Reduced Order Drag Modeling of Liquid Drops

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Abstract
In this paper, a reduced order model (ROM) for a freely translating sphere is developed. The goal of the model is to provide improved drag predictions for Lagrangian-Eulerian simulations of sprays or particle-laden flows. In our previous work, we developed ROMs for oscillatory flow over a fixed sphere. In this work, the sphere accelerates according to Newton’s law. The model is created from a direct numerical simulation (DNS) where a sphere with zero initial velocity is released in a free-stream flow. A Proper Orthogonal Decomposition of the simulation data is performed and then a streamwise-upwind-Petrov-Galerkin (SUPG) projection of the incompressible Navier-Stokes equations onto the space spanned by the POD modes is used to create the model. Results for two different solid/fluid density ratios are tested, 1000 and 30. Even when using as few as 5 degrees of freedom in the model, the ROM produces accurate results for this problem with the velocity error being less than 0.1%. It is also shown that time-history effects are not significant even when the particle-fluid density ratio is relatively low.

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Introduction

The study of drops and particles is of importance to many natural and industrial processes such as raindrops and hailstones, atmospheric particle transport, particle transport by rivers and streams, sprays, and aerosols. To simulate these problems, one often uses simplified drag models to predict the coupling between the carrier phase and the discrete particle phase. Simplified models have been developed through analytic, experimental, and numerical studies of individual drops and particles. One such model is the Basset-Boussinesq-Oseen (BBO) equation [1, 3] (BBO equation). The BBO equation includes many terms that govern the motion of the particle. These include: forces due to pressure gradients, an “apparent mass” term, a drag force, a lift force, a Basset time history term, and gravitational effects. This model was derived analytically for low Reynolds numbers. At higher Reynolds numbers, the problem is non-linear and it is more difficult to obtain analytic solutions, thus there is no analytic model for the physical effects included in the BBO equation. There are empirical laws available for predicting the steady drag of a sphere [4], but it is more difficult to accurately model more complex effects.

In our previous work [7], we used “reduced order modeling” techniques [5–10] to develop models for steady flow over a spherical particle at various Reynolds numbers. Specifically, we applied the Proper Orthogonal Decomposition (POD) [8] to detailed numerical simulation data to generate a basis of spatial functions (called “POD modes” or “empirical eigenfunctions”) that could compactly represent steady solutions for flow over a sphere at various Reynolds numbers. These modes were then combined with a weighted integral form of the Navier-Stokes equations to generate a predictive model for the flow. Using only 10 POD modes, we demonstrated that the variation of drag as a function of Reynolds can be predicted with less than 1% error.

We then extended the model to oscillatory flows over fixed particles [11]. It that work, we created a reduced-order model (ROM) that could predict unsteady oscillatory flow over a sphere. The oscillatory flow was parametrized by a mean component and an oscillation amplitude and frequency. It was shown that a model having 40 degrees of freedom could accurately predict the drag response for a Reynolds number range spanning $10^{-1}$ to 200 and a Strouhal number range of 0.1 to 10.

In this work, we develop a model specialized for predicting the drag in Lagrangian-Eulerian particle laden flow or spray simulations. The main difference between this and our previous work is that we allow the particle to be accelerated by flow forces. To develop the model, direct numerical simulations (DNS) of particles accelerating from zero velocity up to free-stream velocity are performed. The ROM is then generated using POD modes generated from the DNS and a streamwise-upwind Petrov-Galerkin (SUPG) projection of the Navier-Stokes equations. The goal is to develop as a compact a model as possible so that it can be used in Lagrangian-Eulerian simulations having millions of particles.

Problem Formulation

In this section, we describe the physical problem to which we apply reduced-order modeling techniques. The problem is that of an unsteady, axisymmetric fluid flow over a spherical particle. The fluid is assumed incompressible with constant density, $\rho_g$, and viscosity, $\mu$. The equations governing the motion of the fluid are the continuity equation and the Navier-Stokes equations. The free-stream velocity is held fixed at the value $v_0$. The particle initially has zero velocity and is allowed to accelerate based on Newton’s law according to

$$m \frac{d^2z}{dt^2} = F$$

where $m$ is the mass of the particle and $F$ is the fluid force in the direction of the flow (the $z$ direction).

The non dimensional parameters of the problem are the Reynolds number, $Re = \rho_g v_0 d / \mu$, and the mass ratio, $\rho_g \pi d^3 / (6m) = \rho_s / \rho_s$ where subscripts of $s$ indicate the sphere and $g$ indicate the surrounding gas. $v_0$ is the initial slip velocity of the particle. For most spray simulations, the maximum particle Reynolds numbers are on the order of $10^2$ [12]. The mass ratio depends on the fluids involved, but for typical gas liquid system it is on the order of $10^3$ at atmospheric pressures to as low as $O(10^3)$ for higher-pressure applications. Here we try to make a model specialized for a single mass ratio as in typical applications the particle-gas density ratio does not change. Two density ratios are examined, a value of 30, and a value of 1000. As the particle accelerates to the free-stream velocity, the Reynolds number based on the slip velocity is continuously decreasing and there is no reason to study a range of Reynolds numbers. The initial Reynolds number for all the calculations will be 100. The flow initial
conditions are generated by solving the steady-state Navier-Stokes equations for flow over a sphere at \( Re = 100 \). This state is then used as the initial condition for an unsteady simulation where the particle is allowed to accelerate to free-stream velocity.

The numerical formulation of the above problem follows the work presented in [13]. We write the governing equations in terms of curvilinear coordinates

\[
    r = r(\xi, \eta), \ z = z(\xi, \eta) \tag{1}
\]

where \( r \) and \( z \) corresponds to our two-dimensional Cartesian coordinate system (since we are dealing with axisymmetric flow they are the radial and axial directions respectively) and \( \xi, \eta \) are independent curvilinear coordinates. Using this notation the incompressible Navier-Stokes equations in curvilinear coordinates can be expressed as

\[
    \text{diag}[0, 1, 1] \frac{\partial \vec{w}}{\partial t} + \frac{\partial \vec{e}}{\partial \xi} + \frac{\partial \vec{f}}{\partial \eta} - \vec{\theta} = 0 \tag{2}
\]

where \( \vec{w} \) is the vector of unknowns given by \((p, pu, pv)\) where \( p \) is the pressure and \( u \) and \( v \) are the radial and axial velocity components. \( \vec{e} \) and \( \vec{f} \) are the total flux vectors of mass and momentum in the \( \xi \) and \( \eta \) directions and \( \vec{\theta} \) is a source term required because the flow is axisymmetric.

An \( hp \)-finite element method is used to perform the detailed numerical simulations [13]. The discrete form of Eq. 2 is written using a streamwise-upwind-Petrov-Galerkin (SUPG) variational approach [14]. This allows us to seek solutions for the velocity and the pressure in the same polynomial space [15, 16] without pressure decoupling problems. The form of the equations is as follows

\[
    0 = \sum_{e=1}^{n_e} \left\{ \int_{\Omega} \nabla T \left[ \text{diag}[0, 1, 1] \frac{\partial \vec{w}}{\partial t} - \vec{\theta} \right] \quad \right.
\]

\[
    - \frac{\partial \phi^T}{\partial \xi} \vec{e} - \frac{\partial \phi^T}{\partial \eta} \vec{f} \right\} d\Omega + \int_{\Gamma} \phi^T \left( \vec{c} \cdot \vec{n} \right) d\Gamma
\]

\[
    + \int_{\Omega} \left[ \frac{\partial \phi^T}{\partial \xi} A_\xi + \frac{\partial \phi^T}{\partial \eta} A_\eta \right] T \left[ \left( \text{diag}[0, 1, 1] \frac{\partial \vec{w}}{\partial t} - \vec{\theta} \right) + \frac{\partial \vec{e}}{\partial \xi} + \frac{\partial \vec{f}}{\partial \eta} \right] d\Omega \right\}
\]

\[
    \forall \phi
\]

where the sum is performed over all of the elements in the mesh, 1 to \( n_e \). The solution for \((p, u, v)\) is sought in the space \([\Phi]^3\) where \( \Phi \) is a globally continuous finite element space. Each integral in the sum is performed over either the standard triangle area \( \Omega \) or the standard triangle perimeter \( \Gamma \). The matrices \( A_\xi, A_\eta \) and \( T \) are associated with the SUPG stabilization. For more information on these matrices see [13]. If the term involving \( T \) is removed, we recover the standard Galerkin formulation.

For the calculations presented in this study we use a basis composed of quartic polynomials on each element \( (P = 4) \). Quartic polynomials are used because they allow rapid convergence to the exact drag value with increasing mesh resolution (5th order spatial accuracy). An unstructured triangular mesh on a rectangular domain is used in all the calculations. Figure 1 shows the element mesh used to calculate the detailed solutions for the POD study of flow over a sphere. For the calculations, an inflow condition is enforced at the lower boundary of the mesh with \((u, v) = (0, v_0)\) such that the flow is from bottom to top. At the downstream and right boundary, the total stress is set to zero. Along the centerline, a symmetry boundary condition is imposed, and on the sphere, which initially is centered at \((0,0)\), a no slip boundary condition is imposed. The downstream boundary is from \((0, 30)\) to \((20, 30)\), and the inflow boundary is from \((0, -20)\) to \((20, -20)\) where the units are sphere diameters. It is shown in [17] that we are able to obtain values of drag with at least 1% accuracy using this configuration.

![Figure 1. Typical element mesh and magnified region around the sphere](image)

The entire problem is discretized implicitly in time using a 3rd order accurate diagonally implicit Runge Kutta scheme [17]. At each time step the particle motion equations for the velocity and position are solved simultaneously with the Navier-Stokes equations. The entire mesh is moved rigidly with the particle so that there is no change in struc-
ture of the mesh as the sphere moves.

**POD Based Modeling**

The POD was introduced by Lumley [8] as a means to extract the large scale structure of turbulent flows. It uses data obtained in experiments or numerical simulations to generate an orthogonal set of spatial basis functions that optimally describe the flow’s energy. The POD finds functions (herein called POD modes) that maximize the mean square inner product of the flow solutions with the POD mode, \( \vec{\varphi} \).

\[
\frac{\langle (\int_{\Omega} \vec{u} \cdot \vec{\varphi} d\Omega)^2 \rangle}{\int_{\Omega} \vec{\varphi} : \vec{\varphi} d\Omega}
\]

where \( \vec{u} \) is the spatial flow field \((u, v)\), \( \Omega \) is the physical domain, and the angled brackets \( \langle \rangle \) indicate an averaging process. The average is taken over all of the unsteady solutions obtained. The POD mode is optimal because it will represent all of these solution as well as possible in the mean square sense.

Solutions to the above maximization are obtained by solving the Fredholm equation

\[
\int_{\bar{x}'} R(\bar{x}, \bar{x}') \vec{\varphi}(\bar{x}') d\bar{x}' = \lambda \vec{\varphi}(\bar{x}),
\]

where \( R(\bar{x}, \bar{x}') \) is an autocorrelation tensor

\[
R(\bar{x}, \bar{x}') = \langle \vec{u}(\bar{x}, t) \vec{u}(\bar{x}', t) \rangle^T.
\]

Because the autocorrelation function is symmetric, this problem generates an orthogonal series of POD modes similar to an algebraic eigenvalue problem. The first POD mode satisfies the maximum property given above. The next POD mode is orthogonal to the first, and satisfies a similar maximum property except that it maximizes against the remainder of the flow field that can not be captured using the first mode. The higher modes are similar. In this way, a hierarchy of functions is generated that can represent the transient or parametric flow variations with as few degrees of freedom as possible. The eigenvalues, \( \lambda \), of the Fredholm equation represent the mean energy captured by each mode, \( \vec{\varphi} \).

When applied to data obtained from numerical simulations or experiments, the discrete form of Eq. [5] becomes an \( N \) dimensional eigenvalue problem where \( N \) is the number of data points. Often numerical and experimental data sets are highly resolved \((N \gg 1)\), which makes it difficult to solve this problem. A more efficient method proposed by Sirovich [18] allows us to reduce the size of the eigenvalue problem. The main idea of Sirovich’s method is to write the POD modes as a linear combination of “snapshots” of the instantaneous flow field

\[
\vec{\varphi} = \sum_{k=1}^{M} \psi_k \vec{u}_k,
\]

where the sum is performed over the number of snapshots, \( M \), used in the discrete time average for Eq. [9].

By substituting this equation into Eq. [5] we arrive at the following analogous eigenvalue problem

\[
C \vec{\psi} = \lambda \vec{\psi},
\]

whose discrete matrix entries are given as

\[
C_{kl} = \frac{1}{M} \int_{\bar{x}} \vec{u}(\bar{x}, t_k) \cdot \vec{u}(\bar{x}, t_l) d\bar{x},
\]

This method involves solving an eigenvalue problem that has dimension \( M \). The snapshot method is thus more efficient whenever the number of snapshots, \( M \), is smaller than the number of grid points, \( N \).

**Implementation of POD**

In this section we give an overview of the numerical procedure used to determine the POD modes. We always use the snapshot method because we typically have fewer snapshots than grid points in the computational mesh. A component \((u, v)\) of the \( hp \)-finite element flow solution, \( \vec{u} \), in equation [8] can be represented as follows

\[
u_i(\bar{x}, t_t) = \sum_{j=1}^{N} c_{i,t,j} \gamma_j(\bar{x}),
\]

where \( c_{i,t,j} \) is the solution coefficient for flow component \( i \), at time step \( t_t \), for \( hp \)-finite element basis function, \( \gamma_j(\bar{x}) \). If we substitute this expansion into Eq. [9] and integrate over the domain we arrive at the following integration formulation

\[
C_{kl} = \frac{1}{M} \int_{\bar{x}} \sum_{i=1}^{2} \sum_{j=1}^{N} c_{i,k,j} \gamma_j(\bar{x}) \sum_{j=1}^{N} c_{i,t,j} \gamma_j(\bar{x}) d\bar{x},
\]

which can be numerically integrated using Gauss integration. Details of the discrete integration formulation can be found in [19]. The eigenvalue problem given by eq. [9] is solved using Lapack’s DSPEV routine modified using the method discussed in [11].

A final permutation of the POD formulation is to change the definition of the inner product as proposed in [7]. The standard inner product of \( \vec{u} \cdot \vec{\varphi} \) is to include only velocity components in the dot product so that \( \vec{u} \cdot \vec{u} = u^2 + v^2 \). In our POD formulation we include the pressure in the POD decomposition so \( \vec{u} \) is defined as \((u, v, p)\) where \( p \) is the pressure.
The problem with this definition is that the inner product is not dimensionally consistent having the addition of velocity squared with pressure squared. In [7], a low Mach number expansion was performed with \( \vec{u} \) defined as \( (u, v, \sqrt{p/\rho}) \). This resulted in a definition of the inner product that only included the velocity components such that \( (u, v, p) \cdot (u, v, p) \) is defined as \( u^2 + \sqrt{v^2} \).

Once the eigenvalues and eigenvectors of eq. 8 are found we generate a set of POD modes for the velocity and the pressure as

\[
\varphi = \sum_{k=1}^{M} \psi_k \begin{bmatrix} p_k \\ u_k \\ v_k \end{bmatrix}, \tag{12}
\]

where \( k \) is the index of the snapshot. These modes are then normalized such that \( \int \varphi^m \cdot \varphi^n d\vec{x} = \delta_{nm} \).

The exact flow field for \( (u, v, p) \) can now be reconstructed as follows

\[
\begin{bmatrix} p(\vec{x}, t_k) \\ u(\vec{x}, t_k) \\ v(\vec{x}, t_k) \end{bmatrix} = \sum_{n=1}^{M} a_n (t_k) \begin{bmatrix} \varphi^m_p(\vec{x}) \\ \varphi^m_u(\vec{x}) \\ \varphi^m_v(\vec{x}) \end{bmatrix}, \tag{13}
\]

where \( a_n \) is some expansion coefficient associated with each mode. If we want to further reduce the dimensionality of the approximation, we can use only \( S \) of our POD modes instead of the full sum up to \( M \) where \( S < M \).

**Low-dimensional Model**

To obtain a low-dimensional model of the flow we perform a streamwise-upwind-Petrov-Galerkin projection of the incompressible Navier-Stokes equations onto the space spanned by the POD modes. We use this approach because it yields better results than the standard Galerkin projection. In certain cases, the standard Galerkin projection suffers from decoupling problems.

The solution for \( (u, v, p) \) is sought in the space spanned by a subset of our POD modes, \( \varphi \). By inserting the expansion given in Eq. 13 into the total flux vectors of the SUPG formulation of the Navier-Stokes equation (Eq. 3) and also using the POD modes as the test functions, we obtain \( S \) scalar equations for the expansion coefficients \( a_n \). If we define \( R(a_n) \) as the residual error of the Navier-Stokes equations evaluated using the current estimate of the solution, our system becomes

\[
R(a_n) = 0, \tag{14}
\]

which is solved using a Newton-Raphson iterative technique. After we find these coefficients, we are able to reconstruct the flow field (Eq. 13) and calculate the drag.

**Results**

Two DNS simulations were run, both with initial Reynolds number of 100, but one had a solid-gas density ratio of 1000 and the other with a solid-gas density ratio of 30. The simulations were performed with a time step of \( \Delta t = \rho_s/\rho_g/120 \) where all quantities from here on in are made non-dimensional by the particle diameter, the initial particle slip velocity, and the gas-phase density. This time step is larger for more dense solid particles as these will accelerate more slowly. For both cases, 600 time steps were calculated. This allowed the Reynolds number based on the slip velocity to decrease from 100 to 10 over the course of the simulation. Every 5\(^{th} \) time step was used as a snapshot for the POD, thus each case had 120 snapshots. Figure 2 shows the eigenvalue spectrums from the two cases. For each case the eigenvalues are calculated using two different methods, the standard method described above and a “deflation” method which is described in [11]. The location where the curves deviate shows where numerical round-off error has a significant effect on the calculated eigenvalues. In both cases, this occurs when the eigenvalues are on the order of \( 10^{-8} \). The eigenvalue spectrum shows a rapid decay in the energy contained by each mode, thus only a few modes should be necessary to reproduce the DNS solution.

![Figure 2](image.jpg)

**Figure 2.** POD mode eigenvalues. solid curve is for \( \rho_s/\rho_g = 1000 \) and dash-dot curve is for \( \rho_s/\rho_g = 30 \).

ROMs are created for both cases using the POD modes and the procedure described above. For each case, models were created with 5 and 10 modes. Figure 3 shows the position of the particle as a function of time for the case of \( \rho_s/\rho_g = 30 \) calculated by the DNS and the ROMs. There are actually four curves on the figure although only two are visible.
The solid curve is the DNS solution, the 5 mode ROM solution, and the 10 mode ROM solution. To the resolution of the figure, these curves are identical, thus showing that a low dimensional model can accurately predict the unsteady drag response of a sphere. The dashed curve on the figure is a correlation based prediction of the particle location where the drag correlation used was from [4] and is given by

$$C_D = \frac{24}{Re} \left( 1 + 0.1935 Re^{0.6305} \right)$$

There are two possible reasons for difference between the correlation based prediction and the model predictions. The first is that there is error in the quasi-steady drag correlation. The second is that the time-history effects which are included in the DNS and ROM's are significant. This will be investigated subsequently.

**Figure 3.** Vertical position of the particle as a function of time for the case $\rho_s/\rho_g = 30$. The solid curve is the DNS solution and the 5 and 10 mode ROM solutions. The dashed curve is the prediction based on a drag correlation.

Figure 4 shows the particle velocity as a function of time. Again we see that the DNS and ROM results are indistinguishable. To better see the errors in the ROMs, Figure 5 shows the difference between the DNS and ROM velocity predictions as a function of time for the 5 and 10 mode ROMs. This figure shows that even with only a 5 mode model, the maximum error in velocity is less than 0.2%. For the 10 mode model the maximum error is 0.04%. Similar results held for the case of $\rho_s/\rho_g = 1000$. For the 5 and 10 mode model, the maximum error was 0.02% and 0.005%. Thus for the larger density ratio case, the results were more accurate. This is in agreement with the eigenvalue spectrum behavior in that the higher density ratio case had a more rapidly decaying energy spectrum. Thus, in both cases, the ROM procedure can accurately reproduce the DNS with few degrees of freedom.

**Figure 4.** Vertical velocity of the particle as a function of time for the case $\rho_s/\rho_g = 30$. The solid curve is the DNS solution and the 5 and 10 mode ROM solutions. The dashed curve is the prediction based on a drag correlation.

**Figure 5.** Difference between the DNS and ROM predictions of vertical velocity of the particle as a function of time for the case $\rho_s/\rho_g = 30$. The two curves are for the 5 and 10 mode ROMs.

To determine the reasons for the difference between the correlation-based predictions and the DNS predictions, we compare the two density ratio cases. If time history effects are the main source of error between the correlation and DNS predictions, then the differences should be smaller for the higher density ratio. Figure 6 shows the velocity predictions of the DNS (as well as the ROMs) and the correlation-based predictions. The differences between the DNS results and the correlation-based results are approximately the same order of magnitude as that shown in Figure 4 which indicates that the main source of error is not time-history effects but rather inaccuracies in the drag correlation. Thus, although the
ROM does include time-history effects, they are not significant for these problems. It is still not clear whether time-history effects are important in turbulent particle-laden flow calculations, however, because the turbulent fluctuations occur on time scales over which time history effects may be important. Our future work will evaluate the magnitude of time-history effects for particles in a turbulent flow.

Figure 6. Vertical velocity of the particle as a function of time for the case $\rho_s/\rho_g = 1000$. The solid curve is the DNS solution and the 5 and 10 mode ROM solutions. The dashed curve is the prediction based on a drag correlation.

Conclusions
We have applied a new modeling technique based on the Proper Orthogonal Decomposition (POD) to predict the evolution of a freely translating sphere. This approach allows one to systematically create compact models from detailed solutions. These models can then represent physical phenomena such as unsteady effects that are difficult to model using empirical approaches. Because the models are low-dimensional they can be used in more complex simulations such as spray or particle-laden flow simulations.

For the problem investigated here, a single particle injected into a uniform stream, time-history effects do not play a strong role. This is mainly because the mass of the particle is large relative to the mass of the displaced fluid. Our future work, will examine whether this remains true when the particle is injected into a turbulent flow. In spite of the fact that time-history affects are not significant, the ROM developed showed that quasi-steady predictions of drag forces can be made that are significantly more accurate than correlation-based approaches with little increase in computational cost.

References