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Singularities in Contact line Motion: From molecular simulations to continuum theories

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When the contact line at the intersection between a fluid interface and a solid moves, traditional continuum calculations predict a diverging dissipation. Experiments and continuum theories cannot reveal how this singularity is removed, but proposals are based on very different mechanisms: Shear-induced slip or diffusive transport. We present detailed molecular simulations and atomistically-derived mesoscale models [1] of contact line motion in the conditions assumed for diffusive models [2]. The singularity is primarily eliminated by slip, but there is a Marangoni-like contribution to slip that has not been observed previously. Diffusion is present, but perpendicular to the expected direction. We also find an interesting dynamic dewetting transition at a finite dynamic contact angle. [1] C. Denniston and M.O. Robbins, PRL 87, 178302 (2001); ibid, PRE 69, 021505 (2004). [2] H.-Y. Chen, D. Jasnow, J. Vinals, PRL 85, 1686 (2000).