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Computer Simulation Studies of Polyurethane Film Formation SHIHAI YANG, RAS PANDEY, MAREK URBAN, University of Southern Mississippi — Three types of particles (hydrophobic (H, R-NCO), polar (P, R'-OH), aqueous (A) solvent) are used to describe the constituents involved in a polyurethane film formation. Characteristics such as attractive (P,A) and repulsive (H,A) interactions, reaction kinetics, and molecular weight ratios are captured by the model. Each constituent is mobile and forms covalent bonds with appropriate constituents with specific kinetics. Bonded units move and corresponding bonds fluctuate within limits. The aqueous components are also allowed to evaporate. The mobility allows stabilization (equilibration), covalent bonding captures the constituents, and evaporation destabilizes the system. Effects of temperature, initial water concentration, and stoichiometry are considered. With increasing the temperature, film thickness hs increases while its roughness Ws decreases. With increasing the initial water concentration and NCO:OH ratio, both film thickness hs and its roughness Ws increases. Simulation data suggest that higher NCO:OH ratios lead to higher urea and urethane contents, however, higher initial water concentration results in higher urea but lower urethane concentration in the film.

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