APPENDICES

APPENDIX A

A.1 Modeling of Blood Cell Trajectories in a Non-Uniform Transient Flow Field

For a bio-particle system, where the continuous to dispersed phase density ratio is near unity, the pressure and drag terms are the most influential in a point-force model (Buchanan, 2000) neglecting near-wall and inter-particle effects. To investigate the interaction of these and other terms in the point-force particle trajectory model, the annular expansion geometry of Karino and Goldsmith (1977) was selected.

A.1.1 System Description

A sketch of the system is provided as Fig A.1. The sinusoidal pulse shown has a frequency of 540 degrees/sec (1.5 Hz) and a period of $T = 0.666\overline{6}$ s. The release time of Karino and Goldsmith (1977), ω = -71.4°, translates to $t = .53\overline{4}s$ and $t/T = 0.801\overline{6}$. Properties of the hardened red blood cell (rbc) are summarized in Table A.1.

Table A.1: Properties of the Hardened Red Blood Cell in the Karino and Goldsmith (1977) Experiment

	Response Time	Density Ratio	Virtual Mass Coefficient
Formula	$\tau_p \equiv \frac{2\rho_d a^2}{9\mu_c}$	$\alpha \equiv \frac{\rho_c}{\rho_d}$	$\beta = \frac{1}{1+\alpha/2.}$
Value	3.531×10^{-6}	0.885	0.693

The governing dimensional equation, assuming only pressure and drag effects, can be written

$$\frac{dv_i}{dt} = \alpha \frac{Du_i}{Dt} + \frac{1}{\tau_p}(u_i - v_i) \tag{A.1}$$

where v_i and u_i are the components of the particle and local fluid element velocity, respectively. If virtual mass effects are to be included, the above equation can be written

$$\frac{dv_i}{dt} = \frac{3}{2}\beta\alpha \frac{Du_i}{Dt} + \frac{\beta}{\tau_p}(u_i - v_i) \tag{A.2}$$

A.1.2 Particle Trajectories

The results of sequentially adding drag, pressure and virtual mass terms over separate runs are illustrated in Figure A.2. The pathline track is nearly identical to the hbc trajectory of Karino and Goldsmith (1977). The inclusion of only the drag term under identical release conditions reduces the number of particle loops by one and slightly modifies the location at which the particle ends its recirculating trajectory. Furthermore, the computational effort required has increased 40 times, as indicated in Fig. A.2 by the number of steps required by the quality control integration routine. Including both pressure and drag effects modifies the particle trajectory such that it again very nearly resembles that of the hbc. Interestingly, both pressure and drag terms have an influence on particle trajectory; however, their net effect is essentially represented by the motion of a pathline in this geometry. The extent to which these terms cancel one-another is of interest.

Buchanan (2000) found that the inclusion of the virtual mass term in the particle equation caused serious deviations in the particle trajectory. Buchanan (2000) then postulated that the virtual mass approximation is invalid for the case of blood particles where $\alpha \approx 1.0$. This conclusion is in contrast to the work of Hyun (1998) who included the virtual mass approximation. Considering Eqs. (A.1 & A.2) it seems likely that the virtual mass effect simply diminishes as the value of α approaches one. In fact, a minor discretization error correction in the trajectory code produced the expected result. That is, the virtual mass term does not significantly influence the particle trajectory. Figure A.2 illustrates that the inclusion of the virtual mass term has a relatively minor influence, i.e., the number of loops

and the particle exit location are unchanged. This result supports the observation that the virtual mass approximation is valid for cases such as this, where the density ratio is very near one. However, the virtual mass term does not significantly contribute to the particle trajectory and can be neglected. Exclusion of this term is also partially based on the grounds that it is an approximation derived for systems in which there is a large density discrepancy (Buchanan, 2000). Therefore, including this term does not necessarily improve the accuracy of the calculation.

A.2 Need for the Pressure Term in Bio-Particle Simulations

The preceding results indicate that when both pressure and drag terms are included in a point-force model of particle motion the computed trajectory matches the motion of a fluid element pathline as well as the experimental results of Karino and Goldsmith (1977) for consistent initial conditions. A possible explanation for this phenomenon is that the pressure term and the drag term cancel one-another. However, this is an unlikely scenario due to the fact that these terms arise from different mechanisms yet typically result in forces that act in the same direction. The mechanism responsible for the drag force arises from both shear and pressure effects that are induced on the fluid by the presence of the particle. The pressure term results entirely from pressure and shear gradients that would be present in the fluid if the particle was absent and can accordingly be represented by the acceleration of a fluid element. The interrelated effects of the pressure and drag terms are discussed further below.

Buchanan (2000) used a numerical experiment to demonstrate the importance of the pressure term in a sinusoidal oscillating flow. The necessity of this term is now illustrated using a more heuristic argument for the motion of bio-particles ($\alpha \approx 1.0$) in a general nonuniform flow field. The limiting case of a neutrally buoyant particle under the influence of only drag in a 1-D *uniform* flow field is considered first. The representative point-force equation is

$$\frac{dv}{dt} = \frac{1}{\tau_p}(u - v) \tag{A.3}$$

If the initial condition is set such that $v(t = 0) = u_L(t = 0)$ (where $u_L(t)$ represents the Lagrangian velocity of a fluid element at time t) the acceleration of the particle is zero always, i.e.,

$$\frac{dv}{dt} = 0 \tag{A.4}$$

and the particle maintains a constant uniform velocity.

The same neutrally buoyant particle under the influence of only drag is now considered in a *nonuniform* 1-D flow field. Nonuniform flow in a specific direction can be described in a Lagrangian frame as inducing either fluid element acceleration or deceleration. If we set the initial condition as $v(t = 0) = u_L(t = 0)$, Eq. (A.4) remains the solution of Eq. (A.3) for a neutrally buoyant particle. However, Eq. (A.4) provides no physically viable way for the particle to change velocity, i.e., accelerate or decelerate. If the particle is to change velocity, the neutrally buoyant requirement that $v(t) = u_L(t)$ must be violated. Hence, applying only a drag term in a nonuniform flow for the case of $\alpha = 1$ is invalid. This brings into question using only a drag (or drag and added mass) term(s) when $\alpha \approx 1$, as with blood particles.

The above inconsistency is of no surprise due to the fact that Stokes drag is derived in a uniform flow field with no acceleration. However, researchers have had varying degrees of success applying the drag-dominant point-force model to highly nonuniform conditions. Success with this scheme is most likely due to the method of application. When applying this model to a numerical scheme, for the case of $\alpha = 1$, if the fluid accelerates there is an errant velocity difference which elicits a drag force. This force acts to accelerate the particle, however, due to the analytic solution of Eq. (A.3), the particle velocity can now never fully reach the fluid velocity (i.e., asymptotic approach). In this respect, an 'artificial drag' is created to accelerate the particle. However, an error is introduced which can grow without bound depending on the rate and degree of acceleration. The final degree of this error has been quantified for an analytic example (not included).

Clearly, an additional term is needed in the point-force model to account for a nonuniform flow field and which yields a valid equation in the limit of $\alpha = 1$. Nonuniform flow on a fluid element basis in the absence of the particle is a result of pressure and shear induced surface forces that culminate in a change in fluid element velocity. The pressure

term represents the effect of pressure and shear gradients induced by the particle-free flow and can be expressed as proportional to the acceleration of a fluid element. Including the pressure term, the 1-D point-force model becomes

$$\frac{dv}{dt} = \alpha \frac{Du}{Dt} + \frac{1}{\tau_p}(u - v) \tag{A.5}$$

For the case of a neutrally buoyant particle with $v(t = 0) = u_L(t = 0)$ in a nonuniform flow field, the above equation reduces to the analytically correct expression that particle acceleration equals the acceleration of a fluid element

$$\frac{dv}{dt} = 1 \cdot \frac{Du}{Dt} \tag{A.6}$$

Hence, the pressure term is required to correctly account for particle acceleration in the limit of $\alpha = 1$. Furthermore, it is most likely also necessary to include the pressure term to correctly account for fluid acceleration when $\alpha \approx 1$, as with blood particle flow.

The added mass term is associated with the fluid surrounding the particle as the particle changes velocity and can be expressed

$$\frac{m_f}{2}\left(\frac{Du}{Dt} - \frac{dv}{dt}\right) \tag{A.7}$$

This effect is induced by an action of the particle on the flow field and does not arise from the pressure and shear gradients that define a nonuniform flow field. Therefore, this term cannot be used to account for the acceleration of the carrier fluid on the particle. Indeed, for the case of $\alpha = 1$, the added mass term makes no contribution to particle acceleration in a nonuniform flow field. Furthermore, due to the low particle Reynolds number found in blood particle transport (typically, $Re_p = 10^{-4}$), this effect can be neglected, as shown for the looping hbc in the Karino and Goldsmith expansion, cf. Fig. A.2. Similarly, the history integral also accounts for the acceleration effect of the particle on the surrounding fluid and, therefore, cannot be used to replace the pressure term. Again, this unsteady term can be neglected for bio-particle motion due to the extremely small Re_p (Buchanan, 2000).

To illustrate the ideas that the drag term alone is insufficient to model particle motion in a nonuniform flow field and that the pressure term is indispensable, the analytic solution of a simple 1-D test case has been investigated (not included). In summary, this example

illustrates that with the inclusion of the pressure term, a physically appropriate mechanism is provided to account for particle acceleration and deceleration in nonuniform flow. Hence, the velocity difference between the particle and fluid is dramatically reduced. This reduction in velocity discrepancy conceptually explains why the simulation of the hbc that contained drag and pressure terms was nearly identical to the pathline trajectory. Therefore, it is reasonable to assume that for a similar system but with a density ratio $1 \geq \alpha > 0.885$ the particle trajectory will be almost identical to the motion of a fluid element. For platelets and for monocytes $\alpha = 0.983$ and $\alpha = 0.964$, respectively. A fluid element approximation is then justified for the motion of platelets and monocytes in a nonuniform hemodynamic system of sufficient characteristic dimension in the absence of near-wall and inter-particle effects. Furthermore, such an approximation is ***more*** accurate than the use of drag alone in the case of blood particles.

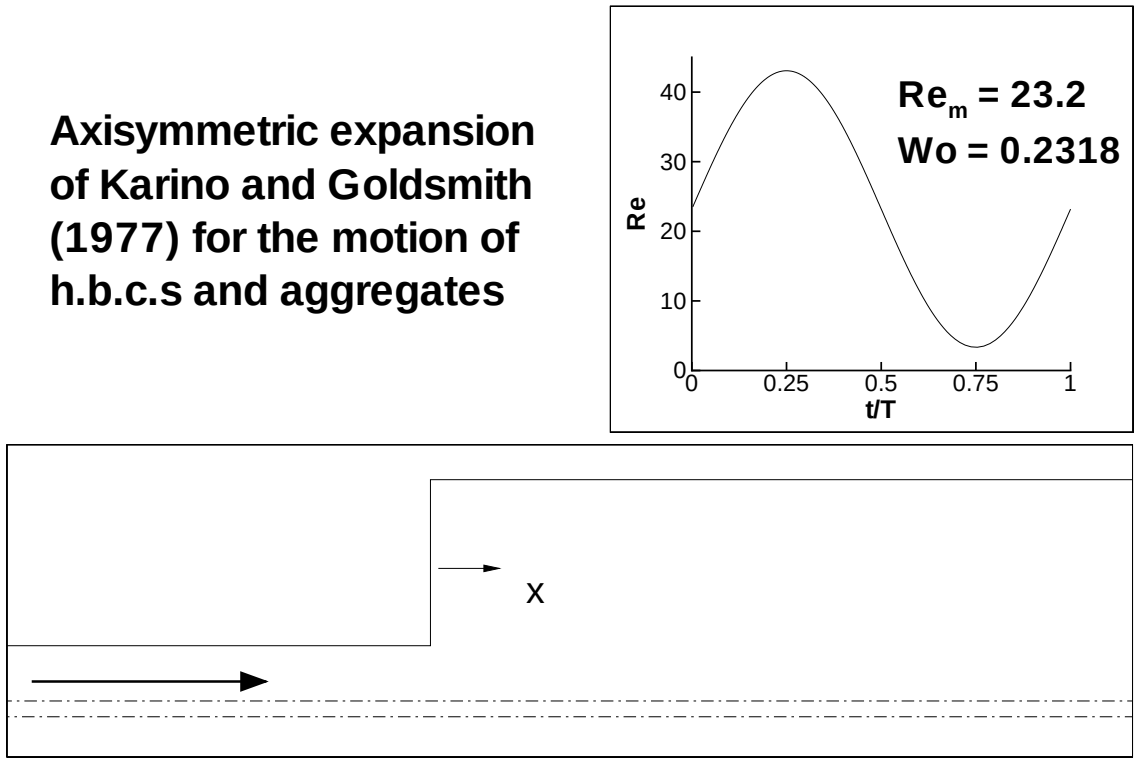

Figure A.1. Annular expansion geometry of Karino and Goldsmith (1977) and the sinusoidal input pulse.

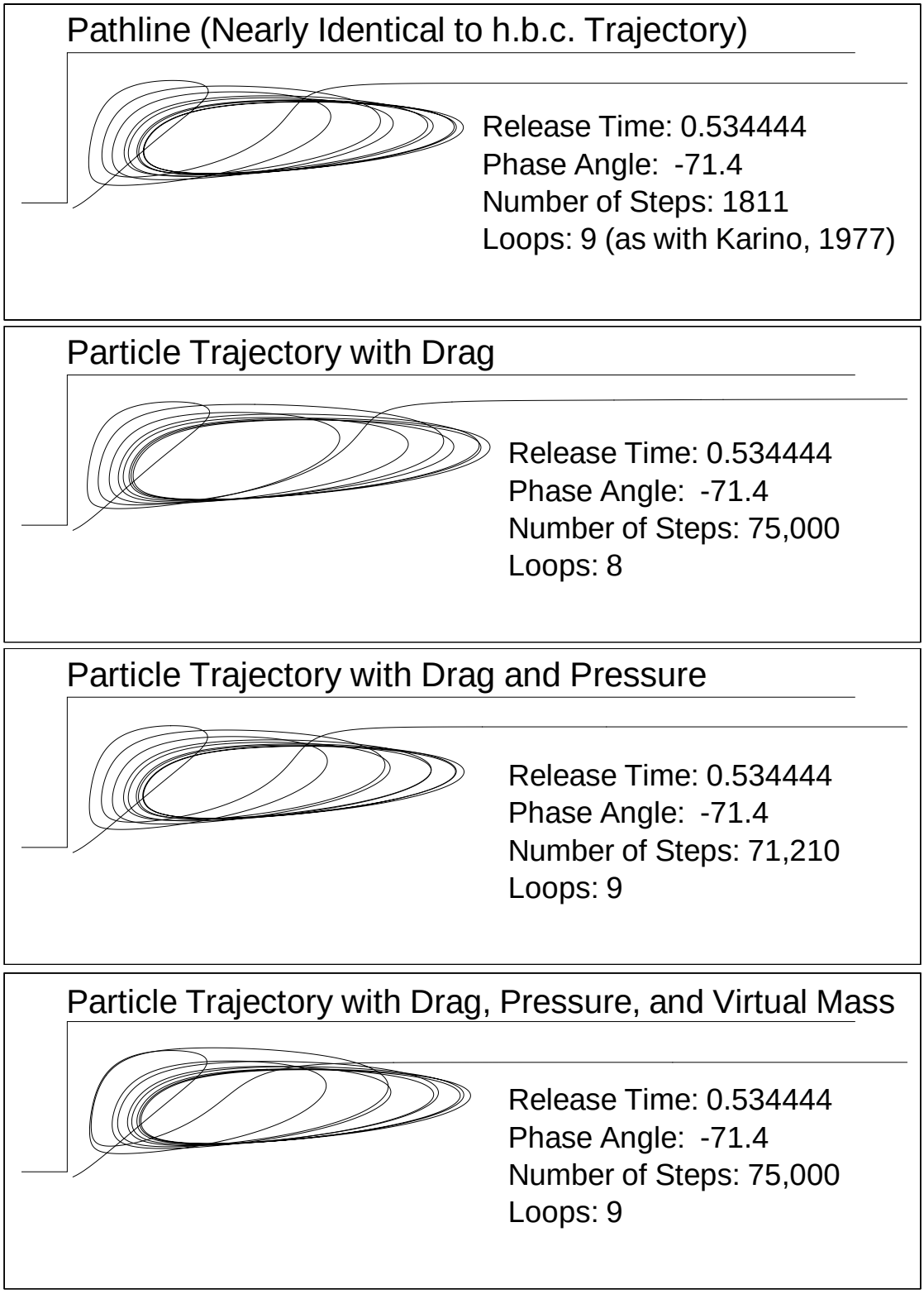

Figure A.2. Hardened blood cell motion in the Karino and Goldsmith (1977) annular expansion as simulated using a pathline and various particle motion equation approximations.