

Unraveling fluid-fluid interfaces through molecular dynamics and machine learning

Dan Ni Lin

EP USP

dan_lin@usp.br

Supervisor: Prof. Dr. Caetano Miranda (IFUSP)

Collaborator: Dr. Alessandro Kirch (IFUSP e EP USP)



IFUSP
Instituto de Física da USP

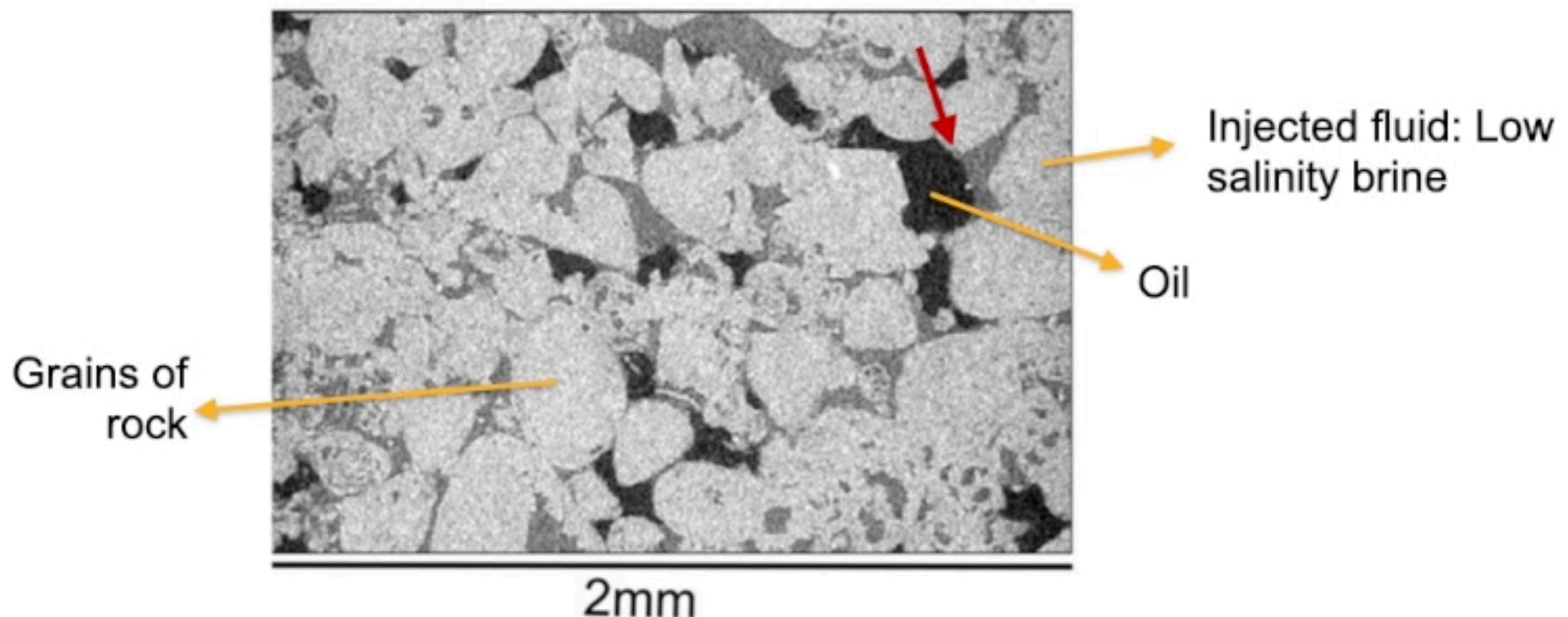


Research Centre for
Greenhouse Gas Innovation



Why study interfaces?

Microscopic level image of a porous rock containing oil



What purpose of the project?

Brine–Oil Interfacial Tension Modeling: Assessment of Machine Learning Techniques Combined with Molecular Dynamics

Alexsandro Kirch, Yuri M. Celaschi, James M. de Almeida, and Caetano R. Miranda*



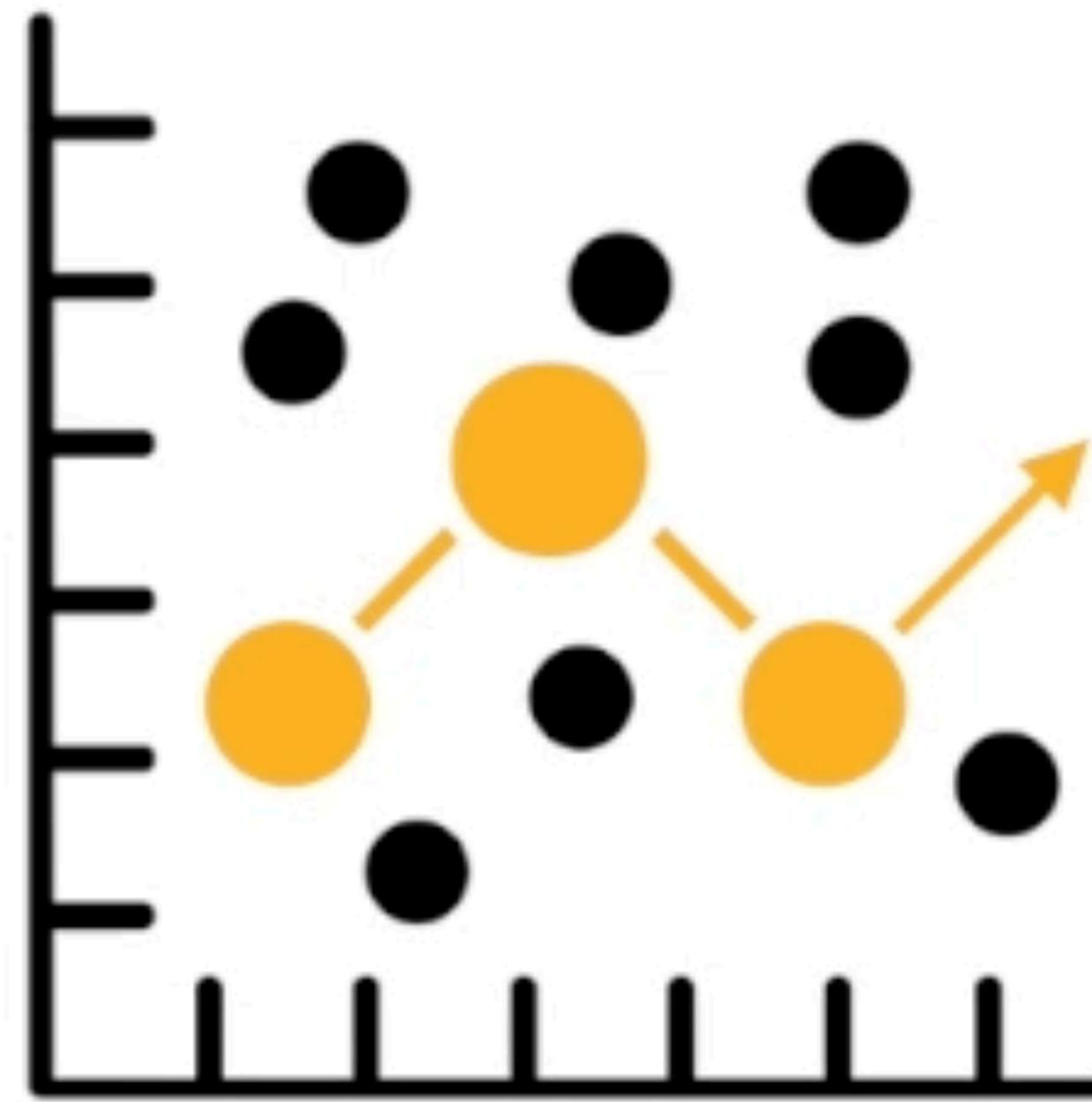
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What purpose of the project?

- ▶ Create machine learning models capable of predicting interfacial tension by correlating structural properties



Methodology and procedures

Post-processing data from
previous simulations



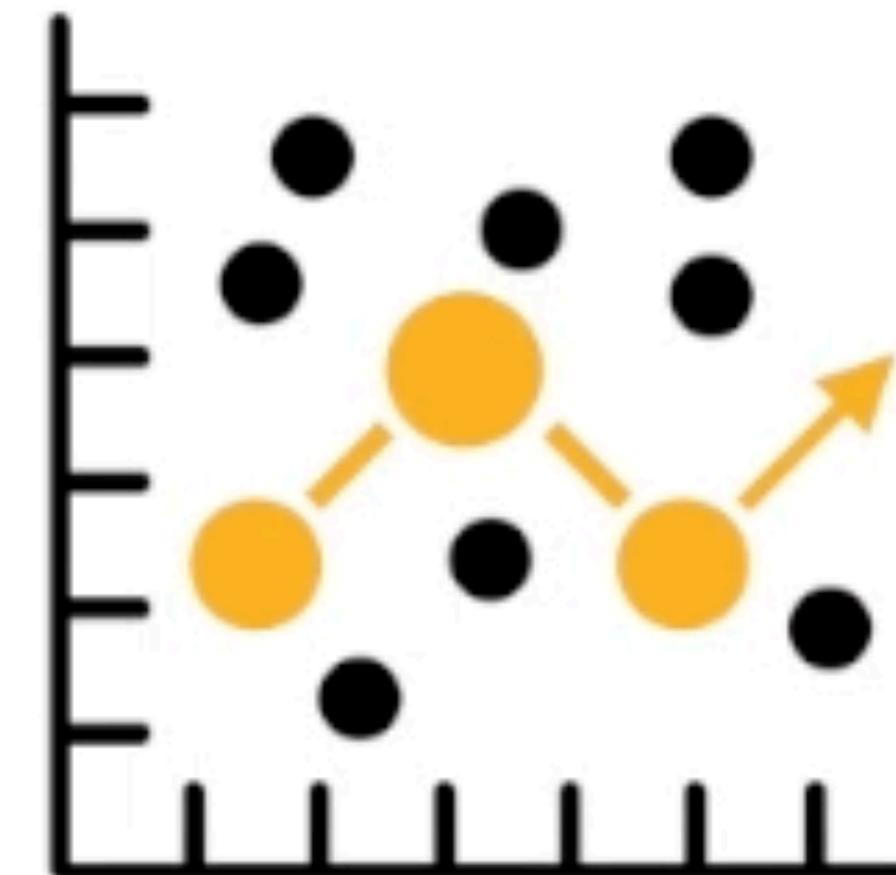
Machine Learning



Used ML methods

XG Boost and Linear
Regression

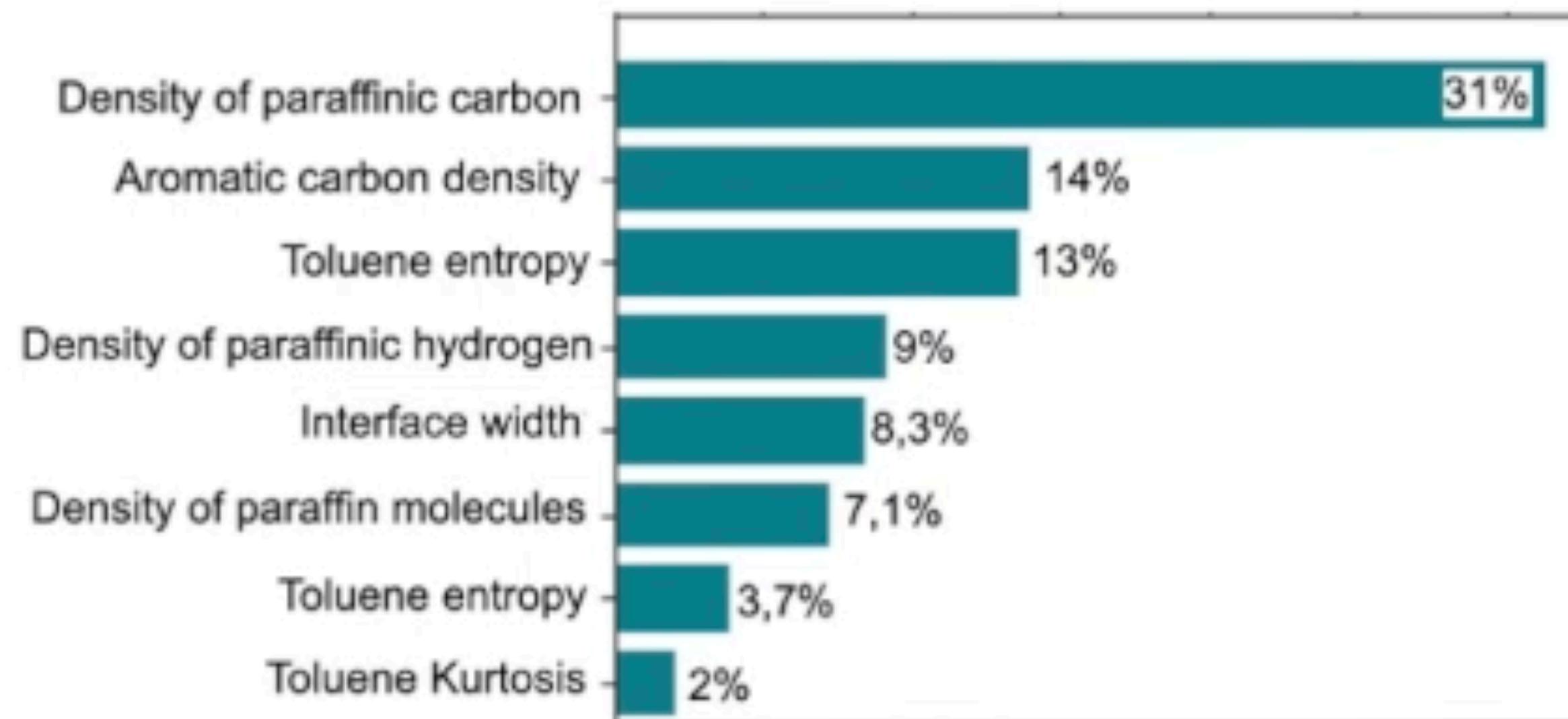
Correlation of structural
data with interfacial tension



Results and Conclusion

✓ Feature Importance

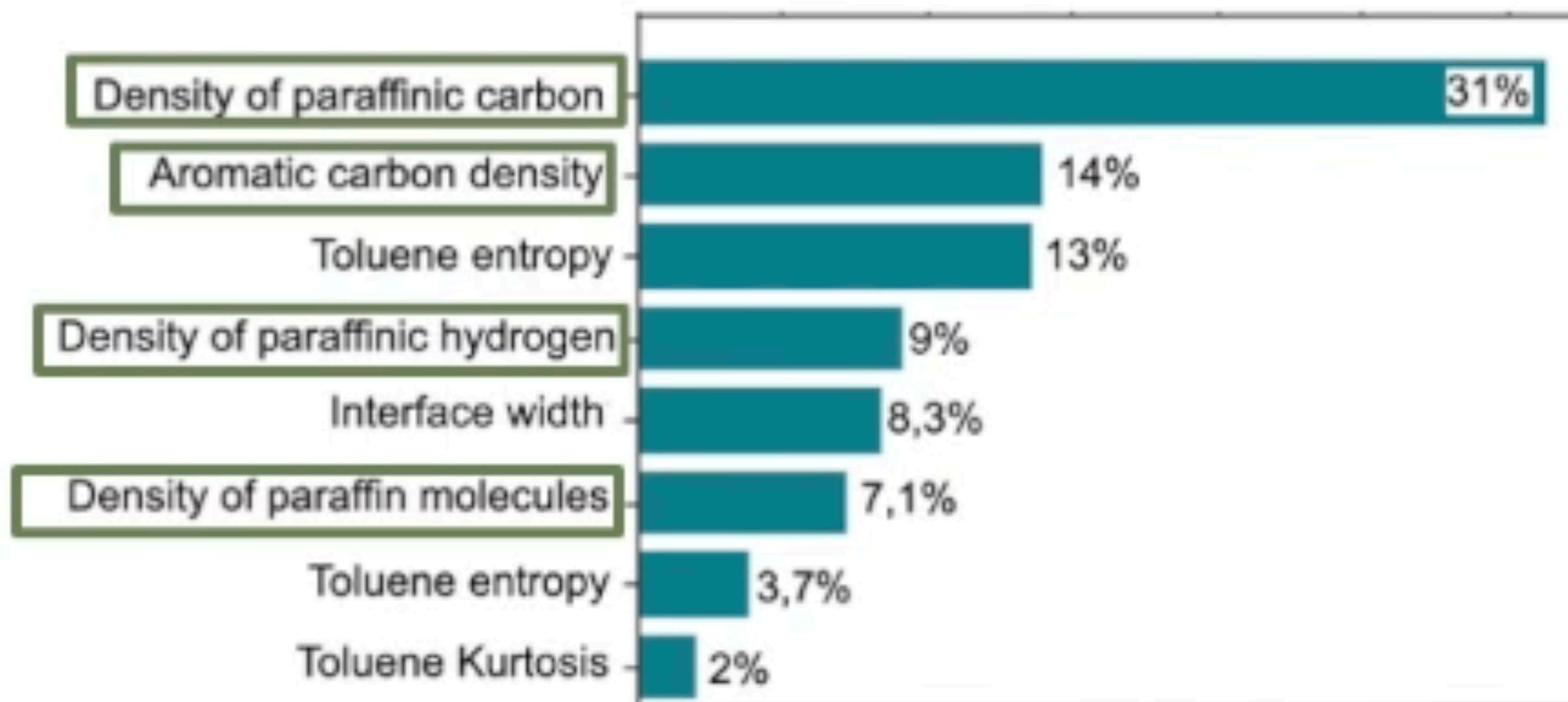
Interfacial properties more correlated with Interfacial Tension



Results and Conclusion

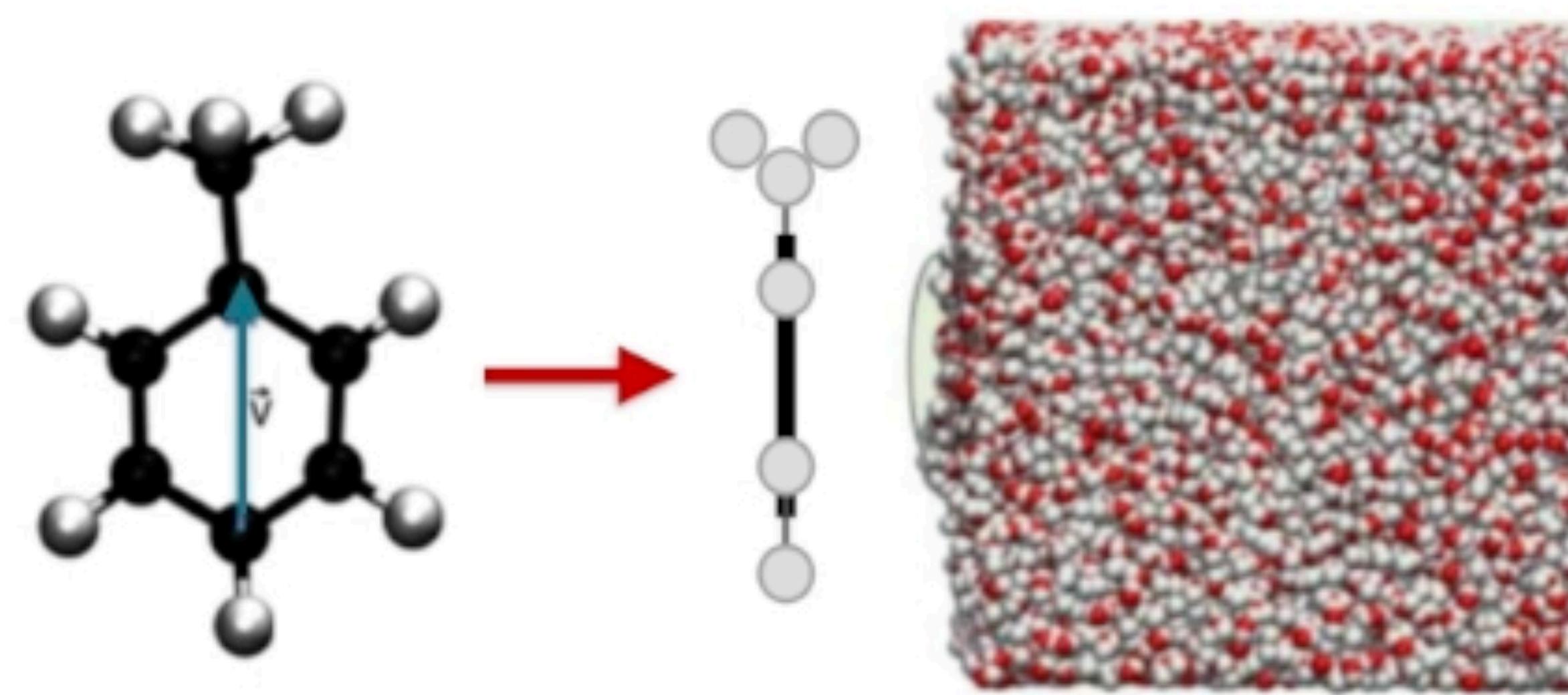
- ✓ Feature Importance
- ✓ Density of aromatics and paraffins

Interfacial properties more correlated with Interfacial Tension



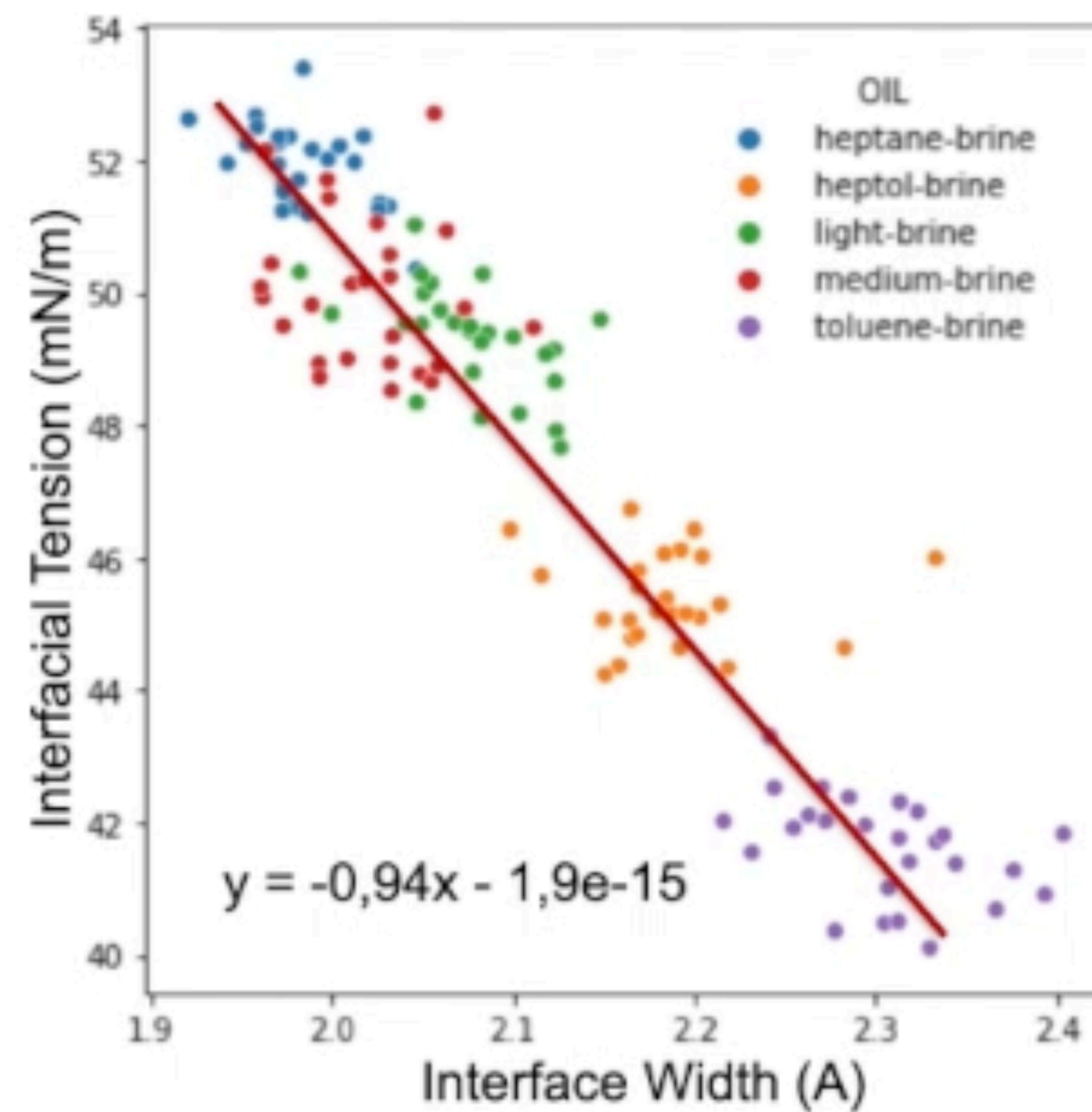
Results and Conclusion

- ✓ Feature Importance
- ✓ Density of aromatics and paraffins
- ✓ Order parameter



Results and Conclusion

- ✓ Feature Importance
- ✓ Density of aromatics and paraffins
- ✓ Order parameter
- ✓ Interface Width x Interfacial Tension



Results and Conclusion

- ✓ Feature Importance
- ✓ Density of aromatics and paraffins
- ✓ Order parameter
- ✓ Interface Width x Interfacial Tension
- ✓ Linear regression for interfacial tension prediction

Multiple Linear Regression

Error = 0,5 mN/m e $R^2 = 0,95$

Simple Linear Regression

Error = 1,1 mN/m e $R^2 = 0,86$