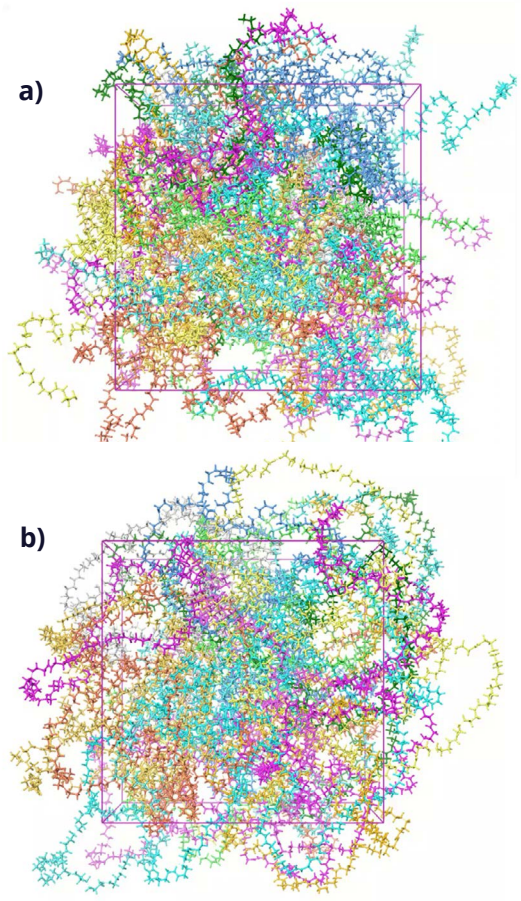
CASE STUDY

Molecular dynamics simulations accelerate the development and optimization of recyclable tire materials

Scientists from Evonik and Schrödinger gain a deeper understanding of the impact of additives and macrocyclic structures on trans-polyoctenamer rubber (TOR)

Executive Summary

- **Accurately predicted key thermophysical and structural properties** such as glass transition temperature (T_g), density, free volume, and diffusion coefficient for rubber mixture systems
- **Explored the miscibility** of trans-polyoctenamer rubber (TOR) with different crosslinkers and base polymers
- **Developed an understanding of the impact** of macrocyclic polymer chains on the structural and thermophysical properties
- **Accelerated rational design** of high-performance rubber formulations and provided insights into the key factors for processability of recycled rubbers



Snapshots of final configuration after the production MD run for a) linear chains, and b) macrocyclic chains of 2000 molecular weight.[1]

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Challenges

Trans-polyoctenamer rubber (TOR), commercially known as VESTENAMER®, has been widely used as a tire additive to improve the processability and recyclability of tire rubbers. In order to efficiently co-vulcanize different rubbers to obtain improved properties, it is vital to understand the interaction of TOR with different components of rubber formulations, including crosslinkers and base polymers. However, experimental characterization of these formulations is time-consuming and resource-intensive.

Approach

Molecular modeling provides an economical alternative to long experiments and lengthy development cycles for new tire formulations. Scientists from Evonik and Schrödinger worked together to digitally evaluate the miscibility of TOR with various crosslinkers and polymers, and to look into the impact of macrocyclic polymer chains on TOR properties. With GPU-accelerated molecular dynamics (MD) engine, scientists were able to run the simulations at high-speed, e.g. 50ns of diffusion calculations, in only a few hours.

All models and simulations were performed using the Schrödinger Materials Science Suite and Desmond for MD according to the following procedure:

Constructed models for polymers and crosslinkers included in **Figure 1**, and equilibrated the systems

Computed cohesive energy, solubility parameter distance, energy of mixing, and interaction energy for different mixtures to predict miscibility

Predicted thermophysical (T_g) and structural (density, diffusion, free volume) properties to understand the impact of macrocyclic chains (greater than 8000 g/mol molecular weight) on TOR

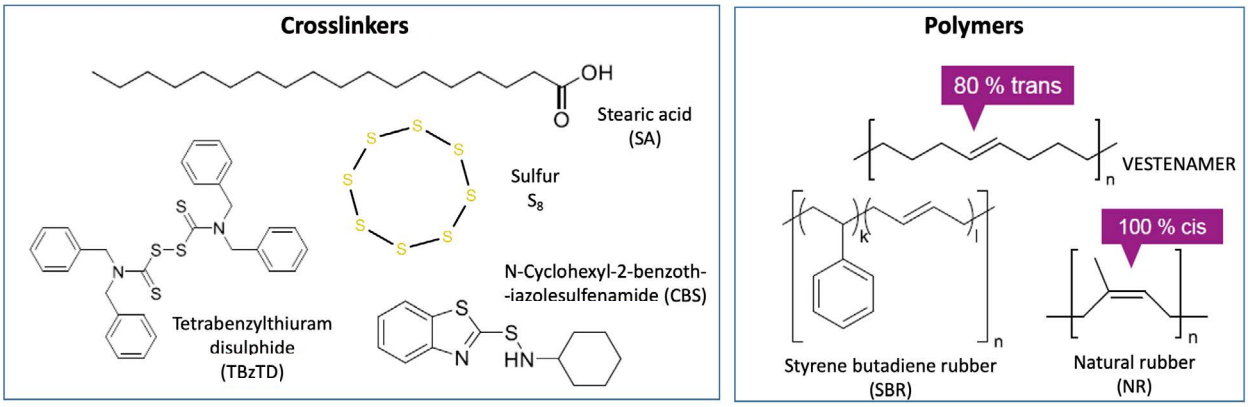

Figure 1. Structures of crosslinkers and polymers used in simulations.[1]

Results

The computational approach revealed new insights into the compatibility of various polymers/crosslinkers and provided an accurate evaluation of the structural and thermophysical properties of TOR systems as summarized to the right. The work serves as an example of how digital molecular simulations can provide unique insights that are not readily available or economical to study in an experimental setting.

The simulation methods and workflows presented in this work can be easily extended to study other polymer/crosslinker systems.

Summary

- The miscibility order for the crosslinkers in SBR, NR, and TOR is TBzTD > SA > CBS > S8, suggesting S8 likely has a limited miscibility in all three polymers, which is also demonstrated by computing the energy of mixing
- Crosslinkers diffuse more in TOR when compared to SBR and NR allowing for better crosslinking
- SBR, NR, and TOR are likely not miscible with each other. A mixture of these three polymers would most likely result in a three-phase system, which is in line with experimental studies
- Interaction energy and density analysis indicated ideal mixing at low crosslinker concentration for all the mixtures
- TOR macrocycles can potentially affect the viscosity as well as other mechanical properties, and may contribute to lower glass transition temperature of TOR

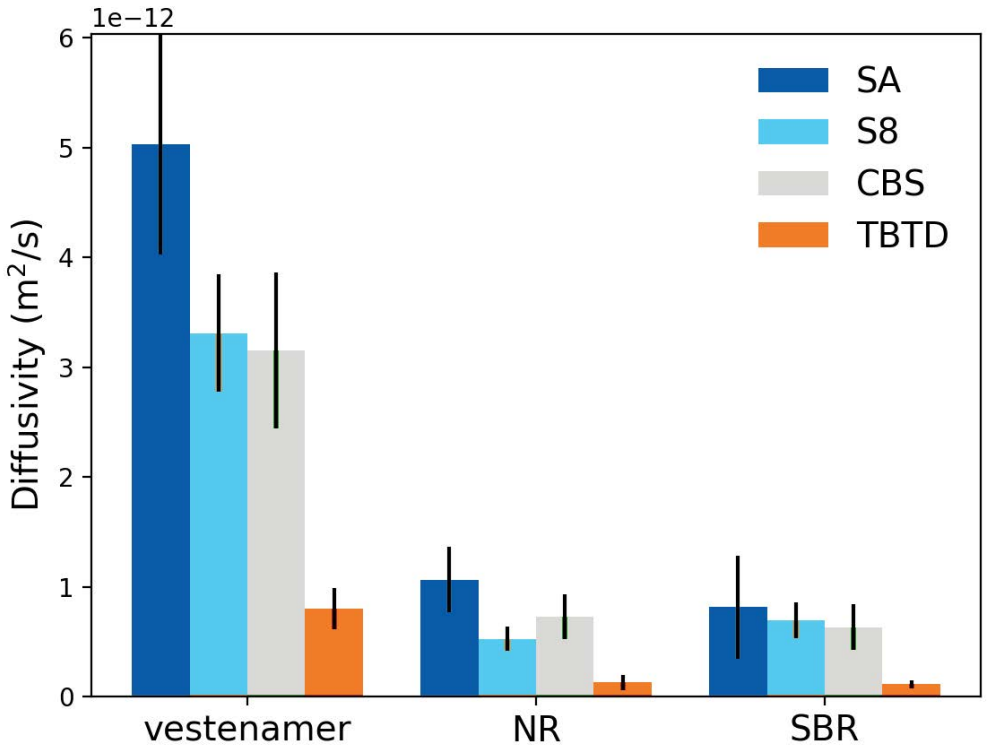

Figure 2. Predicted diffusivity of different crosslinkers in TOR, NR, and SBR

References

1. Using molecular simulation to assess the impact of additives and macrocyclic structures on trans-polyoctenamer rubber (TOR)
Mohammad Atif Faiz Afzal, Benjamin J Coscia, Andrea R Browning, Thomas S. Asche, Alexander Paasche, Mathew D. Halls
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