Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Coil-Globule Transition of Polymer – Tricriticality of Theta ASHOK DASMAHAPATRA, Department of Chemical Engineering, Indian Institute of Technology Guwahati, Guwahati-781039, Assam — We demonstrate the tricriticality of the theta point in the coil-to-globule transition of a single flexible polymer chain by dynamic Monte Carlo (DMC) simulation. For homopolymer, at the tricritical point, the second order theta transition line approaches the first order collapse transition line as the chain length approaches the thermodynamic limit. Theta point of homopolymer has been estimated by following the ideal behavior of chain at the theta point. Temperature at which the constant volume specific heat (Cv) shows a peak is considered as the collapse temperature and the transition is of first order. In T-N plane, collapse temperature approaches towards the theta temperature as the chain length approaches to the thermodynamic limit. For copolymer (with periodic distribution of comonomer along the chain), the collapse temperature increases with increasing the stickiness parameter (viz., higher solvophobicity of the comonomers relative to monomers) and approaching towards the theta as the value of the stickiness parameter increases. Theta points of copolymers have been estimated from the theta point of homopolymer under the condition of the ideality of the theta point. The collapse temperatures for copolymer have been in a manner similar to homopolymers. Theta temperature vs. stickiness parameter represents a second order line whereas collapse temperature vs. stickiness parameter represents a first order line. We demonstrate that as the stickiness parameter increases, these two lines meet each other, close to the "tricritical" theta temperature.

Ashok Dasmahapatra
Department of Chemical Engineering, Indian Institute of Technology
Guwahati, Guwahati-781039, Assam

Date submitted: 18 Oct 2011 Electronic form version 1.4