

Laminar flow past a simplified viral capsid structure model

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ABSTRACT

Viruses enclose their nucleic acids by a protein coat, named viral capsid, that may also shelter viral proteins involved in infection. The viral capsid has two remarkable features in its structure: icosahedron and capsomers. Icosahedral capsid structures are found more frequently in the viruses of relatively larger radius. A few attempts have already been made to explain why larger viruses prefer the icosahedron. In this presentation, our focus is laid on the other characteristics of viral capsid, i.e., the capsomers which are the complexes of diverse viral proteins. We look into the role of capsomers from the perspective of fluid mechanics, by solving the 2D incompressible Navier-Stokes flow past a bumpy circle which represents our simplified model of the viral capsid. By varying the number of capsomer-like protuberances, the changes in drag coefficients are investigated in order to implicate the effect of capsomers on the flow change around a virus. There is a certain range of bump numbers that maximizes the drag coefficient in association with the given characteristic radius and the low Reynolds number. This preliminary deduction is not totally consistent with the patterns of turbulent flows around V-grooved surfaces that decrease drag forces. The capsomers on nanoscale viral capsids may therefore play the reversal role in comparison of macroscopic riblets immersed in turbulent flow. This study on flows around a viral capsid will enhance our fundamental understanding of the highly optimized motion of viruses in blood flow. It will also contribute to the development of the design of nanoscale drug delivery systems for the biomedical purposes such as gene therapy. Clear feasibility will accordingly suggest more comprehensive future studies on the role of capsomers in the free flow of virus particles within the framework of the interaction between blood flow and soft materials. Supports by the Korea Research Foundation (KRF) under the grant of KRF-2005-015-C00052, and by the US Air Force Office of Scientific Research (AFOSR) are gratefully acknowledged.

WHY DO VIRUSES HAVE THEIR OWN STRUCTURE ? : MECHANICS POINT OF VIEW

A gallery of identified viruses by T.S. Baker et. al. is shown in *Microbiol. Mol. Biol. Rev.* 63, 862 (1999), which is depicted in Figure 1. A large set of viruses is known to have the icosahedral structure. The surface of virus is covered by a bumpy structure as shown in Figure 1.

We look into the role of capsomers from the perspective of fluid mechanics, by solving the 2D incompressible Navier-Stokes flow past a bumpy circle which represents our simplified model of the viral capsid.

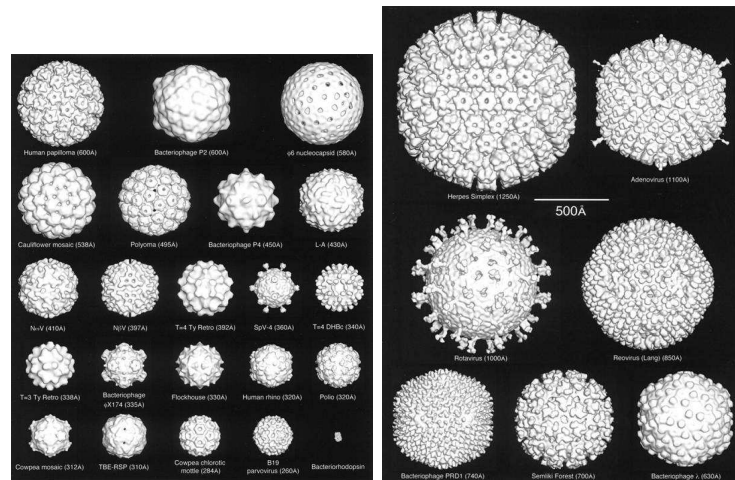


Figure 1. A gallery of viruses : T.S. Baker et. al., Microbiol. Mol. Biol. Rev. 63, 862 (1999)

From the accurate numerical experiments using the meshfree point collocation method to solve the stream-vorticity equation in 2D, we have found out that there is a certain range of bump numbers that maximizes the drag coefficient in association with the given characteristic radius and the low Reynolds number. This feature is totally different from that of golf ball with grooved surface.

This study on flows around a viral capsid will enhance and enlarge our fundamental understanding of the highly optimized motion of viruses in blood flow. Additionally, this result will also contribute to the development of the design of nanoscale drug delivery systems for the biomedical purposes such as gene therapy. Consequently speaking, this will be the first step toward truly mathematical and computational biology.

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