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Interphase coupling in polydisperse evaporating sprays using the generalised Fully Lagrangian Approach

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Abstract

A novel methodology is presented for the modelling of polydisperse evaporating droplet flows by combining the generalised Fully Lagrangian Approach (gFLA) with the statistical learning technique of kernel regression. This procedure is shown to retain the detail of the structures inherent in the droplet concentration field for such systems, whilst offering a reduction in computational cost due to the lower droplet seeding required by the gFLA in comparison to conventional methods. The developed approach is further applied to the scenario of tracking the droplet vapour field arising due to droplet evaporation, with the interphase coupling source terms being constructed using the droplet probability density provided by the gFLA.

Introduction

The behaviour of evaporating spray systems is fundamental to many industrial and environmental processes including internal combustion engines, aerosol dispersion of pathogenic droplets, and droplet condensation within atmospheric clouds. The modelling of such processes naturally has to account for details such as treatment of polydisperse droplets, evaporation effects, and mass and momentum transfer between the droplets and background carrier flow. For the post-secondary atomisation region of a spray consisting of only discrete droplets, the modelling typically requires a large number of droplets to be present in simulations in order to achieve statistical convergence. This has the consequence of leading to long computational runtimes to obtain the required behavioural information about systems, presenting a barrier to more widespread use of these simulations.

Modelling Framework

The generalised Fully Lagrangian Approach (gFLA) offers an alternative means of describing polydisperse droplet behaviour in simulations by representing the dispersed phase as a continuum. This has the advantage of being able to provide the local droplet probability density p along individual trajectories using the Lagrangian form of conservation of mass for droplets with position $\boldsymbol{x}_d$ and radius r_d (Osiptsov 2000)

$$p(\boldsymbol{x}_d, r_d, t) = \frac{p(\boldsymbol{x}_0, r_0, t_0)}{|\det(\boldsymbol{J}(\boldsymbol{x}_0, r_0, t))|} \tag{1}$$

in which $\boldsymbol{J}$ is the Jacobian tensor that represents the Eulerian-Lagrangian transformation along trajectories with respect to the initial conditions $\boldsymbol{x}_0$ and r_0. The evolution of $\boldsymbol{J}$ is determined according to the equations governing the motion and evaporation of individual droplets. In this work a linear drag law is used, along with an idealised evaporation model in which all heat that reaches the droplet surface is assumed to be spent on its evaporation (Li 2021).

As the gFLA directly provides the instantaneous value of p along trajectories by Eq. (1), it offers the benefit of requiring relatively few droplets to reproduce the droplet concentration field in comparison to box-counting methods (Healy & Young 2005), whilst remaining applicable for all values of particle inertia and mass loading. The novelty of the present research comes from using kernel regression to reconstruct the probability density field by accumulating the contributions from individual droplet trajectories using the Nadaraya-Watson estimator (Hastie, Tibshirani & Friedman 2009)

$$p(\boldsymbol{x}, r, t) = \frac{\sum_{i=1}^{N} K_{\boldsymbol{H}}(\boldsymbol{x}, r, \boldsymbol{x}_d^i, r_d^i) p(\boldsymbol{x}_d^i, r_d^i, t)}{\sum_{j=1}^{N} K_{\boldsymbol{H}}(\boldsymbol{x}, r, \boldsymbol{x}_d^j, r_d^j)} \tag{2}$$

where N is the number of droplets that contribute at $(\boldsymbol{x}, r)$, and $K_{\boldsymbol{H}}$ is the kernel with bandwidth matrix $\boldsymbol{H}$. The advantage offered by this approach is the ability to adaptively scale the kernel directly in accordance with the droplet probability density field by specifying $\boldsymbol{H}$ in terms of $\boldsymbol{J}$. This enables the kernel size and shape to vary with the Eulerian-Lagrangian transformation, thereby making it possible to distinguish the structures in the droplet concentration field and retain a high level of detail at a reduced computational cost.

Application to Interphase Coupling

For evaporating droplets, it is desirable in many applications to track the evolution of the droplet vapour field c, and this is achieved by treating c as a passive scalar governed by

$$\frac{\partial c}{\partial t} + \nabla \cdot (D \nabla c) + \nabla \cdot (\boldsymbol{u} c) = S_{\text{Mass}} \tag{3}$$

where D is the mass diffusivity of droplets, $\boldsymbol{u}$ is the carrier flow velocity, and S_{Mass} is a source term accounting for the transfer of mass as droplets evaporate to vapour. It is possible to write S_{Mass} in terms of the probability density p in the form

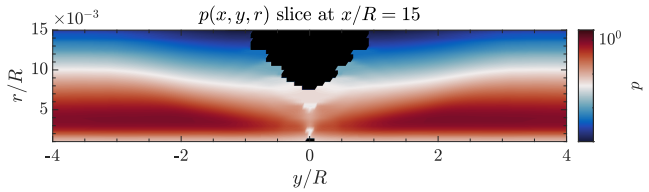
$$S_{\text{Mass}} = -\int_r p(\boldsymbol{x}, r, t)\dot{m}(r)\, dr \tag{4}$$

where $\dot{m}(r)$ is the droplet evaporation rate. This provides a procedure for utilising the reduced particle seeding associated with the gFLA to reproduce S_{Mass} with an improved computational efficiency, whilst still accounting for the polydispersity of droplets and retaining physical accuracy.

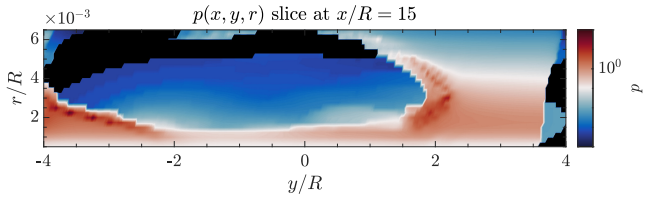
Results and Discussion

The developed modelling framework has been implemented within OpenFOAM, and is applied to the prototypical configuration of two-dimensional incompressible gas-droplet flow past a cylinder of radius R for both steady-state ($Re = 20$) and transient ($Re = 100$) cases.

Reconstruction of the droplet probability density field $p(x, y, r)$ using the kernel regression estimator in Eq. (2) provides the complete droplet size distribution, as depicted in Fig. 1 for slices of $p(x, y, r)$ at $x/R = 15$. For the steady-state case, Fig. 1a shows a symmetrical droplet distribution about $y/R = 0$, whilst the transient case in Fig. 1b exhibits asymmetry in both position and droplet size that is characteristic of the vortex street that develops behind the cylinder.



(a) $Re = 20$

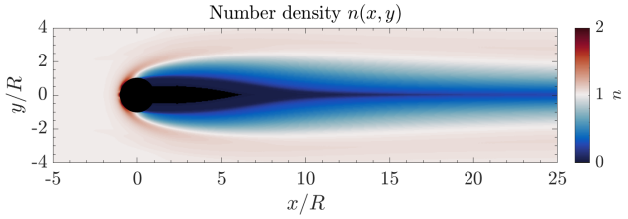


(b) $Re = 100$ at time $t = 30$

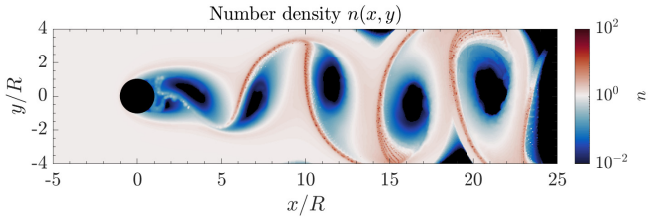
Figure 1: Slices of the probability density field $p(x, y, r)$ obtained using kernel regression for polydisperse droplet flow around a cylinder at $x/R = 15$

Calculation of the number density field $n(\boldsymbol{x}, t)$ by integrating out the size dependence in $p(\boldsymbol{x}, r, t)$ produces the droplet concentration distributions illustrated in Fig. 2. The kernel regression is seen to capture well both the areas with no or few droplets (the cylinder wake in Fig. 2a and centre of vortices in Fig. 2b), and also the areas of higher droplet number density (in front of the cylinder in Fig. 2a and along curves in between the vortices in Fig. 2b).

From Fig. 2 it is seen that the gFLA used in conjunction with kernel regression provides a reliable means of reproducing the droplet number density field. This approach has



(a) $Re = 20$



(b) $Re = 100$ at time $t = 30$

Figure 2: Reconstruction of the number density field $n(x, y)$ for polydisperse droplet flow around a cylinder

also been shown to require $\mathcal{O}(10^3)$ times fewer trajectories than a conventional box-counting Cloud-In-Cell method to statistically converge in the steady-state case, representing a considerable saving in the computational cost required to obtain n. Construction of the mass source term S_{Mass} from the droplet probability density field further demonstrates the efficacy of this methodology for tracking the droplet vapour which is accumulated as a result of droplet evaporation.

Conclusion

This work presents a novel procedure for modelling polydisperse evaporating droplet flows using the gFLA and kernel regression. The approach is seen to retain a physically accurate description of droplet behaviour across the range of droplet sizes, whilst providing an improvement in computational efficiency owing to the gFLA requiring fewer droplets to achieve statistical convergence. The procedure is applied to studying the evolution of the droplet vapour field by constructing the interphase coupling source terms from the droplet probability density provided by the gFLA.

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