

Abstract Submitted  
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**MD simulations of chemically reacting networks: analysis of permanent set** DANA ROTTACH, University of New Mexico, JOHN CURRO, JOANNE BUDZIEN, GARY GREEST, AIDAN THOMPSON, Sandia National Laboratories — The Independent Network Model (INM) has proven to be a useful tool for understanding the development of permanent set in strained elastomers. Our previous work showed the applicability of the INM to our simulations of polymer systems crosslinking in strained states. This study looks at the INM applied to theoretical models incorporating entanglement effects, including Flory's constrained junction model and more recent tube models. The effect of entanglements has been treated as a separate network formed at gelation, with additional curing treated as traditional phantom contributions. Theoretical predictions are compared with large-scale molecular dynamics simulations.

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