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AGENT-BASED SIMULATION OF THE DIFFUSION DYNAMICS AND CONCENTRATION OF TOXIC MATERIALS FROM QUANTUM DOTS-BASED NANOPARTICLES

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ABSTRACT

Due to their favorable electrical and optical properties, quantum dots (QDs) nanoparticles have found numerous applications including nanomedicine. However, there have been concerns about their potential environmental impacts. The objective of this study is to develop an agent-based simulation model for predicting the diffusion dynamics and concentration of toxic materials released from QDs. Reaction kinetics is used to model the stability of surface capping agent particularly due to oxidation process. The diffusion of toxic Cd^{2+} ions in aquatic environment was simulated using an adapted Brownian motion algorithm. A calibrated parameter to reflect sensitivity to reaction rate is proposed. The model output demonstrates the stochastic spatial distribution of toxic Cd^{2+} ions under different values of proxy environmental factor parameters.

1 INTRODUCTION

Quantum Dots applications in medicine and life sciences (i.e. nanomedicine) range from drug delivery to bio-imaging using nanoparticle labels and from tissue repair and replacement to implantable sensors.The risks of toxicity of QD based nanomedicine and PV cells stem from their potential to cause undesirable health effects, contaminate the environment (air, water, and land), and adversely affect susceptible parts of the population (e.g. workers at nano-manufacturing and healthcare facilities) (Oberdorster 2010).

2 AGENT-BASED SIMULATION MODEL AND SET-UP

When released in the environment, QDs nanoparticles may undergo several transformation processes ranging from chemical transformations, biological transformations, physical transformations, to transformations that may occur by interactions of nanoparticles with macromolecules (Lowry et al. 2012). Fig. 1 summarizes a scenario for QD nanomaterial release and subsequent transformation in aquatic environment.

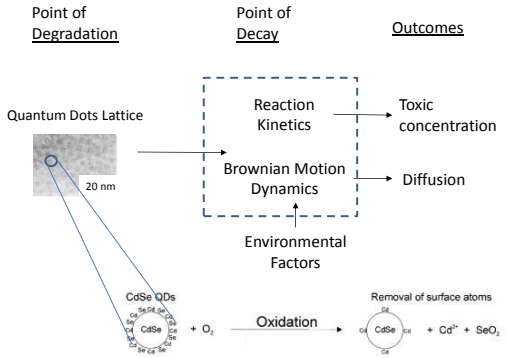

Figure 1. The transformation of CdSe QD-based nanoparticles and the diffusion of Cd^{2+} ions

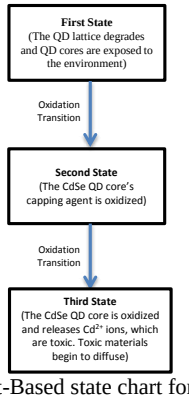

Fig. 2. Agent-Based state chart for CdSe QDs

The transformation process is captured using a state chart diagram (Fig. 2). The first state describes the

status of an agent (i.e. CdSe QD core with capping agent) when it is oxidized. A similar study about the Thiol-capped photo-oxidation kinetics of CdSe quantum dots is used as a reference (Chen 2010).

The Cd^{2+} diffusion model of CdSe-based QD is based on an adapted computational algorithm of Brownian motion model developed by Azimi et al. (Azimi, Jamali, and Mofrad 2011). Reaction kinetics algorithm for oxidation reaction is based on the work of Klann et al. (Klann, Lapin, and Reuss 2011). The agent-based approach is implemented in AnyLogic software (www.anylogic.com).

3 RESULT AND ANALYSIS

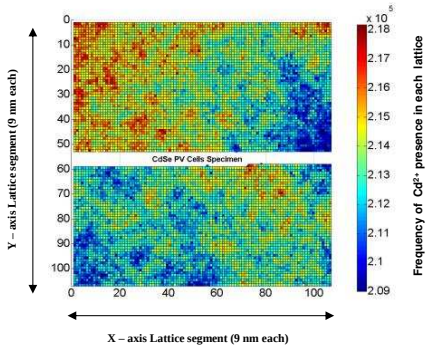

Fig. 3. The frequency distribution of diffusion trajectory of toxic material release

A calibrated of model parameter is obtained in order to approximate the simulation results to reality. Limited data is available for the context of CdSe –based Nanomedicine as a basis for calibration. As a proof of concept, the value of model parameter $F_{multiplier}$ was calibrated to closely represent the reaction rate observed by (Derfus, Chan, and Bhatia 2004).

From the perspective of diffusion dynamics, the distribution of Cd^{2+} ions across the spatial dimension is established. Fig. 3 shows a snapshot of such a distribution for the baseline $F_{multiplier}$. To take into account the stochastic nature of the dynamics, median value of five simulation runs was used.

The color map for each set up represents different frequency of Cd^{2+} ions presence during the simulation period and hence indicates most likely location of the toxic materials. Each lattice in 100 x 100 matrix has the size of 9nm x 9nm. The QD specimen is located in the middle section of the matrix.

4 CONCLUDING REMARK

The modeling simulation approach is built upon sound methods for modeling fundamental processes that have been verified and validated based on experimental data (Derfus et al., 2004). Specifically within this context, this work contributes to add a modeling tool to complement existing tools available for quantifying and visualizing the fate and transport of Cd^{2+} ions. The modeling approach adds simplicity of the solubility and rate of release of Cd^{2+} ions by essentially relegating the chemistry to a single adjustable coefficient. At the same time, it also deals with the complexity of tracking of individual atoms of Cd.

REFERENCES

Azimi, M., Y. Jamali, and M. R. K. Mofrad. 2011. "Accounting for Diffusion in Agent Based Models of Reaction-Diffusion Systems with Application to Cytoskeletal Diffusion." Plos One 6 (9).

Chen, Jixin. 2010. "Nanofabrication, Plasmon Enhanced Fluorescence and Photo-Oxidation Kinetics of CdSe Nanoparticles." DOCTOR OF PHILOSOPHY, Chemistry, Texas A&M University.

Derfus, A. M., W. C. W. Chan, and S. N. Bhatia. 2004. "Probing the cytotoxicity of semiconductor quantum dots." Nano Letters 4 (1):11-18.

Klann, M. T., A. Lapin, and M. Reuss. 2011. "Agent-based simulation of reactions in the crowded and structured intracellular environment: Influence of mobility and location of the reactants." Bmc Systems Biology 5. doi: 10.1186/1752-0509-5-71.

Lowry, G. V., K. B. Gregory, S. C. Apte, and J. R. Lead. 2012. "Transformations of Nanomaterials in the Environment." Environmental Science & Technology 46 (13):6893-6899.

Oberdorster, G. 2010. "Safety assessment for nanotechnology and nanomedicine: concepts of nanotoxicology." Journal of Internal Medicine 267 (1):89-105.