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Project Title: Early Failure of Elastomers: Understanding Damage Accumulation toward Failure

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Abstract

Elastomeric joints, seals and hoses and their failure are a menace to hydrocarbon transfer systems. Modeling of damage in elastomers is based on a single-phenomenon, single-model approach where a model covers only a specific damage mechanism such as aging. Current predictive models are relevant mainly when damage occurs via only one mechanism. Despite being popular, this approach is limited since it cannot accommodate real-life failures that are typically induced by several parallel damage mechanisms. Elastomer components experience different damage types due to low-frequency dynamic loads, aging/degradation, ozone cracking, and shock loads of repeated reeling under high hose tension. The complexity of coupling of damage models to each other, and lack of a systematic approach toward creating a multi-model multi-phenomena framework are the main challenges we face in understanding damage accumulation in elastomers. This proposal aims to tackle those challenges.

The goal is to devise a theoretical basis that allows integration of different damage mechanisms into one framework, and accounts them at the same time. The advantage is that the damage mechanisms can be derived from some of the existing models in literature and then coupled together. In the 2 years of this project, a framework will be assembled to couple multi-scale models of different damage mechanism to predict damage accumulation and provide input to fatigue models of ENCs. In the context of the framework, we will also study how parallel micro-structural phenomena influence crack propagation and how the material matrix evolves accordingly.

Accordingly the 2 year scientific Plan was set as follows

1. Construct Visco-elastic Platform.
2. Model (i) strain induced crystallization, (ii) deformation induced anisotropy of NP network, and describe their role on crack propagation.
3. Derive module of ozone/temperature matrix degradation from existing models.
4. Implement derived modules into the platform to form the framework.
5. Derive a new failure model and bridge it to the framework.
6. Evaluate framework performances using FEM by changing the content, distribution, and geometry of NPs.

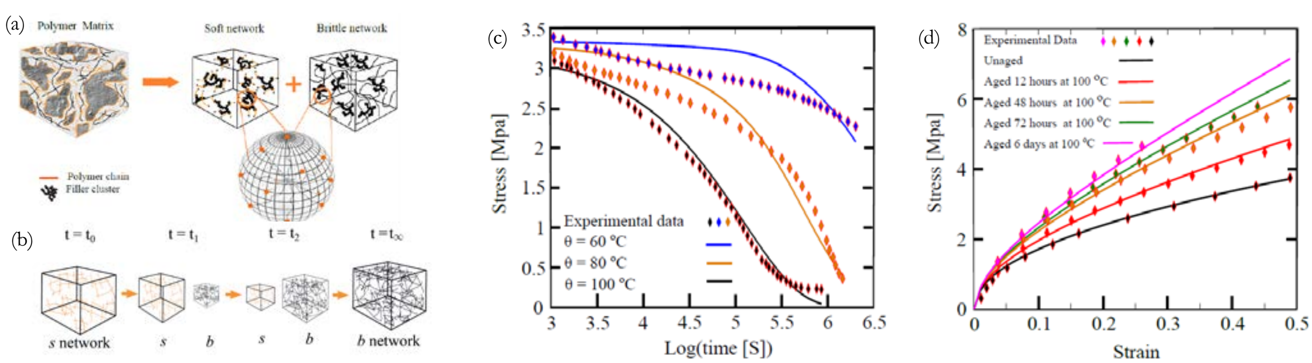

Figure 1. (a) Schematic breakdown of a polymer matrix into two networks; soft (s) and brittle (b). (b) Transformation of the soft polymer matrix into the brittle matrix in the course of thermos-oxidative aging. (c) Model prediction of experimental tests on relaxation test at e = 50% and (d) intermittent tension test at q = $100^{o}C$ taken from our paper at Int. J. Plasticity.

In the second year of this project, the efforts has been directed in 3 main tasks. Each task has been done by one or two graduate students that were partly involved in this project. In task 3, we also used the help of one visiting faculty.

1. Modeling Damage and inelasticity in constitutive behaviour of elastomers: While failure is often induced by several parallel damage mechanisms, the damage resulted by each of them is modeled individually to avoid extreme complexity of interacting damage mechanisms. Micro-mechanical models often describe damage with respect to the changes in the entropic energy of the polymer chains, clusters or networks and the changes in the enthalpic energy of the nano-particle structures. These models, despite having similar view of the polymer matrix, are usually not compatible to each other for the following reasons (i) incompatible description of the structural changes across multiple scales, (ii) incompatible understanding of mechanics of micro-structure, and (iii) different coupling approaches that are used to address time- and scale-consistency problems in the bridging of atomistic to continuum-scale parts. Moreover,

current models of rubber elasticity usually are based on different approximation methods which contains considerable error for chains under high extension rates. This fact initiates three independent studies on

a. Predicting the entropic energy of single polymer chain–see figure 1.b (Phys. Rev. E 2019)

b. Approximating the behaviour of inverse Langevin function near singularity –see figure 1.a (MMS)

c. Predicting inelastic behaviour of soft materials with cross-linked polymeric matrix such as hydrogel –see figure 1.c (Int. J. Solids Struct. 2019)

2. Modeling damage accumulation in aging: Cyclic loading of ENC generates a significant quantity of heat, and depending on the dissipation rate, a significant temperature increase. In elevated temperatures, matrix dominated properties are especially vulnerable and could be greatly reduced by thermal and ozone degradation,80–85 particularly at temperatures close to the glass transition temperature (T_g). Oxidation breaks down the polymer chains and crosslinks, and gradually degrades the overall mechanical performance of elastomers. In contrast to ozone degradation, thermal degradation and its role on mechanical properties of ENCs have been extensively studied. However, despite efforts to link these effects, it remains a challenge to combine the effects of thermal degradation on progressive damage of elastomers, which is the very goal of this part. This task is mainly focused on two subjects

a. Understanding damage induced by matrix degradation (ECCMR 2019)

b. Modeling the effect of aging on mechanical behaviour of elastomers (Int. J. Plasticity 2019)

3. Failure modeling through the platform: Models of damage in elastomers are often based on a single phenomenon approach where one model only covers damage mechanisms induced by one phenomenon, e.g. time, temperature, or deformation. Despite its popularity, this approach has limited accuracy in prediction of real-life failures that are formed by parallel damage mechanisms. Current models are relevant when damage occurs due to only one mechanism. The complexity of the coupling of damage phenomena to each other, and lack of a systematic approach toward creating an integrated framework are the main challenges faced in understanding damage accumulation in elastomers. This proposal aims to tackle those challenges. The aim of this task is to devise a theoretical platform that provides a consistent space to define damage mechanisms, integrates them into one framework and describes the current state of damage accumulation as input for failure models. Such a platform transforms our modeling abilities in predicting failure due to the accumulated damage of parallel mechanisms. Many existing multi-scale models of other groups can also be imported to the platform and then coupled to each other.

This task is mainly focused on three subjects

a. Design of systems for detection of the early failure in elastomers through Micro-electro-mechanical systems (Mechanics of Advanced Materials and Structures 2018)

b. Development of Platform assembly process for seamless coupling of models of different damage mechanisms (Rubber Chemistry & Technology 2019)

c. Development of a predictive software to predict early failure of elastomers due to accumulated damage (SoftwareX 2019)

In all the aforementioned tasks, the research topics have formed the basis of the PhD thesis of the involved PhD students. PI's group will graduate two experts in the fields of elastomer degradation, and constitutive modeling, Mr. Vahid Morovati in 2019 and Mr. Hamid Mohammadi in 2020. All the experimental and theoretical efforts reported in this work has been carried out at the PI's Lab.

Impact: the developed framework will be released to industry and academia through release of the open-source code and the manual through SoftwareX.org, and the PI's website. After validation, the PI has provided the code and the database on his group website that contains materials for the quasi-static network evolution framework, the code on ageing will be released shortly by the first quarter of 2020. The database should be further expanded to work as an online exchange center which is able to host, sort, and disseminate the modified codes, and models uploaded by any group and not only the PI.

Main industrialization is expected to start after public release. New validation tests enforced for industrial adoption, integration of models and updates provided by other groups require continuous improvement of the framework and the database. These efforts places PI's group and consequently MSU in a key position in the exploding field of virtual design and testing of nanocomposites.

The advancement of nanocomposite research is particularly important in the state of Michigan, which has historically been the hub of the auto industry. These materials are crucial to the auto industry that thrive for more fuel-efficient and safe vehicles. Several national research centers on polymeric matrix composites have been established in Michigan, many of which are placed at MSU such as the Composite Materials and Structures Center, Composite Vehicles Research Center, and the new center of excellence, Institute for Advanced Composites Manufacturing Innovation. These centers are mainly focused on compounding, process, and manufacturing optimization. Thus, enabling virtual design through improved simulation capabilities can strongly enhance the position of MSU in this field.