag law in ODT line-direction is used, which is given as

$$\begin{aligned} y_d &= y_{d0} + v_g t + \tau_p g_y t - \tau_p(\tau_p g_y + v_g - v_{d0})(1 - e^{-t/\tau_p}), \\ v_d &= v_g + \tau_p g_y - (\tau_d g_y + v_g - v_{d0}) e^{-t/\tau_p}. \end{aligned} \tag{13}$$

where v_{d0} and y_{d0} are the initial droplet velocity and location, respectively. τ_p includes here the correction factor f (Eq. 12). As during the diffusive advancement the relative velocity in ODT line direction was assumed to be zero and with a new defined gas velocity for the droplet-eddy interaction (DEI), so-called eddy velocity, the resulting correction over the integral time t_{dei} are

$$\begin{aligned} \Delta y_d &= v_g t_{\mathrm{dei}} - v_g \tau_p (1 - e^{-t_{\mathrm{dei}}/\tau_p}), \\ \Delta v_d &= v_g (1 - e^{-t_{\mathrm{dei}}/\tau_p}), \end{aligned} \tag{14}$$

and the post-DEI location and velocity are $y_d = y_{d0} + \Delta y_d$ and $v_d = v_{d0} + \Delta v_d$, respectively.

Now, it is required to define an eddy velocity in lateral direction v_{e} and an interaction time t_{dei}, which determines the time interval in Eq. 11, to correct the integration over the time interval t_{dei}. Determining the eddy velocity v_e during the eddy event, the concept of the displacement of a mass-less droplet governed by the mapping method (Eq. 3) is used. The triplet map provides three possible mass-less droplet positions and a unique position is sampled randomly with a uniform distribution from those three possible ones. The final displacement $\triangle Y_{TM}$, see Fig. 3, divided by the eddy time scale τ_e defines the gas velocity during the DEI.

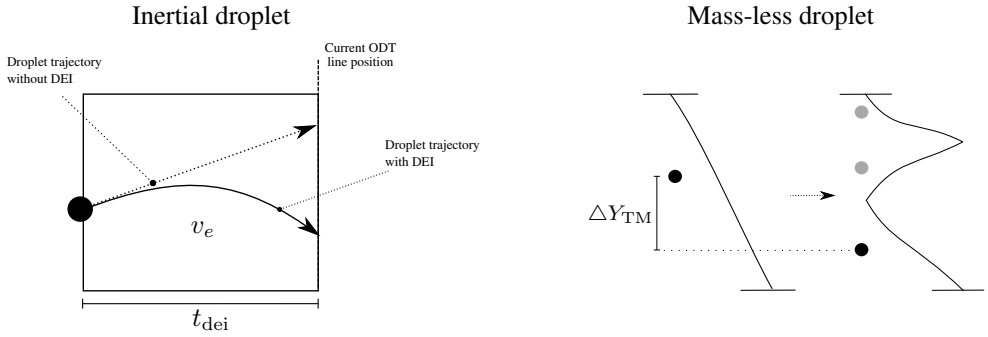

Figure 3: Example of re-integration of drag law (Eq. 11) over droplet-eddy interaction time t_{dei}. Eddy velocity v_e is defined as the mass-less droplet displacement $\triangle Y_{\mathrm{TM}}$ by the triplet map divided by the eddy time scale t_e. For the displacement one (black circle) of three possible positions (grey circles) is chosen randomly.

As a next step the integral time scale t_{dei} has to be determined and therefore a so-called eddy box is introduced with the dimensions $[l \times l \times l]$. The DEI integration time t_{dei} is given as the time the particle needs to exit the box. Therefore, the analytical solution (Eq. 13) is used again to compute the exit time in each direction. For the non-lateral eddy velocity components the local gas velocity at the droplet position is used. The minimum of the resulting exit times and the eddy time scale $\tau_e \beta_p$, where β_p is a model parameter, defines the droplet-eddy interaction time t_{dei}.

	DNS	ODT
k	0.55*	0.4
ϵ	0.088*	0.055
$\langle u^2 \rangle / k$	1.07**	1.06
$\langle v^2 \rangle / k$	0.37**	0.47
$\langle w^2 \rangle / k$	0.56**	0.47

Table 1: Comparison of DNS and ODT data for a single-phase homogeneous shear turbulence test case. (*Gualtieri et al. [7] , **Tavoularis and Corrsin [19])

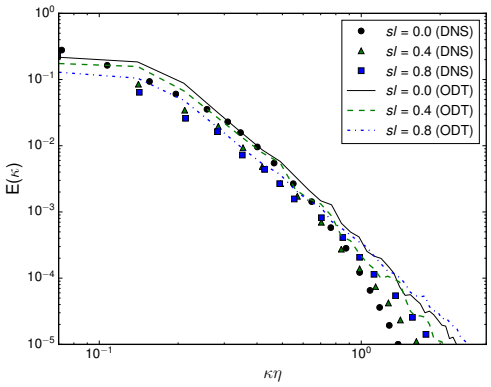

Figure 4: Energy spectrum for different droplet ($St \sim 1$) mass-loadings compared to DNS data of Gualtieri et al. [7].

ODT setup and preliminary results

For the general setup of ODT for homogeneous shear turbulence we chose the height h of the ODT domain to 2π and it goes from $-\pi$ to π. The initial gas velocity profile in streamwise direction is $u_g = S \cdot y$, where S is the shear rate (see also Fig. 1). The two other velocity profiles are zero and the following Dirichlet boundary conditions are used:

$$\begin{aligned} u_g(y = -\pi) &= S \cdot -\pi, & u_g(y = \pi) &= S \cdot \pi, \\ v_g(y = -\pi) &= 0, & v_g(y = \pi) &= 0, \\ w_g(y = -\pi) &= 0, & w_g(y = \pi) &= 0. \end{aligned} \tag{15}$$

Special boundary conditions are required for the eddy events to ensure an equal distribution of them over the domain. Therefore, periodic jump boundary conditions are implemented. This means during an eddy event over the positive domain boundary the profile outside the domain will be mapped to the other side of the domain and reduced by the velocity difference of both boundaries. The initial velocities of each droplet is equal to the gas-phase at its position due to a aimed stationarity of the flow. For showing the capability of ODT to capture droplet-laden homogeneous shear turbulence a first test case is evaluated below.

For evaluating a first test case for droplet-laden homogeneous shear turbulence ODT simulations are compared with DNS data of Gualtieri et al. [7] for $Re_\lambda = 50$. The kinematic viscosity is $\nu = 0.0125$ and the density is $\rho = 1.0$ kg/m^3. To capture similar behavior for the turbulent values the viscous penalty parameter is $Z = 500$ and the eddy frequency parameter is $C = 8.5$. The maximum eddy size is limited by the domain size. As seen in Tab. 1 the turbulent kinetic energy $k = 0.5(\overline{u_i' u_i'})$ and the dissipation rate $\epsilon = \nu \overline{(\partial u_i'/\partial x_j)^2}$ fairly agree with the DNS data for the single-phase. It is essential to achieve firstly agreeing results for the single-phase to provide a reasonable base for the multiphase simulations. Due to the anisotropic character of homogeneous shear turbulence the turbulent kinetic energy budgets are not equally distributed like in homogeneous isotropic turbulence. As in this study our main concern is the turbulent kinetic energy budget in streamwise direction it is important that ODT captures its share very accurately. This is done by defining the distribution parameter $\alpha = 1.06$. For more details we refer to Kerstein et al. [9].

Regarding the dispersed phase the energy spectrum for different mass loading are shown in Fig. 4. For these cases the droplet diameter is $d_p = 0.7$ mm and the ratio of the densities is $\rho_d/\rho_g = 2 \cdot 10^5$. The ODT parameter β_p for the dispersed phase is 0.5. The energy spectra shows that ODT is capable to predict the same trend as the DNS data for increasing mass loading. The dispersed phase attenuates the larger turbulent scales in the inertial subrange and augments the smallest ones in the dissipative regime which agrees with the DNS data. This is unique for Stokes number below unity. Due to these preliminary but promising results ODT seems to be capable to provide quantitative data to evaluate turbulence modulation.

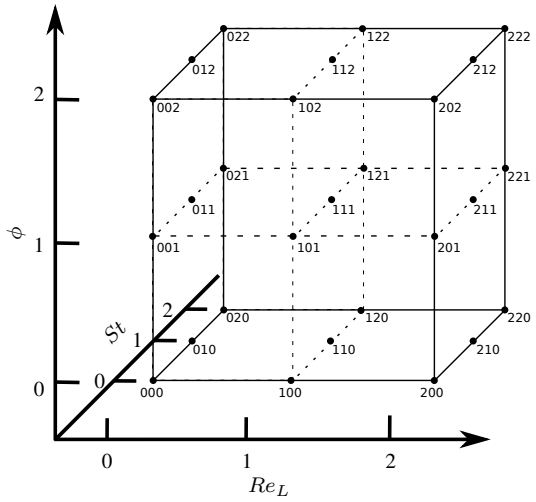

Figure 5: Treatment combinations in a 3^3 design using the three factors unladen flow Reynolds number Re_L, droplet mass loading ϕ and droplet Stokes number St. The low, intermediate and high state are represented as 0, 1, 2, respectively. (Adopted from Montgomery [11])

Empirical SGS model using Design of Experiments

Due to the simplification of the flow phenomena at the sub-grid level by assuming homogeneous shear turbulence the turbulence modulation model provides only an update for the turbulence intensity values saved in the LES cell (or at the cell edge). Fulfilling the requirements for a cost-effective SGS model it is necessary to be accessible on the flight and not producing a significant overhead in computational costs. One way to ensure these properties is to derive a function for turbulence intensity depending on predefined parameters which can be computed based on the variables saved in each LES cell. As mentioned before previous studies regard the following parameters as most significant regarding turbulence modulation by droplets: unladen flow Reynolds number Re_L, droplet mass loading ϕ and droplet Stokes number St. The resulting function for turbulence intensity can be seen as a regression model with empirical coefficients. To determine the order of the turbulence modulation function (TMF) for the SGS model we use an approach which is commonly used by chemical engineers. The broad field is called Design of Experiments (DoE) and the tool we are using is Factorial design (FD) (Montgomery [11]). FD describes the design of experimental realizations with multiple factors (parameters) to see their effect on a process variable. For our specific case we will use a 3^3 design, which means we investigate three (base) factors on three (exponent) different levels for each factor. The levels are defined by a low, intermediate and high state represented as 0, 1, 2, respectively. Each treatment combination will be denoted by three digits, where the first digit indicates the level of factor Re_L, the second digit indicates the level of factor St and the third digit indicates the level of factor ϕ. All treatment combinations are illustrated in Figure 5. The results achieved by ODT for the various combinations facilitate fitting a regression model of second order, which is given as

$$u_i' = \beta_0 + \sum_i \beta_i x_i + \sum_i \sum_{j>i} \beta_{ij} x_i x_j + \sum_j \beta_{jj} x_j^2 + f, \tag{16}$$

where x_i is the i^{th} parameter (either Re_L, St or ϕ) and f summarizes additional higher order terms. These terms are assumed to be very small and can be neglected. This regression model depending on the computed parameters of each LES cell provides a new turbulence intensity value for each component.

Summary and conclusions

We presented a new approach of using ODT to develop a SGS model for turbulence modulation by droplets. For this purpose, we consider the flow inside a LES cell as particle-laden homogeneous shear turbulence. This flow phenomena is analyzed by using ODT to provide quantitative data of the turbulence modulation for a regression model which will be the core of the one-equation SGS model. Therefore, an established experimental design strategy is used which is called Factorial design. The preliminary results show the capability of ODT to capture these flows. The next step is to implement this model into a LES framework and to investigate further requirements and updates for spray applications. Additional studies on general turbulence modulation of particle-laden flows will help to understand the mechanisms of this phenomena better.

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