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Multi-scale understanding the rejuvenation efficiency and mechanism of different rejuvenators in aged bitumen for RAP reusing

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2022/11/10

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Support from:

TU Delft Delft University of Technology

Rijkswaterstaat Ministry of Infrastructure and Water Management

Contents

I. Background introduction

Reclaimed asphalt pavement (RAP) is the removed pavement materials containing bitumen and aggregates.

Asphalt pavement distresses

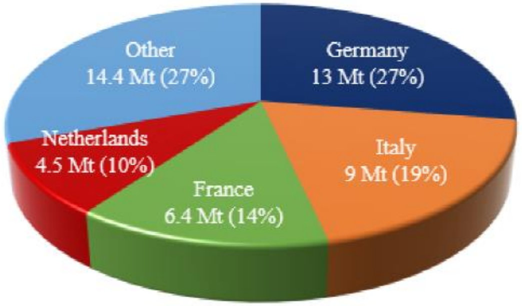
Repair/Reconstruct

Result

Reuse

New asphalt road

Production of RAP materials

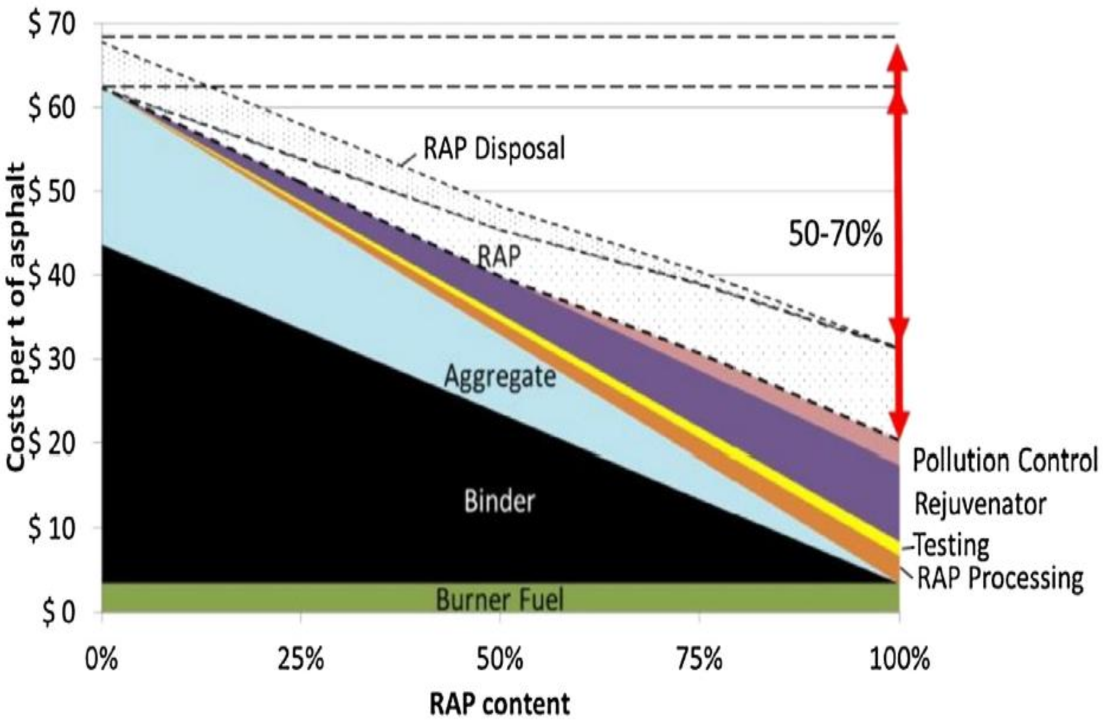


RAP amount per year in Europe

I. Background introduction

Recycling benefits of the sustainable pavement

Material related costs of virgin and 100% RAP mixtures



Environmental

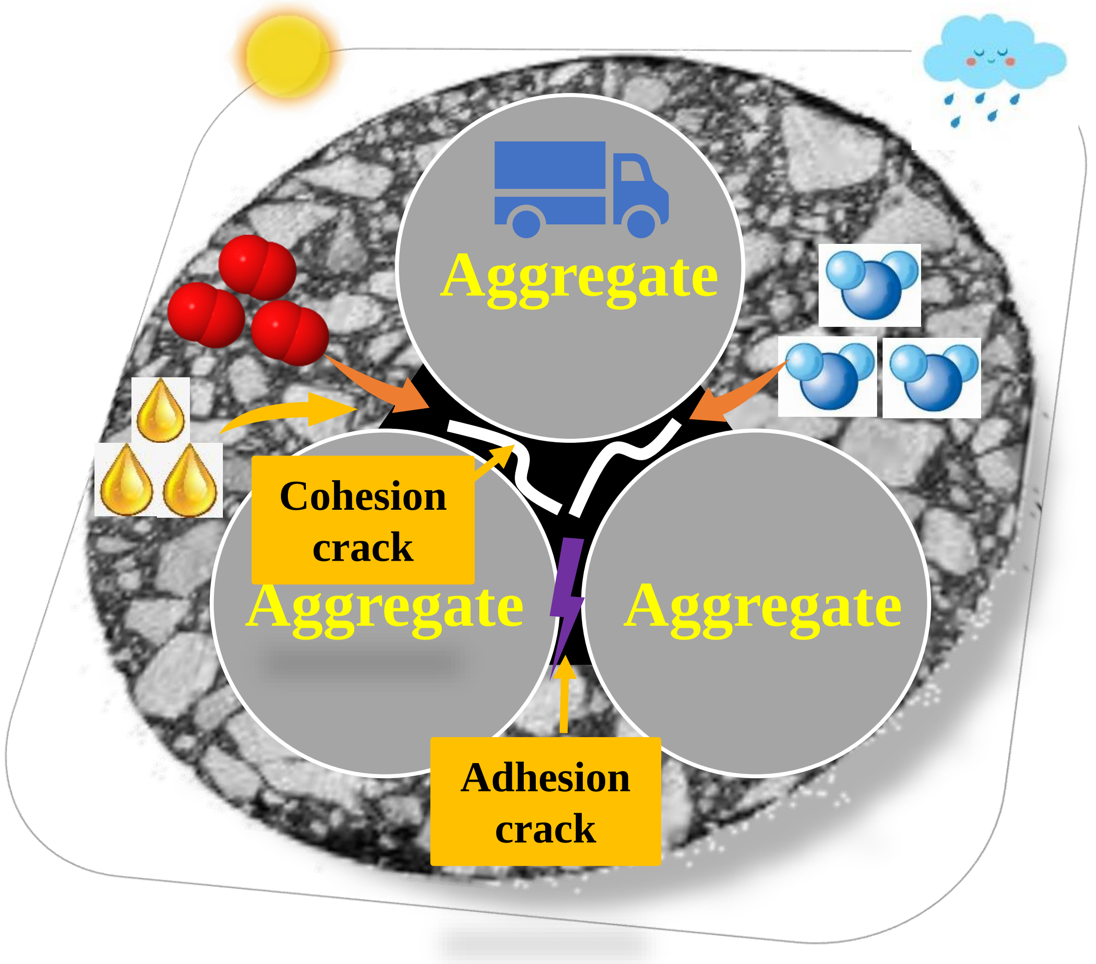
- Reduce the pavement construction **cost**
- Improve the **mechanical properties** (rutting resistance) of pavement

Economical

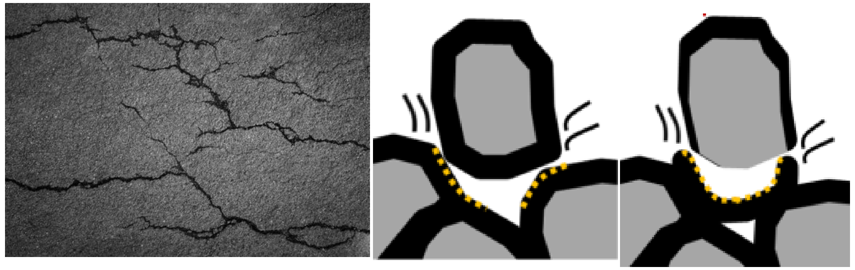
- Reduce emissions and fuel usage
- Cut down the demand on non-renewable resources
- Save landfill space for disposal of RAP

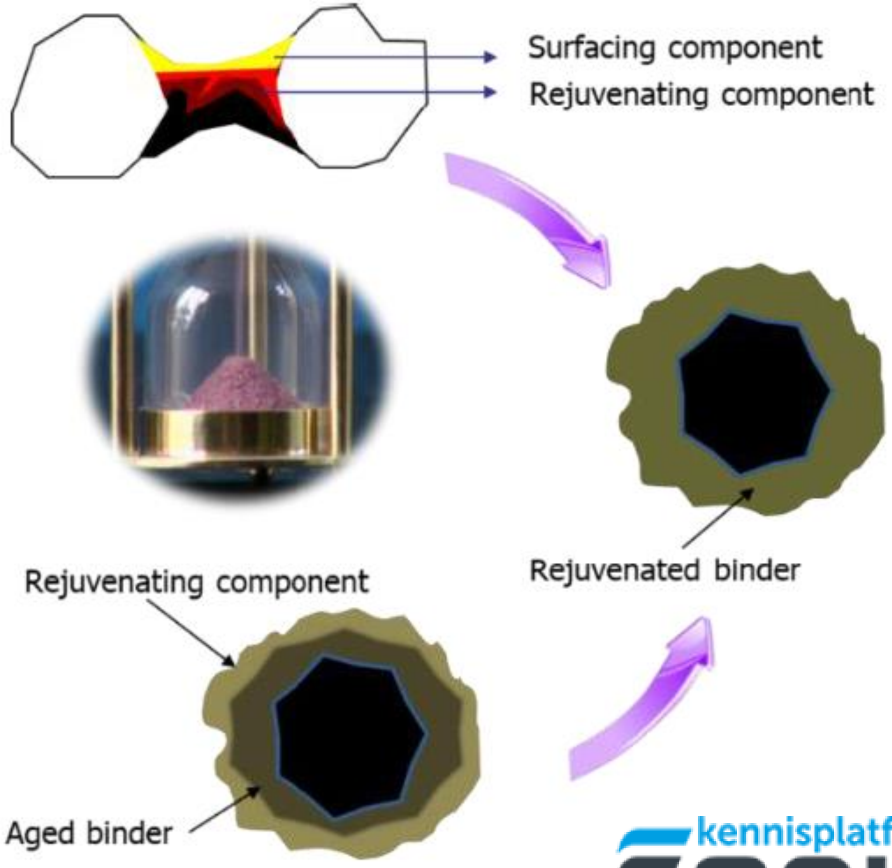
I. Background introduction

What happens of asphalt road during its service life ?



Rejuvenation





I. Background introduction

Binder level

Can the rejuvenator totally restore the performance of aged bitumen to the virgin bitumen ?

Elixir !!!

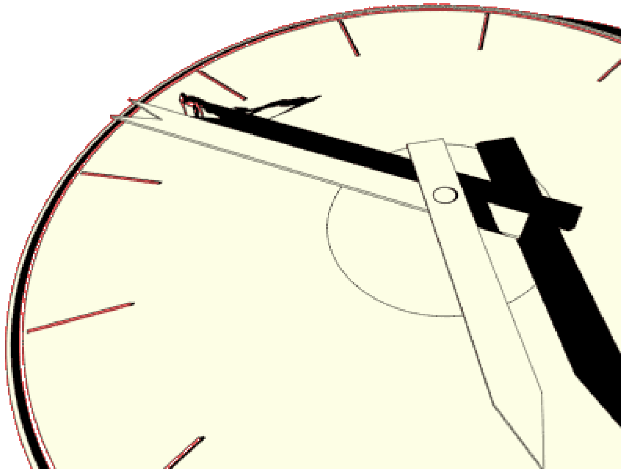
Rejuvenator

Aged bitumen

Virgin bitumen

Expectation

- High temperature rutting and deformation resistance
- Low temperature cracking resistance
- Fatigue resistance
- Adhesion performance (including moisture resistance)
- Aging resistance
- Self-healing performance
- Workability



Do U believe that one rejuvenator can restore all performance of all aged bitumen from RAP?

Heavy load !

I. Background introduction

Sample diversity

Mechanism uncertainty

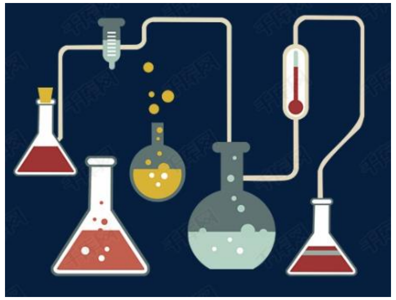
Disease diversity

Solution diversity

Selection basis ?

Different aged bitumen

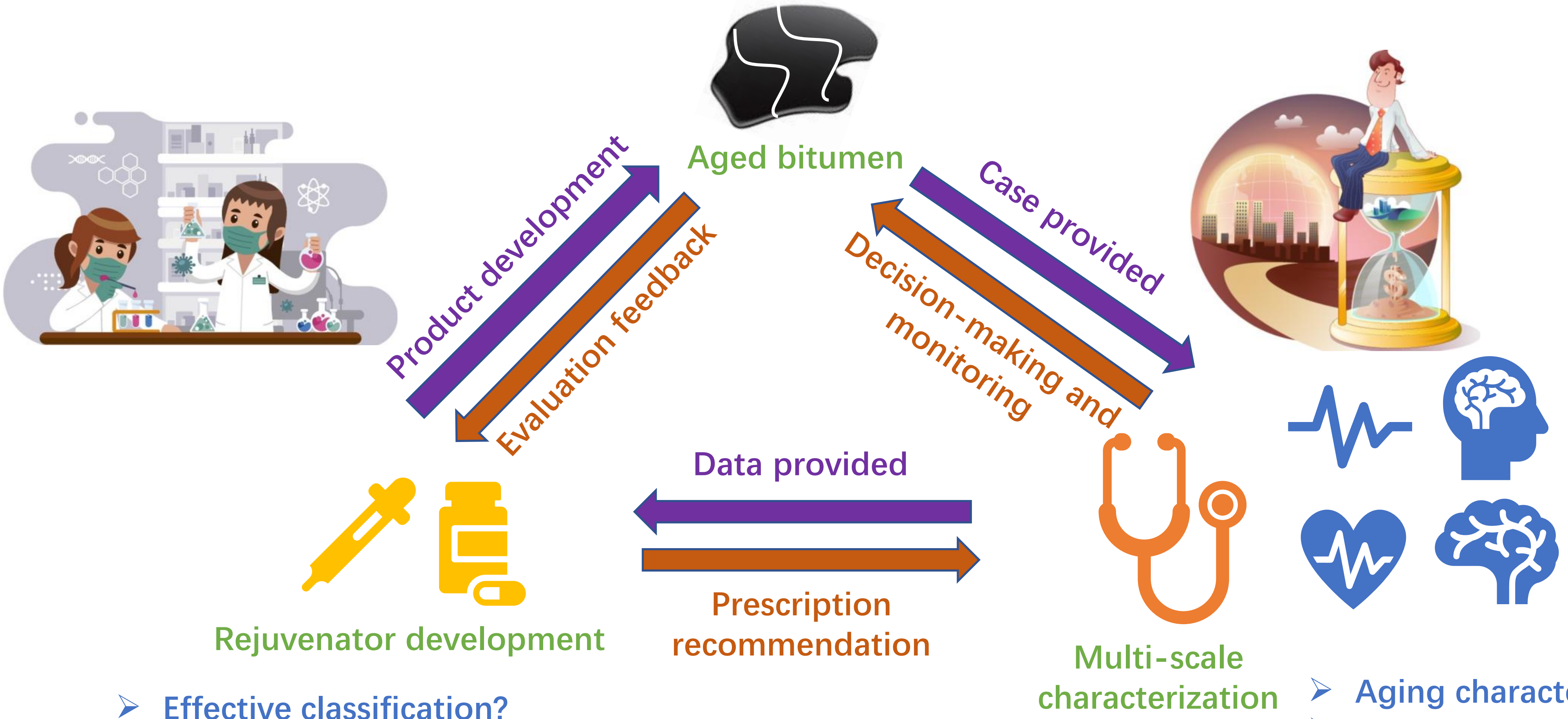
Different rejuvenators



Novel rejuvenator development

I. Background introduction

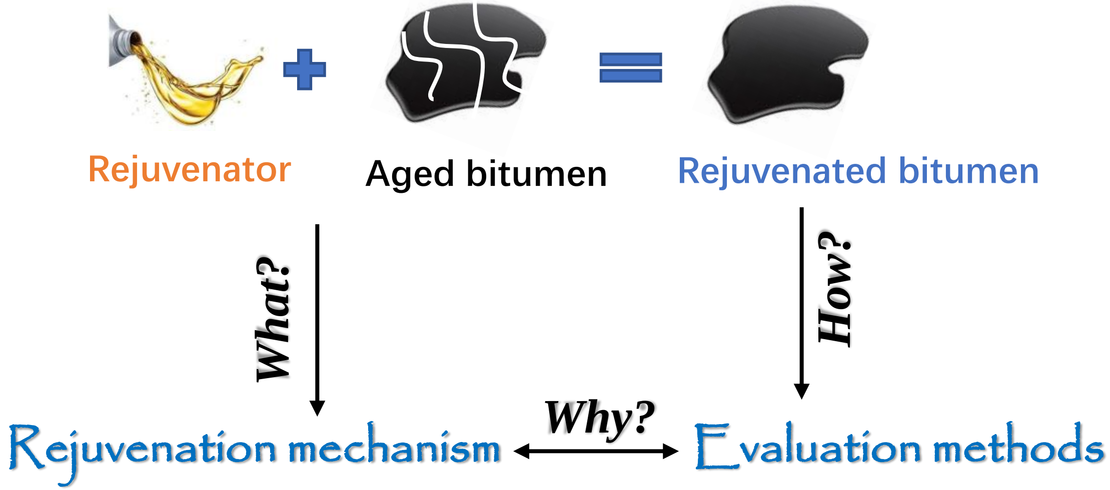
How to effectively evaluate the rejuvenation efficiency and develop high-performance rejuvenators ?



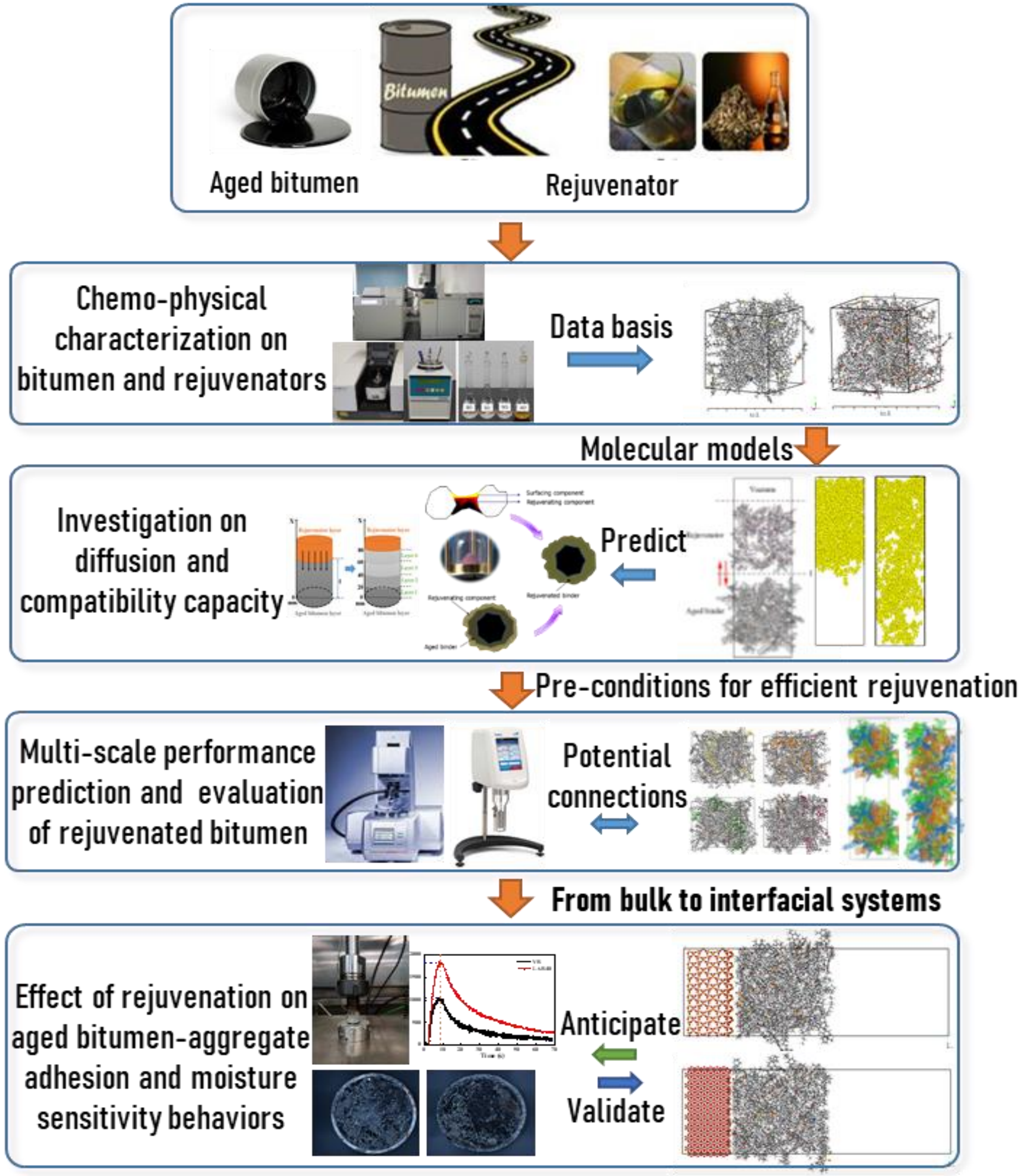
- Effective classification?
- Mechanism explanation?
- Novel rejuvenator development?

- Aging characteristics?
- Distress type and ranking?
- Prescription?

II. Research objective and scheme

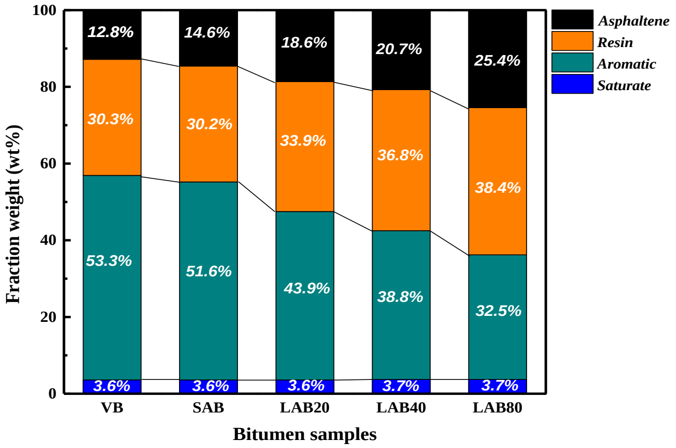


The main objective is the multiscale investigation of the rejuvenation mechanism to develop the advanced evaluation methods for rejuvenated bitumen binder.

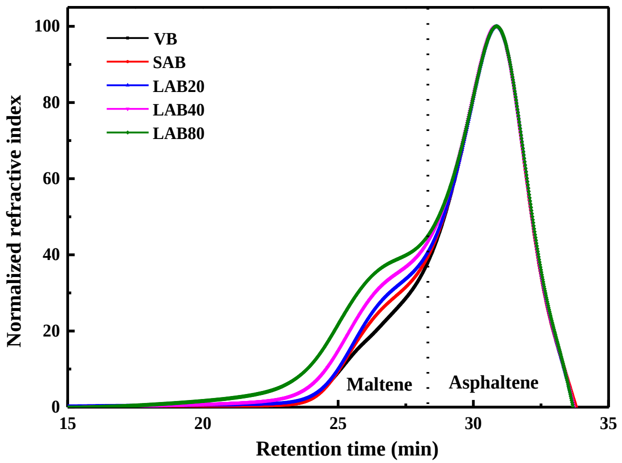


III. Chemo-physical characterizations on aged bitumen and rejuvenators

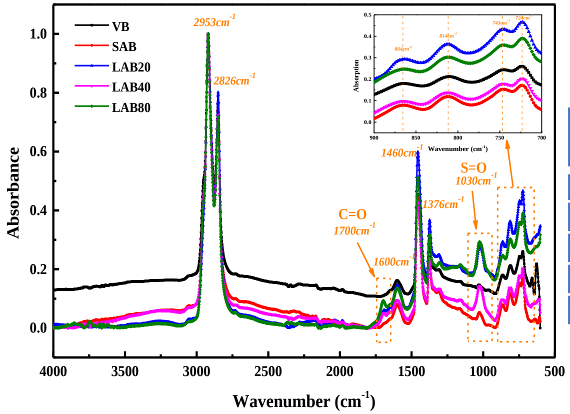
Selected bitumen: 70/100 fresh bitumen from Total energies company.
Aging levels: Virgin bitumen, Short-term aged bitumen, and Long-term aged bitumen with 1PAV, 2PAV, and 4PAV.



SARA fractions



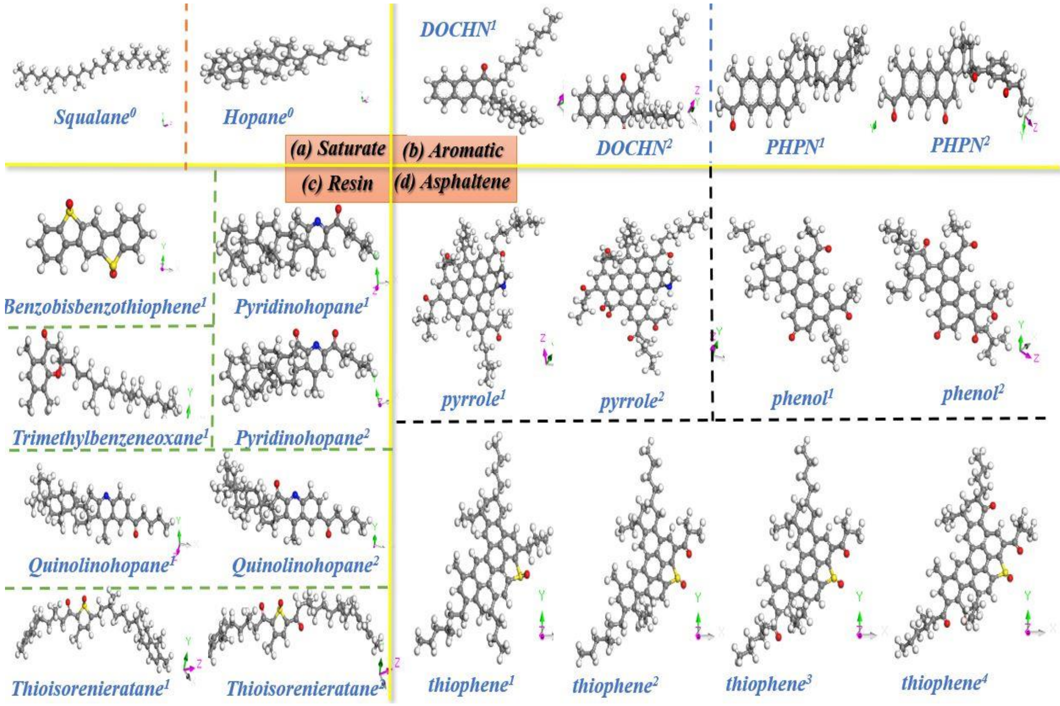
Average molecular weight



Functional group distribution

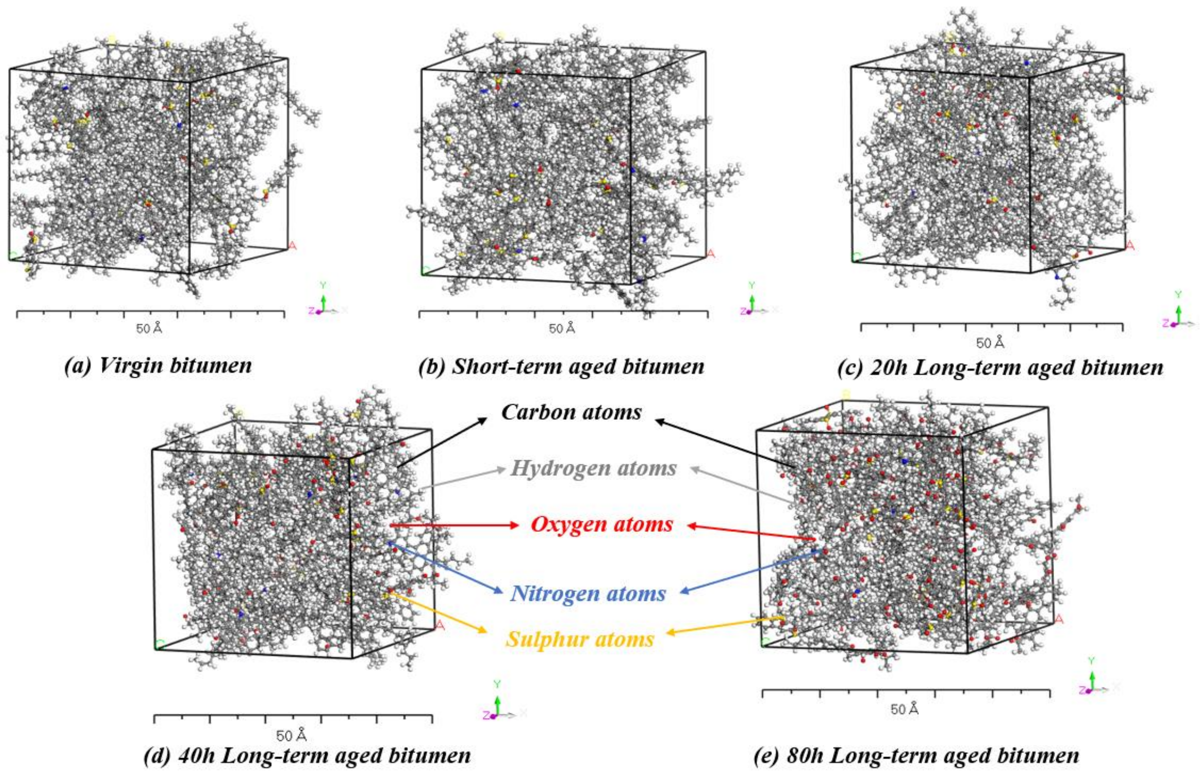
Elemental components distribution

samples	N (wt%)	C (wt%)	H (wt%)	S (wt%)	O (wt%)
VB	0.90	84.06	10.902	3.52	0.618
SAB	0.91	83.72	10.856	3.51	1.004
LAB20	0.92	83.26	10.748	3.49	1.582
LAB40	0.89	83.02	10.437	3.53	2.113
LAB80	0.91	82.14	10.098	3.54	3.312

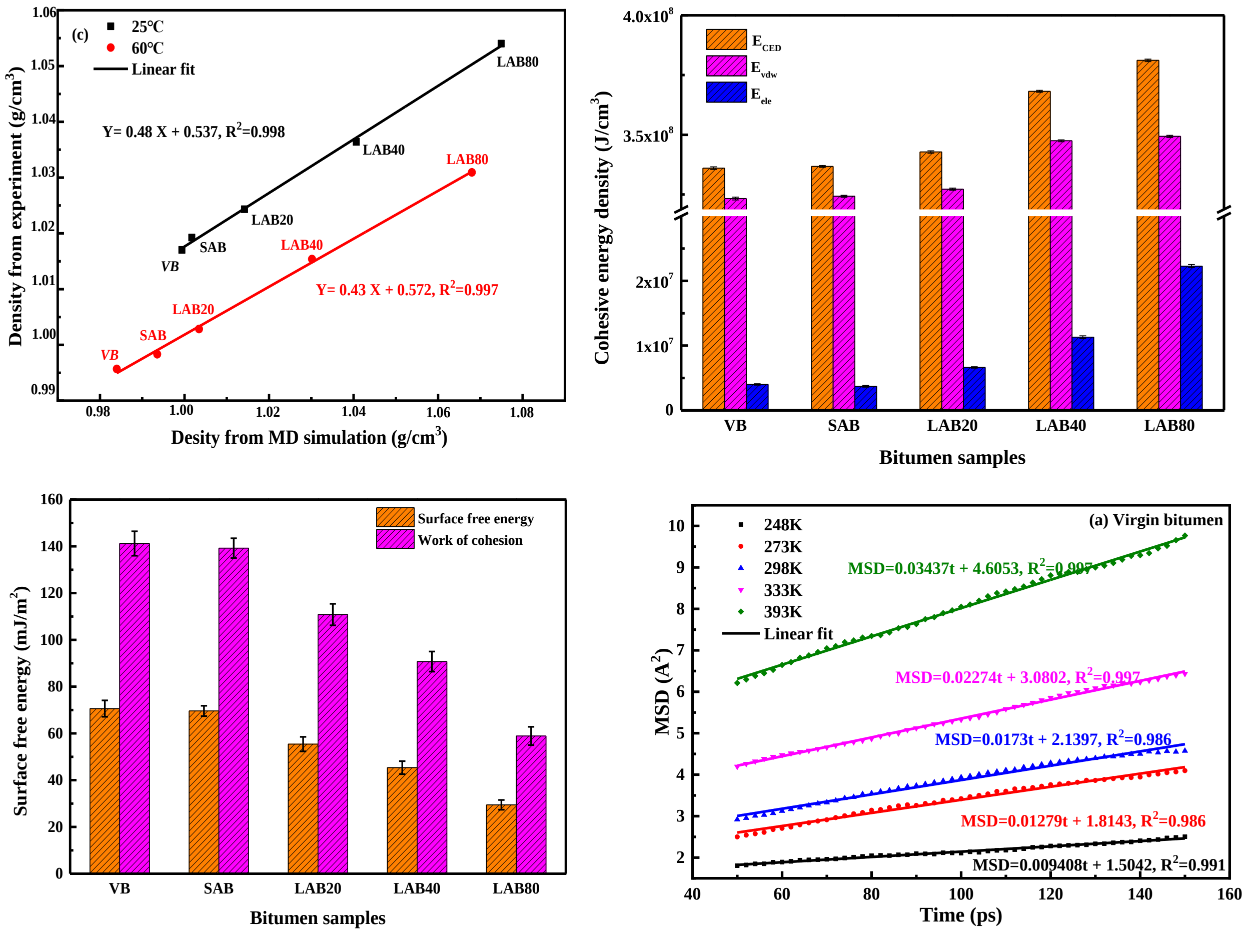


Molecular components in molecular models of virgin and aged bitumen

III. Chemo-physical characterizations on aged bitumen and rejuvenators



Molecular models of virgin and aged bitumen

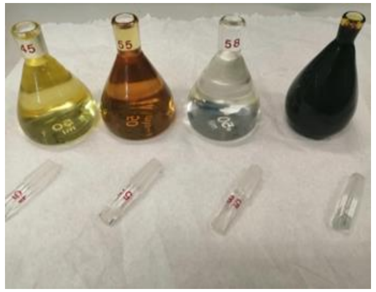


Thermodynamic parameters predicted from MD simulations

1. **Shisong Ren***, Xueyan Liu, Peng Lin, Sandra Erkens, Yue Xiao. (2021).Chemo-physical characterization and molecular dynamics simulation of long-term aging behaviors of bitumen. **Construction and Building Materials.** 302, 124437.

2. **Shisong Ren***, Xueyan Liu, Peng Lin, Sandra Erkens. (2022). Toward the long-term aging influence and novel reaction kinetics models of bitumen. **International Journal of Pavement Engineering.** 2024188, 1-16.

III. Chemo-physical characterizations on aged bitumen and rejuvenators



Selected rejuvenators:
(1) Bio-oil (BO); (2) Engine-oil (EO);
(3) Naphthenic-oil (NO); (4) Aromatic-oil (AO)

Elemental compositions in various rejuvenators.

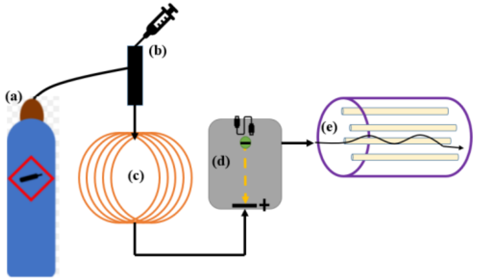
Rejuvenators	N%	C%	H%	S%	O%	H/C	O/C
Bio-oil	0.15	76.47	11.96	0.06	11.36	1.88	0.1114
Engine-oil	0.23	85.16	14.36	0.13	0.12	2.02	0.0011
Naphthenic-oil	0.12	86.24	13.62	0.1	0.1	1.90	0.0009
Aromatic-oil	0.55	88.01	10.56	0.48	0.4	1.44	0.0034

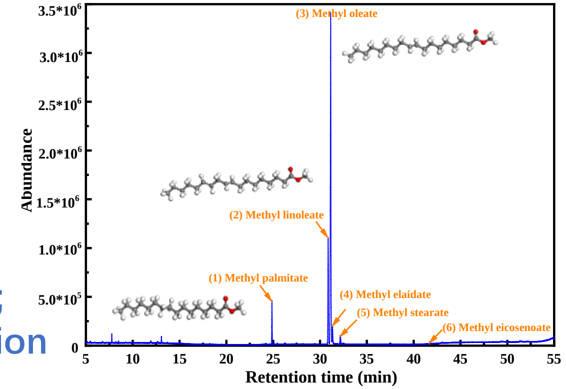
The VPO parameters and average molecular weight of various rejuvenators.

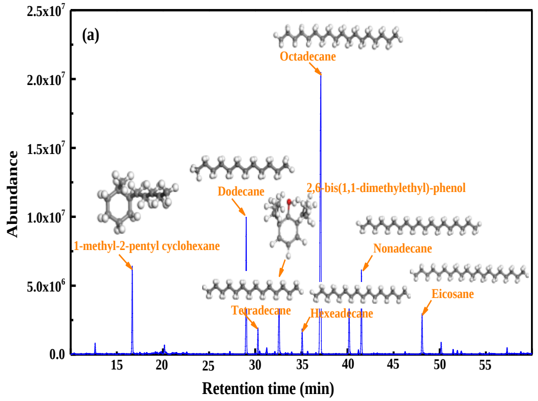
Rejuvenators	Bio-oil	Engine-oil	Naphthenic-oil	Aromatic-oil
m_r (g)	0.0654	0.0577	0.1234	0.0710
m_s (g)	21.3250	23.0800	22.4384	11.8334
v/c	240	180	377	350
c (mol/kg)	0.01026	0.00788	0.0157	0.01463
Mn (g/mol)	286.43	316.48	357.06	409.99

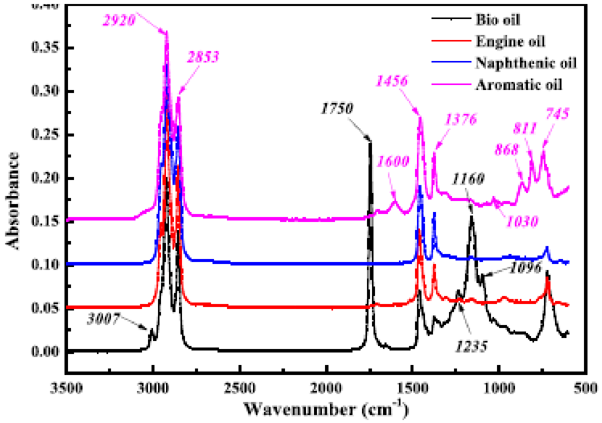
Element analysis;
Average molecular weight;
Functional group distribution

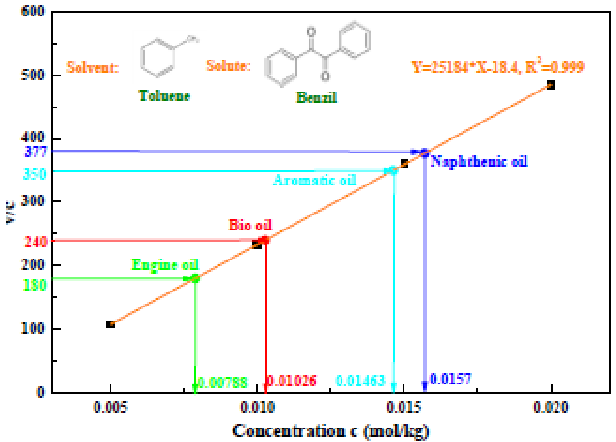
GC-MS test

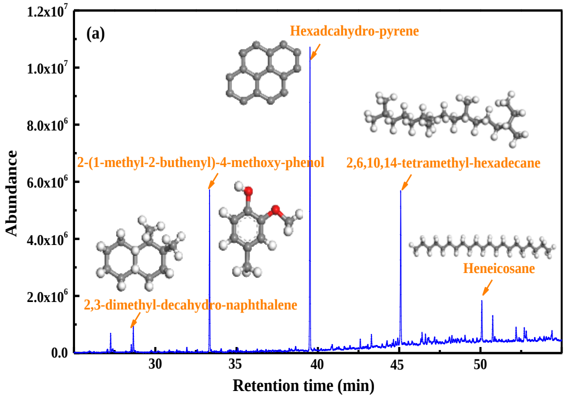


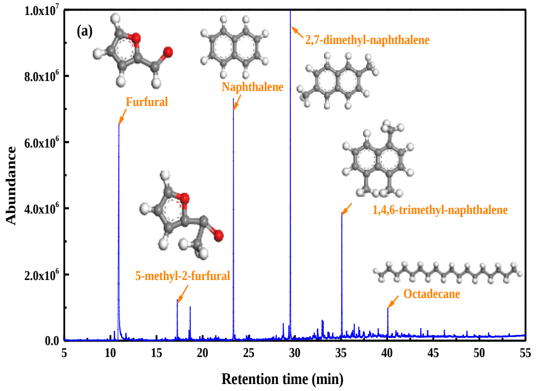






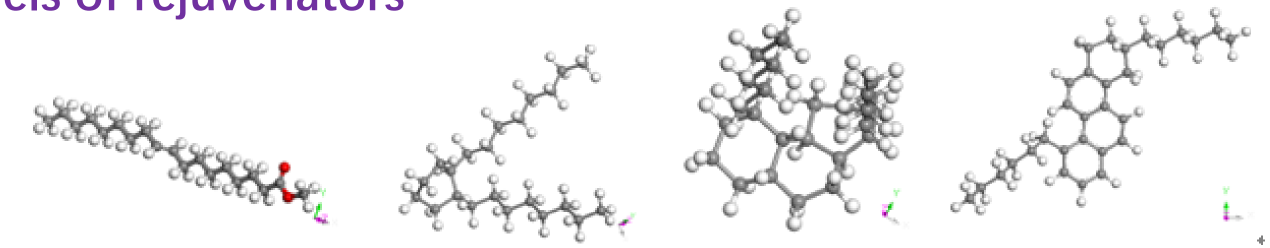






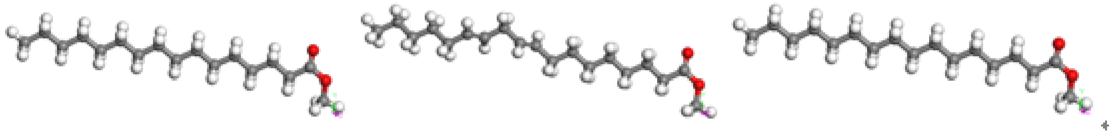
III. Chemo-physical characterizations on aged bitumen and rejuvenators

(a) Average molecular models of rejuvenators



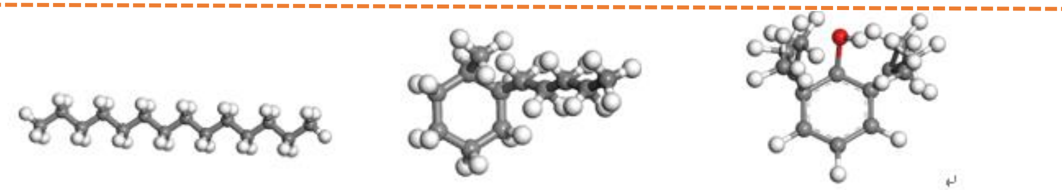
(a) Bio-oil (b) Engine-oil (c) Naphthenic-oil (d) Aromatic-oil

(b) Multi-component molecular models of rejuvenators

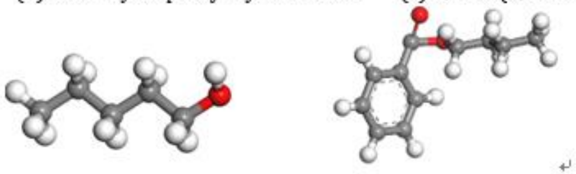


(a) Methyl palmitate (b) Methyl linoleate (c) Methyl oleate

(1) Bio-oil rejuvenator

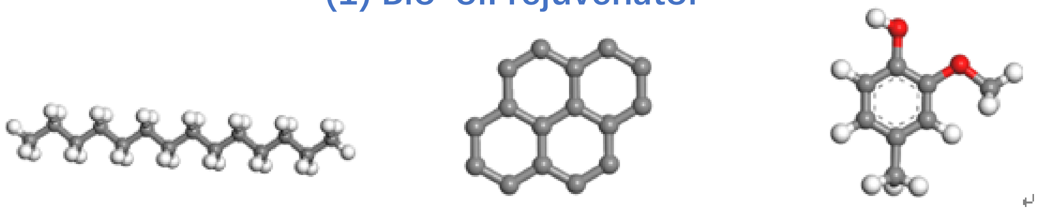


(a) Tetradecane (b) 1-methyl-2-pentyl-cyclohexane (c) 2,6-bis(1,1-dimethylethyl)-phenol



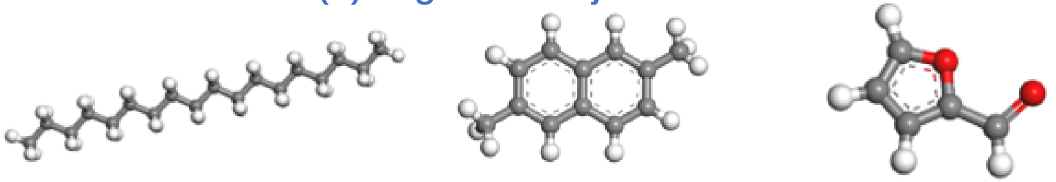
(d) 1-pentanol (e) Butyl benzoate

(2) Engine-oil rejuvenator



(a) Tetradecane (b) Hexadecahydro pyrene (c) 2-methoxy-4-methyl phenol

(3) Naphthenic-oil rejuvenator



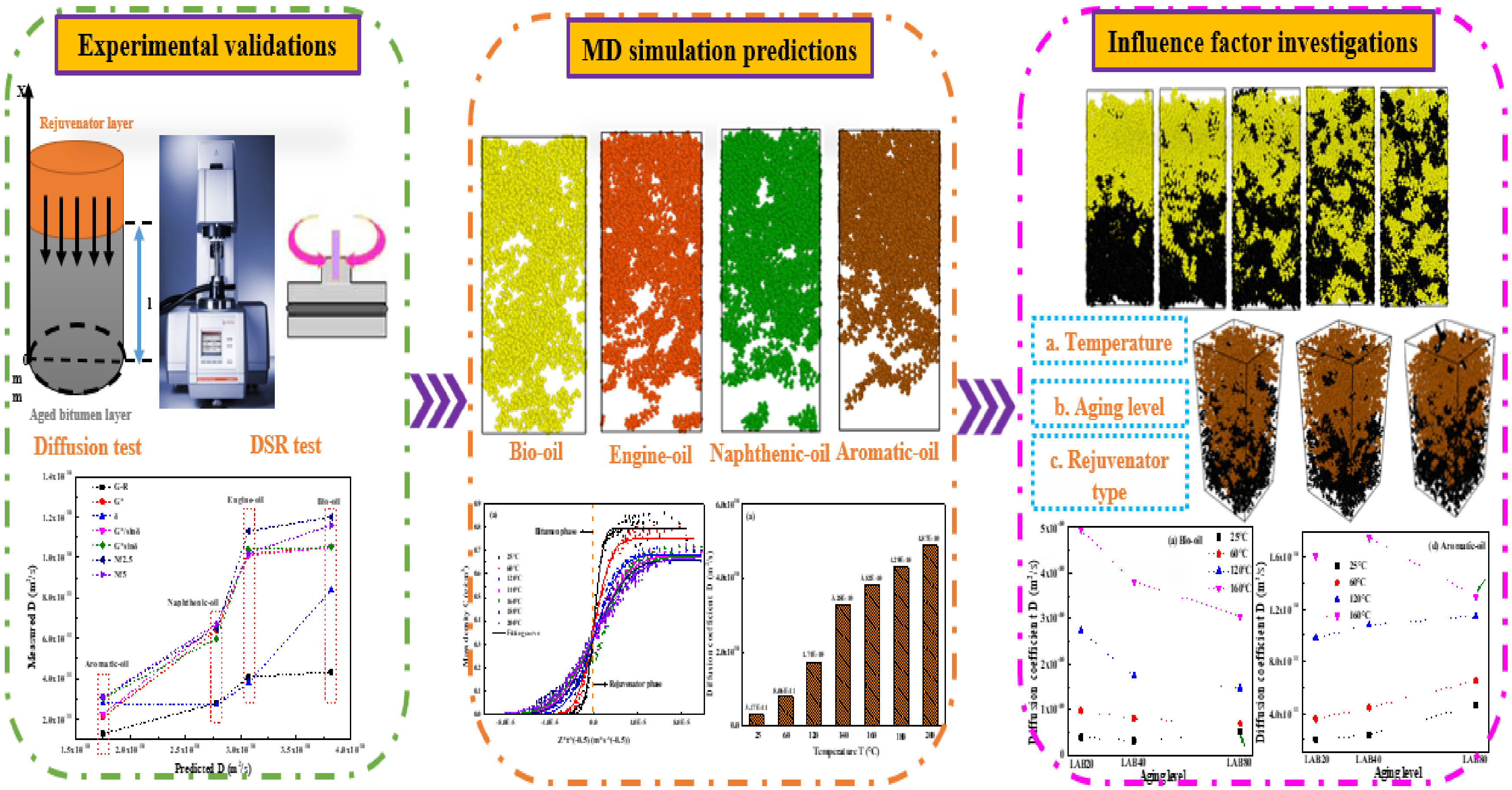
(a) Octadecane (b) 2,7-dimethyl naphthalene (c) Furfural

(4) Aromatic-oil rejuvenator

1. **Shisong Ren*,** Xueyan Liu, Peng Lin, Sandra Erkens, Yangming Gao. (2022). Chemical characterizations and molecular dynamics simulations on different rejuvenators for aged bitumen recycling. **Fuel.** 124550.

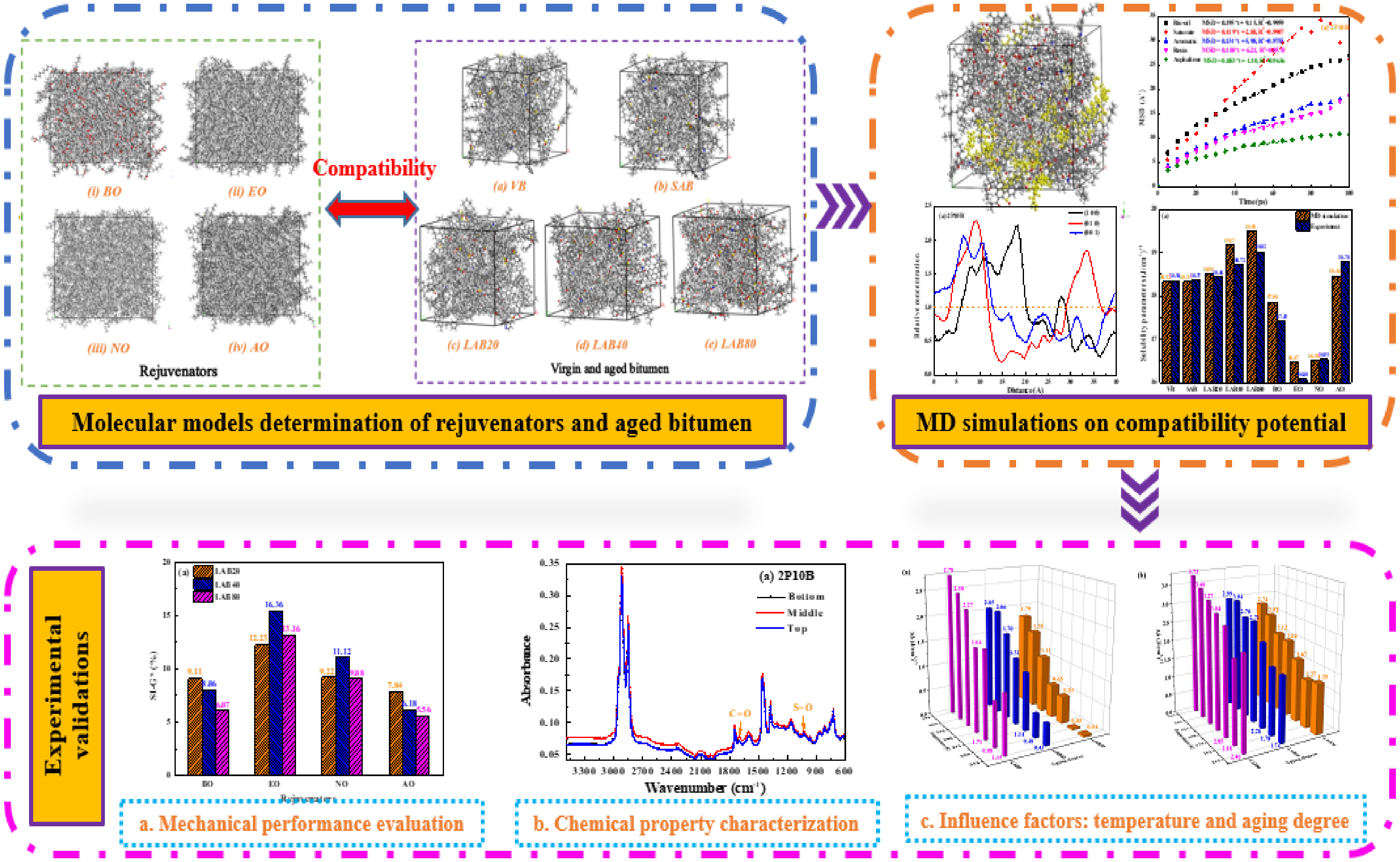
2. **Shisong Ren*,** Xueyan Liu, Sandra Erkens, Peng Lin, Yangming Gao. (2022). Multi-component analysis, molecular model construction, and thermodynamics performance prediction on various rejuvenators of aged bitumen. **Journal of Molecular Liquids.** 119463.

IV. Investigation on diffusion and compatibility behaviors



- At an atomic scale, the mutual but partial interfacial diffusion behaviors between the rejuvenators and the aged bitumen molecules are observed.
- The magnitude of diffusion coefficient D of four rejuvenators varies from 10^{-11} - 10^{-10} m^2/s, which strongly depends on the rejuvenator type, temperature, and bitumen aging levels.
- The order for diffusive capacity of four rejuvenators is BO > EO > NO > AO. The experimental results in both the magnitude and order of D parameters agree well with the MD simulation outputs

IV. Investigation on diffusion and compatibility behaviors

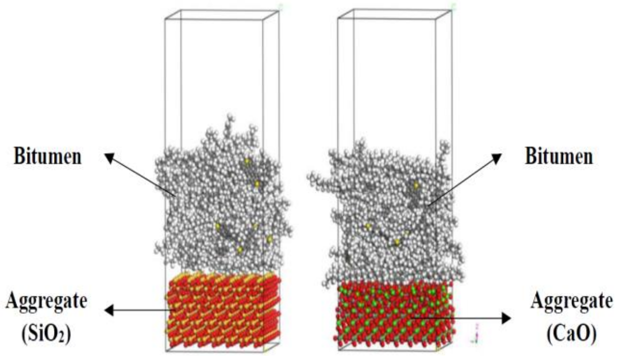


- The ranking on predicted compatibility and experimentally measured thermal stability for four rejuvenators is the same as AO > BO > NO > EO.
- The thermodynamic parameters of solubility parameter difference Δδ, Flory-Huggins parameter χ, and mixing free energy ΔGm are efficient to estimate the compatibility potential of various rejuvenators with aged bitumen.
- At the molecular scale, the compatibility and thermal stability issues between rejuvenators and aged bitumen are complicated and related to different aspects of the intermolecular interaction, dispersion degree, and molecular mobility.

1. **Shisong Ren***, Xueyan Liu, Peng Lin, Yangming Gao, Sandra Erkens. (2022). Insight into the compatibility behaviors between various rejuvenators and aged bitumen: Molecular dynamics simulation and experimental validation. Materials & Design. 2022. 223, 111141.

V. Bitumen-aggregate interface adhesion

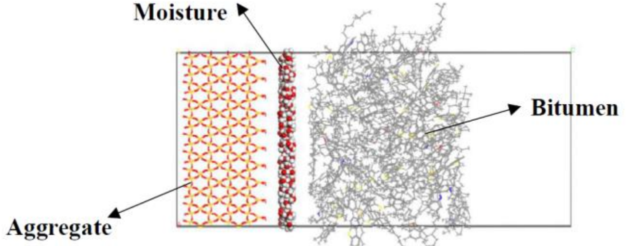
(1) MD simulation method



Adhesion energy (Work of adhesion):

$$W_{BM} = \Delta E_{BA}/A$$

$$W_{dry} = W_{BA} = (E_B + E_A - E_{BA})/A$$

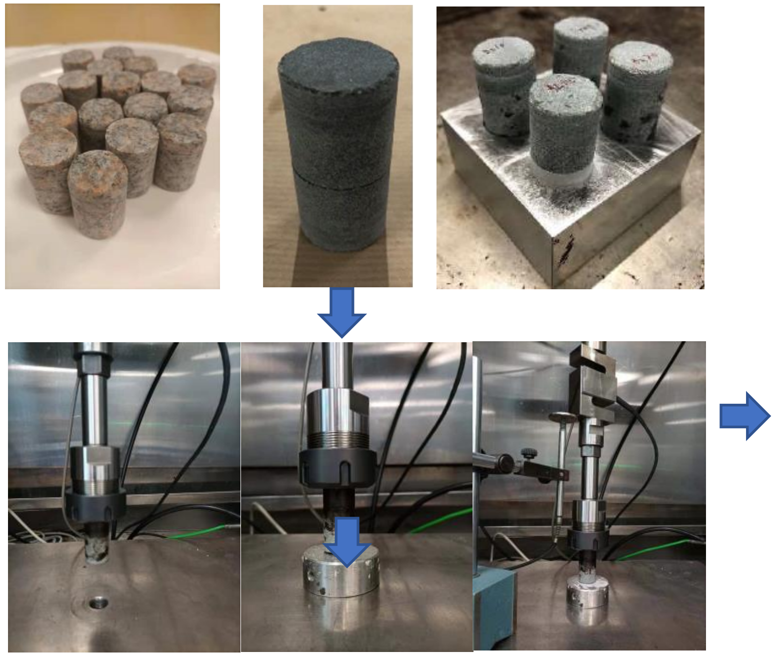


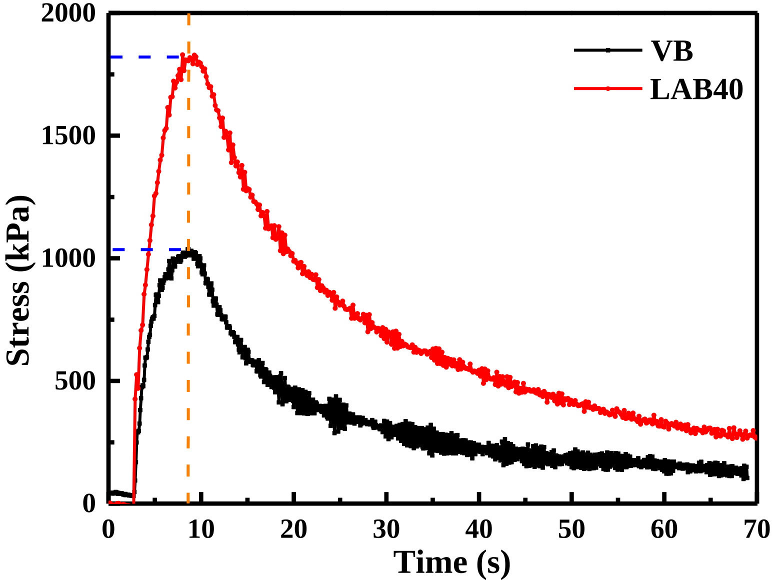
Moisture susceptibility (Work of debonding):

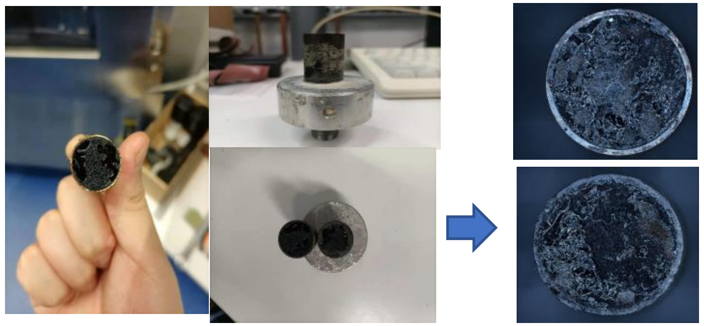
$$W_{wet} = (E_{BA} - E_{AM} - E_{BM})/A$$

$$R_{AD} = (W_{dry} - W_{wet})/W_{dry}$$

(2) Experimental method







Influence factors:

- Temperature;
- Aggregate type;
- Rejuvenator type and dosage;
- Moisture (Freeze-thaw);

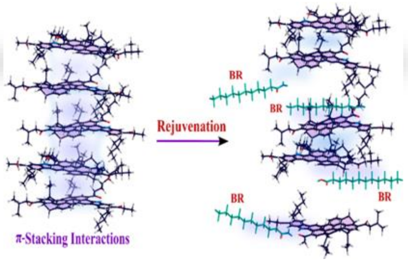
VI. Multi-scale performance prediction and evaluation on rejuvenated bitumen

Chemical characterization — *Provide parameters* → **MD simulation** ⟷ *Validation and correlation* ⟷ **Rheology and morphology**

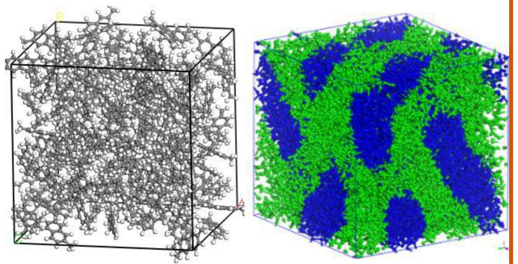
Chemical properties and components

- ***Chemical functional groups (FTIR);***
- ***SARA fractions;***
- ***Molecular weight;***
- ***Element analysis;***

Molecular structure



Agglomeration of asphaltene



Molecular model of rejuvenated bitumen

Thermodynamics and physical properties

- ***Density;***
- ***Glass transition temperature;***
- ***Surface free energy;***
- ***Work of cohesion;***
- ***Free volume;***
- ***Cohesive energy density;***
- ***Solubility parameter;***
- ***Diffusion behaviors;***
- ***Work of adhesion***

Rheological properties and microstructure

- ***Master curves of G* and δ;***
- ***Black diagram;***
- ***Viscosity and flow behaviors;***
- ***MSCR: Jnr, R%, Jnr_{diff} and R_{diff};***
- ***Rutting parameter;***
- ***Relaxation test;***
- ***LAS fatigue test;***
- ***G-R parameter;***
- ***Aging resistance;***
- ***Adhesion performance***

Rejuvenation mechanism ⟷ Evaluation method

Support from:

Delft University of Technology

Rijkswaterstaat
Ministry of Infrastructure and Water Management

Thanks!

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