

Abstract Submitted  
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**Boundary Element Microhydrodynamics: Stagnation of flow in protein cavities**<sup>1</sup> SERGIO ARAGON, DAVID HAHN, San Francisco State University — A very precise boundary element solution of the exact Stokes flow surface integral equation has been implemented in our Fortran 90 program BEST. In our previous work (Aragon & Hahn, *Biophys. J.* 2006, 91: 1591-1603; *J. Chem. Theory and Comput.* 2006, 2: 1416-1428) we obtained very precise values of the tensorial transport properties (translation, rotation, and intrinsic viscosity) for a large set of proteins with a uniform water hydration thickness of 0.11 nm. In this work, we utilize the surface stress distribution thus obtained to evaluate the flow field as a function of distance away from the hydrodynamic surface for a variety of surface features in a dimpled sphere (test case) and for the proteins myoglobin, lysozyme, and human serum albumin. We demonstrate that solvent in small to large pockets on the hydrodynamic surface moves with the protein with distances up to 2 nm for deep pockets regardless of the direction of motion of the protein. On the other hand, the fluid flow pattern on protruding portions of the hydrodynamic surface decays much more rapidly with distance from the surface. The implications of these results with respect to the amount of water associated with the surface and the rate of transport to active enzymatic sites in stirred solutions is discussed.

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