

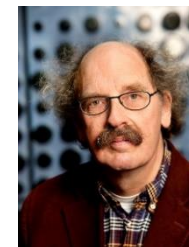
Faculty of Engineering and Applied Science

Chemical Engineering Seminar Series



Polymer modeling for Art and Industry

Dr. Piet Iedema/University of Amsterdam
Thursday, March 14, 2019, 2:30pm
Dupuis Hall, Room 215



ABSTRACT

In this talk a multiphysics approach to mathematical modeling of polymer network based paints will be discussed, as applied to photocuring acrylates (e.g used in 3D printing (art) objects) and linseed oil based binding medium in oil paintings.

Old oil paintings are a precious but vulnerable part of cultural heritage. The binding medium polymer chemically interacting with metal from pigments is degrading over many years of museal exposure and treatments. In order to better understand the chemistry and migration of degradation products models predicting the polymer network structure are developed from atomistic to macroscopic scales. The extreme chemical complexity of the historically interesting binding medium linseed oil is treated using automatic reaction network and kinetic model generation. The link between polymer network topology and thermomechanical properties is provided by Molecular Dynamics.

Understanding the chemistry of the transition, in photocuring of acrylates, from liquid monomer to solid polymer, involving the role of oxygen, network-bound and free unsaturated groups, humidity and metal coordination sites (ionomers), allows predicting the network topology. Simulations on atomistic level serve to compute the increasing diffusion limitation of the reactions which forms input to higher aggregation level models based on Random Graph Theory. Thus, prediction will become possible of old paintings degradation behavior related to metal-based pigments and performance related to structure of acrylates.