

MOLECULAR DYNAMICS SIMULATIONS OF THE CORONAVIRUS SUSPENDED IN MIST AND AIR

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ABSTRACT

The reopening of public services during this pandemic has led to many unique situations for the coronavirus to propagate and spread, especially in warmer, outdoor environments. The consensus is that the virus has limited avenues to spread in outdoor environments, but certain factors may in fact impact the infection capability of the coronavirus in outdoor environments. Some evidence suggests that outdoor venues with large crowds (sports stadiums, theme parks, music concerts, etc.) may give rise to increased rates of infection. This study investigates if one such factor, the use of misting as a form of cooling, can contribute to the spread of the virus using molecular dynamics (MD) simulation techniques. Previous research indicates that the virus is at minimum significantly impeded or at most faces some destruction of its viral structure in humid environments. This study analyzed the spike protein of the Covid-19 virus in an assembly 1 conformation (which is a dormant form of the virus) surrounded by air and water droplets in a cool and low-pressure environment. The simulation was first minimized the total energy of the simulation and then the interaction process was observed using a constant volume and total energy with periodic boundary conditions. The results indicated that the virus deformed notably and that the radius of gyration, taken as an analog for the internal volume of the virus structure, saw a general increase. These findings however are not in the same order of magnitude as suggested by previous studies, which may be caused by a difference in simulation length, construction, or conditions. Future studies would benefit from an increase in simulation domain and inclusion of more complex intermolecular forces such as the coulombic potential..

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