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# BIOFLUID MECHANICS OF VON WILLEBRAND FACTOR INTERACTIONS WITH EXTRACELLULAR VESICLES

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## ABSTRACT

The mechanics of deformable biological macromolecules is central to many physiological processes, yet remains poorly understood when multiple physical interactions coexist. A prominent example is von Willebrand Factor (vWF), a large multimeric polymer whose conformation is altered under shear and extensional flow, transitioning from a compact globular structure to an extended conformation as hydrodynamic forces overcome internal elastic resistance. A key feature of vWF is its A1 domain, which governs interactions with other biomolecules and surfaces through electrostatic charges. In blood flow, vWF coexists with extracellular vesicles (EVs), nanoscale particles with negatively charged surfaces, introducing long-range electrostatic interactions into an already complex fluid-structure system. How these interactions alter polymer dynamics under flow remains an open question in biofluid mechanics.

Here, we investigate coupled hydrodynamic and electrostatic mechanics of a flexible polymer interacting with charged particles in shear flow using multiscale multiphase direct numerical simulations. The polymer is modelled as a bead-spring chain coupled to the lattice Boltzmann solver through Langevin dynamics, enabling resolution of polymer elasticity, hydrodynamic interactions, and thermal fluctuations. Suspended particles representing EVs interact with the polymer through long-range electrostatic coupling. This unified, two-way coupled framework enables systematic analysis of flow-dependent interaction regimes governing polymer conformational dynamics.

The results demonstrate that polymer conformation is governed by a balance between shear-induced hydrodynamic stretching and electrostatic restoring interactions arising from oppositely charged particle–polymer interactions. In the absence of electrostatic interactions, polymer unfolding occurs when hydrodynamic forces exceed the intrinsic elastic restoring force, defining a critical shear rate for extension. The presence of charged particles introduces an additional electrostatic contribution to the effective restoring force, stabilizing compact polymer configurations and shifting the critical shear rate for unfolding to higher values. This stabilization effect increases with particle concentration. As the imposed shear rate increases beyond this modified threshold, hydrodynamic forces dominate the force balance, reducing particle–polymer proximity and weakening electrostatic interaction energy. Under these conditions, electrostatic stabilization becomes ineffective, and the polymer undergoes sustained elongation. Simulations with neutral particles serve as a control case and exhibit no measurable shift in the critical shear rate or conformational statistics, confirming that the observed stabilization and threshold shift arise from electrostatic–hydrodynamic coupling rather than purely hydrodynamic interactions. These results demonstrate how charged particles modify flow-induced conformational dynamics of flexible macromolecules and provide a mechanics framework for understanding polymer behavior in complex biological flows where electrostatic interactions coexist with hydrodynamic forcing.