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Keith A Erickson* (keith.erickson@usma.edu), Department of Mathematical Sciences, United States Military Academy, West Point, NY 10996. *Agent-based model of therapeutic intervention following exposure to botulinum neurotoxin*. Preliminary report.

Neurotoxins produced by the bacterium *Clostridium botulinum* are highly toxic and are potential biological weapons. Symptoms of exposure begin within a few days and include nerve palsies and respiratory failure. Botulinum neurotoxin (BoNT) binds to receptors on nerve terminals at the neuromuscular junction and is taken up into the cell by endocytosis. Inside the cell, BoNT blocks exocytosis of acetylcholine into the synaptic cleft, resulting in paralysis. While much data exists on the in vivo targets of these neurotoxins and the interactions, the mechanisms involved in therapeutic intervention after exposure are not understood. We are developing an agent-based platform to test hypotheses related to treatment and recovery following exposure to BoNT. The foundation of this platform is a quantitative kinetic model simulating the steps of BoNT-induced muscle paralysis. A comparison of model predictions to experimental results indicates points in the model that require refinement. These points include the fate of BoNT inside the cell and the spatial distribution of vesicles containing acetylcholine. We will discuss the current state of our model and our efforts to refine it to account for experimental data. (Received September 26, 2006)