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**A Coarse Grained Model for Methylcellulose: Spontaneous Ring Formation at Elevated Temperature** WENJUN HUANG, RONALD LARSON, Univ of Michigan - Ann Arbor — Methylcellulose (MC) is widely used as food additives and pharma applications, where its thermo-reversible gelation behavior plays an important role. To date the gelation mechanism is not well understood, and therefore attracts great research interest. In this study, we adopted coarse-grained (CG) molecular dynamics simulations to model the MC chains, including the homopolymers and random copolymers that models commercial METHOCEL A, in an implicit water environment, where each MC monomer modeled with a single bead. The simulations are carried using a LAMMPS program. We parameterized our CG model using the radial distribution functions from atomistic simulations of short MC oligomers, extrapolating the results to long chains. We used dissociation free energy to validate our CG model against the atomistic model. The CG model captured the effects of monomer substitution type and temperature from the atomistic simulations. We applied this CG model to simulate single chains up to 1000 monomers long and obtained persistence lengths that are close to those determined from experiment. We observed the chain collapse transition for random copolymer at 600 monomers long at 50C. The chain collapsed into a stable ring structure with outer diameter around 14nm, which appears to be a precursor to the fibril structure observed in the methylcellulose gel observed by Lodge *et al.* in the recent studies. Our CG model can be extended to other MC derivatives for studying the interaction between these polymers and small molecules, such as hydrophobic drugs.

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