University of Victoria | Graduate Studies

Notice of the Final Oral Examination
for the Degree of Doctor of Philosophy

of

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MSc (University of Victoria, 2012)
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"Simulation and Network Analysis of Nanoparticles Agglomeration and Structure Formation with Application to Fuel Cell Catalyst Inks"

Department of Mechanical Engineering

Thursday, April 25, 2019
10:00 A.M.
Engineering Office Wing
Room 108

Supervisory Committee:
Dr. Ned Djilali, Department of Mechanical Engineering, University of Victoria (Supervisor)
Dr. Peter Oshkai, Department of Mechanical Engineering, UVic (Member)
Dr. Irina Paci, Department of Chemistry, UVic (Outside Member)

External Examiner:
Dr. Akeel Shah, School of Engineering, University of Warwick

Chair of Oral Examination:
Dr. David Berg, Department of Chemistry, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

Agglomeration of nanoparticles occurs in a number of colloidal systems related, for example, to material processing and drug delivery. The present work is motivated by the need to improve fundamental understanding of the agglomeration and structure formation processes that occur in catalyst inks used for the fabrication of polymer electrolyte fuel cells (PEMFCs). Particle dynamics simulations are performed to investigate agglomeration under various conditions. The interaction between particles is defined using realistic physical potentials, rather than commonly used potential models, and a novel analysis of the agglomeration and structure formation process is performed using graph theory and network science concepts. The simulated systems correspond to catalyst inks consisting primarily of carbon nanoparticles in solution. The effect of various conditions such as different force magnitude, shape of the force function, concentration etc. are investigated in terms of graph theory parameters such as average degree and shortest path. An “agglomeration timescale” and a “restructuring timescale” introduced to interpret the evolution of the agglomeration process suggest that the structure, which has a strong impact on the performance of the eventual catalyst layer, can be controlled by tuning the rate at which particles are added based on the restructuring timescale.