Abstract Submitted
for the DFD10 Meeting of
The American Physical Society

Microscopic description of a liquid film on a solid substrate using density functional theory ANDREAS NOLD, Fachgebietfur Stromungsdynamik, TU Darmstadt, Petersenstr. 30, 64287 Darmstadt, Germany, ANTONIO PEREIRA, ENSEM, 2 avenue de la foret de Haye, 54516 Vandoeuvre les Nancy, France, ALEXANDR MALIJEWSKY, E. Hala Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals of ASCR, 16502 Prague 6, Czech Republic, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK — We examine the wetting properties of planar and spherical substrates using a mean-field density functional theory. Equilibrium density profiles of a fluid close to an attractive wall are obtained by solving an integral equation resulting from the minimization of the grand potential. Using a novel pseudo-arc length continuation scheme, we compute the complete bifurcation diagram of the adsorption as a function of the chemical potential. For a spherical substrate we demonstrate a second unstable branch approaching saturation from the right, absent in the planar case. Our numerical results are in excellent agreement with analytical predictions obtained from a piecewise function approximation in which the density profile is assumed to be everywhere constant except near the wall-liquid and the liquid-gas interfaces. We also show that the sharp-interface approximation, used often to predict wetting behavior on planar substrates, is inadequate to describe wetting on a spherical substrate.

Serafim Kalliadasis
Department of Chemical Engineering,
Imperial College London, London SW7 2AZ, UK

Date submitted: 09 Aug 2010 Electronic form version 1.4