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Toward a predictive model for the failure of elastomer seals.[1] NICOLA MOLINARI, MUSAB KHAWAJA, ADRIAN SUTTON, ARASH MOSTOFI, Imperial College London, BAKER HUGHES COLLABORATION — Nitrile butadiene rubber (NBR) and hydrogenated-NBR (HNBR) are widely used elastomers, especially as seals in oil and gas industry. During exposure to the extreme temperatures and pressures typical of well-hole conditions, ingress of gases causes degradation of performance, including mechanical failure. Using computer simulations, we investigate this problem at two different length- and time-scales. First, starting with our model of NBR based on the OPLS all-atom force-field, we develop a chemically-inspired description of HNBR, where C=C double bonds are saturated with either hydrogen or intramolecular cross-links, mimicking the hydrogenation of NBR to form HNBR. We validate against trends for the mass density and glass transition temperature for HNBR as a function of cross-link density, and for NBR as a function of the fraction of acrylonitrile in the copolymer. Second, a coarse-grained approach is taken in order to study mechanical behaviour and to overcome the length- and time-scale limitations inherent to the all-atom model. The effect of nanoparticle fillers added to the elastomer matrix is investigated. Our initial focus is on understanding the mechanical properties at the elevated temperatures and pressures experienced in well-hole conditions.

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