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A Langevin model for the Dynamic Contact Angle Parameterised Using Molecular Dynamics[1] EDWARD SMITH, ERICH MULLER, RICHARD CRASTER, OMAR MATAR, Imperial College London — An understanding of droplet spreading is essential in a diverse range of applications, including coating processes, dip feed reactors, crop spraying and biomedical treatments such as surfactant replacement theory. The default modelling tools for engineering fluid dynamics assume that the continuum hypothesis is valid. The contact line motion is very difficult to capture in this paradigm and requires some form of closure model, often tuned *a priori* to experiments. Molecular dynamics (MD), by assuming only an inter-molecular potential, reproduces the full detail of the three-phase contact line with no additional modelling assumptions. This provides an ideal test-bed to understand contact line motion. In this talk, MD results for a sheared liquid bridge are presented. The evolution and fluctuations of the dynamic contact angle are paramterised over a range of wall sliding speeds and temperatures. A Langevin model is proposed to reproduce the fluctuations and evolution of the contact angle. Results from this model are compared to molecular simulation data showing excellent agreement. The potential applications of this model, as well as limitation and possible extensions, are discussed.

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