PARTICLE COLLISION STATISTICS IN TURBULENT FLOWS WITH KINEMATIC SIMULATION

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<u>Abstract</u> Colliding droplets or particles in turbulent flows are important in applications ranging from rain formation in clouds to aerosol production in process engineering. To reduce the computational costs when simulating such flows, kinematic simulation (KS) is frequently applied [1, 2] as a cheap surrogate for direct numerical simulation (DNS) of the turbulent flow field. In this work [5], we provide for the first time a systematic validation of the particle collision statistics that result from KS. We show that while the particle collision frequencies for particles with different Stokes numbers are in good agreement with DNS reference data, a more detailed inspection of the flow field and particle concentration characteristics reveals significant differences between KS and DNS.

INTRODUCTION

The computational cost of turbulent flow DNS scales with the Reynolds number to the power of three [6] and therefore especially for high-Reynolds-number DNS becomes prohibitive. In the context of particle or droplet laden turbulent flows, stochastic Lagrangian models are applicable to determine the fluid velocity seen by the dispersed particle or droplet phase [4]. Alternatively, KS is applicable, which provides unlike the previous option information about velocity gradients or shear rates in addition to the seen velocity [3]. Shear rates are particularly important when studying for example aggregation and breakage of particle clusters [7], which was simulated by means of KS by Dominguez et al. [1]. Moreover, KS was applied to investigate the collision rates of heavy settling particles [2]. Despite these studies, a rigorous validation of KS against detailed DNS is still outstanding and provided in the present contribution.

FORMULATION

In a KS, the flow field does not emerge from the Navier–Stokes equation, but is calculated from the algebraic expression

$$\mathbf{u}(\mathbf{x},t) = \sum_{n=1}^{N_k} \left[\mathbf{A}_n \cos(\mathbf{k}_n \cdot \mathbf{x} + \omega_n t) + \mathbf{B}_n \sin(\mathbf{k}_n \cdot \mathbf{x} + \omega_n t) \right],\tag{1}$$

where N_k is a model parameter, which determines the number of Fourier modes with wavenumber vector \mathbf{k}_n and frequency ω_n [2]. The coefficients \mathbf{A}_n and \mathbf{B}_n are chosen such that $\mathbf{u}(\mathbf{x}, t)$ satisfies the continuity equation and the frequencies ω_n are determined based on the velocity energy spectrum E(k) as

$$\omega_n = \lambda \sqrt{k_n^3 E(k_n)}.$$
(2)

In this expression, λ is the persistence parameter. To perform realistic KS of isotropic turbulence, a Reynolds-numberdependent model spectrum as outlined in [6] is applied.

For the dispersed phase, we apply in agreement with our reference DNS study [8] the point-particle approximation or more precisely the following equations of motion

$$\frac{\mathrm{d}\mathbf{x}^n}{\mathrm{d}t} = \mathbf{v}^n \quad \text{and} \quad m_p \frac{\mathrm{d}\mathbf{v}^n}{\mathrm{d}t} = -\frac{m_p}{\tau_p} [\mathbf{v}^n - \mathbf{u}(\mathbf{x}^n, t)] + \sum_{m \neq n} \mathbf{F}^{mn}, \tag{3}$$

for the position \mathbf{x}^n and the velocity \mathbf{v}^n of the particle with index n. In equation (3), m_p is the particle mass, τ_p the particle relaxation time-scale, and \mathbf{F}^{mn} is the force exerted by particle m on particle n during a perfectly elastic collision.

RESULTS

By solving equations (1) to (3) for an ensemble of 64^3 particles with different Stokes numbers St $\equiv \tau_p/\tau_\eta$ in a turbulent flow field with Kolmogorov time-scale τ_η and Taylor-scale Reynolds number equal to 54.2, particle collision frequencies N_c can be computed and compared with the reference data from the detailed and highly-cited DNS study [8] as depicted in Figure 1. In addition to the collision frequencies recorded for given Stokes numbers (circles), the frequencies



Figure 1. Comparisons of the collision frequencies N_c as a function of the particle Stokes number St. Depicted are results from the KS (filled, red symbols) and the DNS of [8] (hollow, black symbols). The collision frequencies recorded in the KS and DNS runs are provided by circles, whereas the limiting values resulting from the kinetic theory, i.e., equation (4) with $\langle v^2 \rangle$ -values from the KS and DNS runs, are plotted with squares. Also, the value of the Saffman–Turner limit (4) is provided as a horizontal red line.

resulting from the Saffman–Turner limit for light particles with $St \rightarrow 0$ and the kinetic theory limit for heavy particles with $St \rightarrow \infty$, i.e.,

$$N_{c} = \frac{1}{2}n^{2}d^{3}\left(\frac{8\pi}{15}\frac{\varepsilon}{\nu}\right)^{1/2} \text{ and } N_{c} = \frac{1}{2}n^{2}d^{2}\left(\frac{16\pi\langle v^{2}\rangle}{3}\right)^{1/2},\tag{4}$$

respectively, are depicted as well (solid red line and squares, respectively). In equation (4), n is the particle number density, d the particle diameter, ε the dissipation rate, and ν the kinematic viscosity. The kinetic theory provides essentially a validation of the particle velocity variance $\langle v^2 \rangle$ resulting from the KS.

Especially for St \geq 2, the KS predictions are in good agreement with the DNS results. However, a closer inspection of the collision frequency

$$N_c = \frac{1}{2}\pi n^2 d^2 g(d) \underbrace{\int_{-\infty}^0 (-v_r) P(v_r|d) \,\mathrm{d}v_r}_{\equiv \langle v_r|d \rangle},\tag{5}$$

which is essentially resulting from the product of the radial distribution function g(d) evaluated at a radius equal to d and the mean relative velocity $\langle v_r | d \rangle$ at particle separations equal to d, reveals crucial differences in the flow field structures resulting from KS and DNS. These difference in g(d) and $\langle v_r | d \rangle$ cancel out when evaluating N_c as given by equation (5).

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