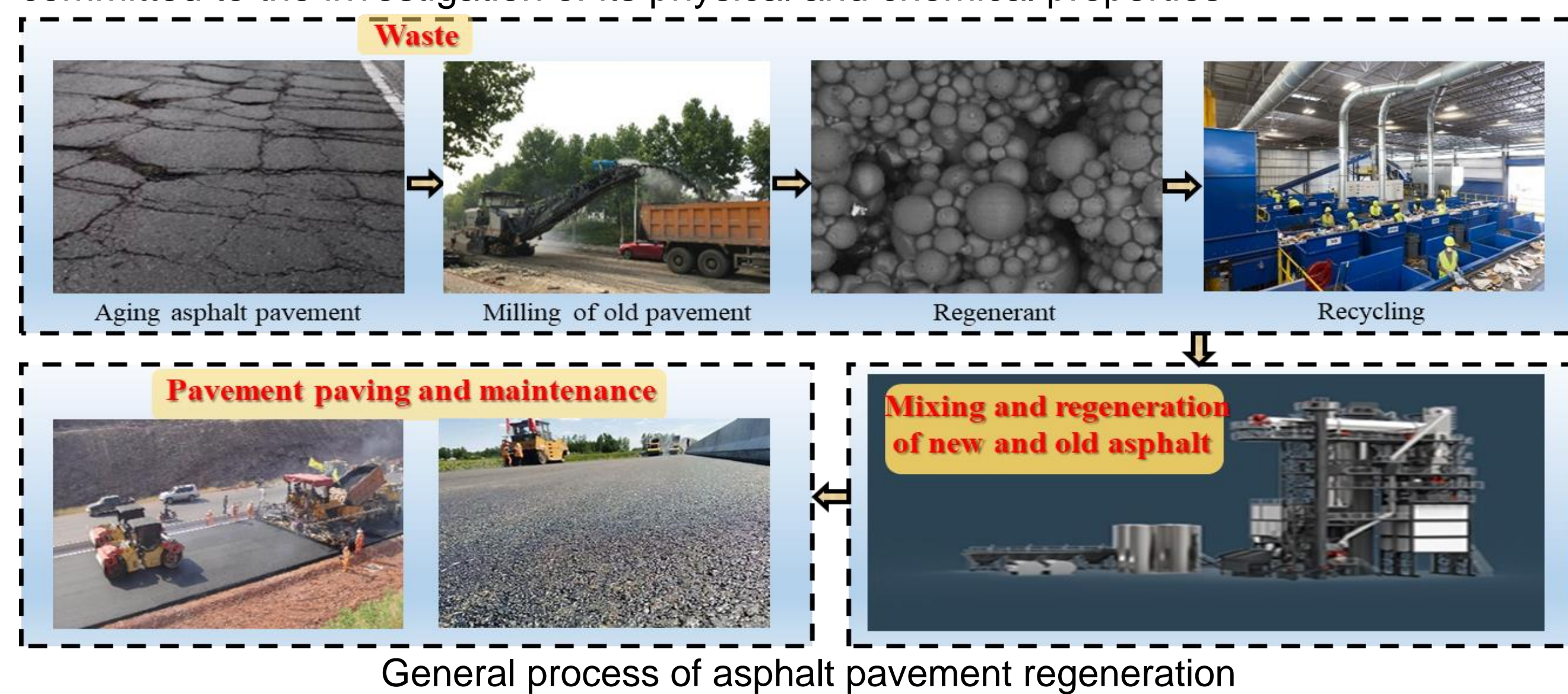


Abstract

The reuse of reclaimed asphalt pavement (RAP) in hot mixed asphalt by means of decrease nature aggregates and bitumen generates environment-friendly production processes. The additive of rejuvenators has the potential to improve the new mixture property as well as allowing a significant increase of RAP reportion.

Background

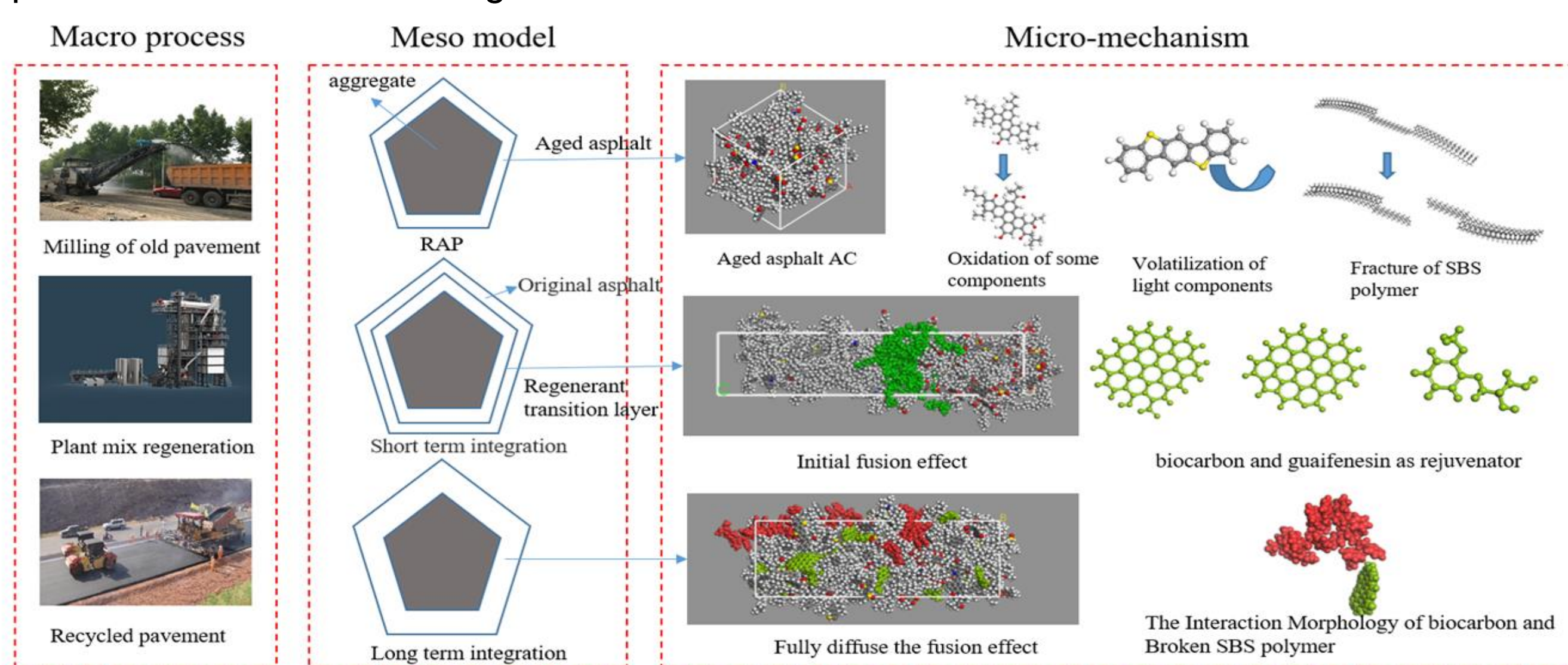
Asphalt pavement is favorably utilized in highway and urban road construction due to its advantages of sound wear resistance, high flatness and excellent performance. Through recent years of construction and development, due to the ever-increasing traffic load and environmental corrosion (for instance ultraviolet radiation, temperature, rain and snow), the continuously served asphalt pavement inevitably enter a maintenance stage. According to the approximate estimation of maintenance institution in US, the average amount of reclaimed asphalt pavement (RAP) produced by resurfacing and widening has reached annually 100 million tons[1]. Due to the depletion of high-quality stone resources, it can be foreseen that the recycling and reuse of RAP possess potential economic and environmental benefits. For this purpose, highway engineering researchers have launched studies on the application of RAP in asphalt mixture [2,3], and are committed to the investigation of its physical and chemical properties



Method and Feasibility

This study focuses on the diffusion of regenerant in aged asphalt. Aiming at the problems of unclear activation mechanism of regenerant on old asphalt and single evaluation scale of regeneration effect in asphalt regeneration project, molecular simulation method is used to analyze the effect of regenerant at molecular level, revealing the driving mechanism of the diffusion of modifier in aged asphalt and the factors affecting its diffusion, It is helpful to select and develop modifiers.

At present, the research on the fusion effect of new and old asphalt is at the initial stage, the evaluation system of fusion degree is not perfect, and the research scale is relatively single. As a micro simulation software, molecular dynamics is expected to provide help for further research. In this paper, molecular dynamics is used as the main research method to reveal the diffusion mechanism of regenerant from the molecular level and realize the quantitative evaluation of regeneration effect.



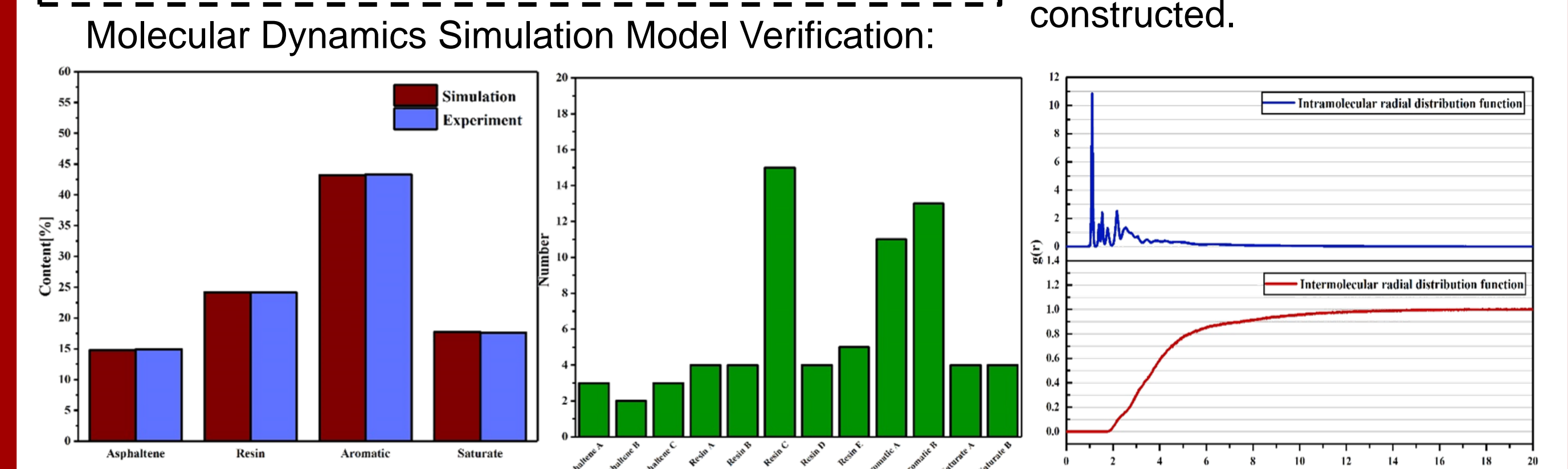
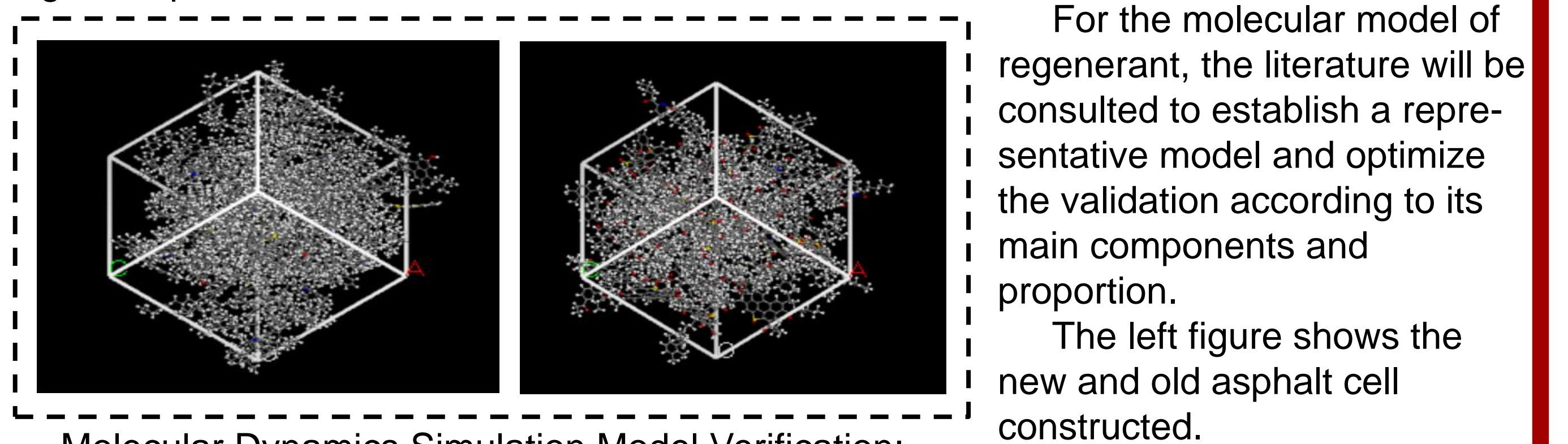
References

- [1]T. Ma, X. Huang, Y. Zhao, Y. Zhang, Evaluation of the diffusion and distribution of the rejuvenator for hot asphalt recycling, Constr. Build. Mater. 98 (2015) 530–536,
- [2]G. Xu, H. Wang, Diffusion and interaction mechanism of rejuvenating agent with virgin and recycled asphalt binder: a molecular dynamics study, Mol.Simul. 44 (2018) 1433–1443,
- [3]Liu, J., et al. (2021). "Molecular dynamics evaluation of activation mechanism of rejuvenator in reclaimed asphalt pavement (RAP) binder." Construction and Building Materials 298: 123898.

Results and Discussion

At present, the density value of AAA-1 asphalt twelve component model system proposed by Greenfield et al. is closer to the density value of real asphalt, and has been widely used in the molecular scale study of asphalt.

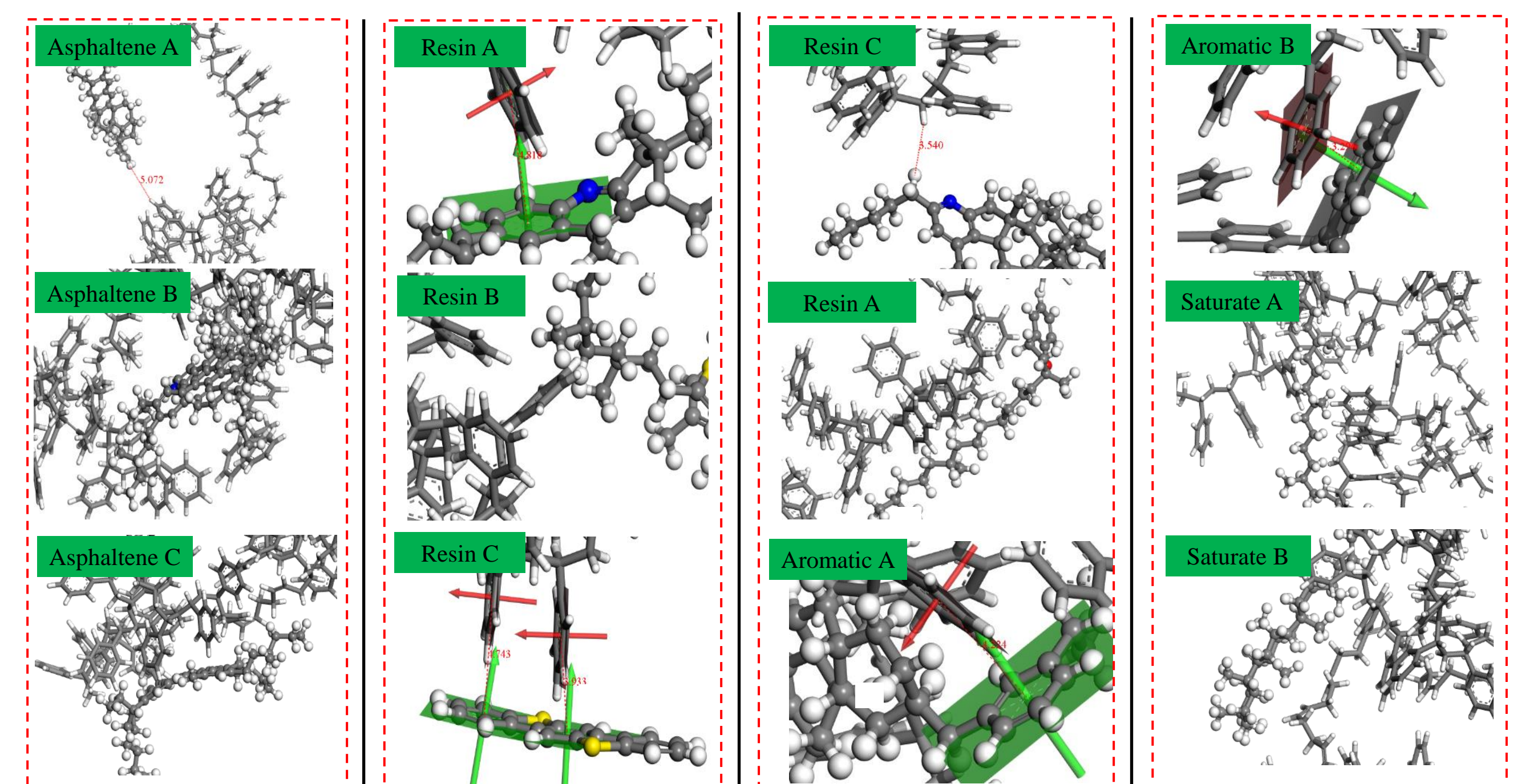
The main products of asphalt aging are sulfites and ketones. Xu et al. built aging asphalt molecules and systematically verified them. Based on this, this study built aging and original asphalt models.



The figures above are the simulated and experimental molecular weights, the molecular numbers of twelve components and the radial distribution functions, respectively.

The molecular models of the virgin asphalt and aged SBS-modified asphalt were constructed based on components collected from time-of-flight mass spectrometry experiment.

Validation of SBS modified asphalt model:



The π - π benzene ring stacking occurs between SBS and aromatic fraction and some gum molecules, and SBS is tightly entangled with saturated fraction, while the interaction with asphaltene is weak.

Conclusion

This study focuses on the diffusion of regenerant in aged asphalt. Aiming at the problems of unclear activation mechanism of regenerant on old asphalt and single evaluation scale of regeneration effect in asphalt regeneration project, molecular simulation method is used to analyze the effect of regenerant at molecular level, revealing the driving mechanism of the diffusion of modifier in aged asphalt and the factors affecting its diffusion, It is helpful to select and develop high-quality modifiers.

The results indicate that the compound rejuvenators not only able to improve the physical properties of aged SBS modified asphalt but also promote to restore the bitumen components. The interface transition zone between aged bitumen and virgin bitumen was expanded as well as the binding energy increased 15%. In considering the rejuvenating effects and cost efficiency, 0.1% biocarbon and 0.3% guaifenesin by the weight of RAP is optimized as the proposed compound rejuvenator.

Since the composition of asphalt and the rejuvenation process are quite complex, this paper only provides a preliminary theoretical explanation at molecular scale of the activation mechanism of rejuvenators on RAP asphalt. It is foreseeable that whether the original structure of aged asphalt can be restored is critical for evaluating the rejuvenation, although the rejuvenators in the engineering applications may not be composed of a single component as assumed in this work.