Abstract Submitted for the DFD12 Meeting of The American Physical Society

General Multi-Species Dynamical Density Functional Theory BENJAMIN GODDARD, ANDREAS NOLD, NIKOS SAVVA, Department of Chemical Engineering, Imperial College London, GRIGORIOS A. PAVLIOTIS, Department of Mathematics, Imperial College London, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London — We extend our recent study on the dynamics of single-species colloidal fluids in the full positionmomentum phase space to the dynamics of multi-species colloidal fluids. We include both inertia and the full hydrodynamic interactions, which strongly influence the non-equilibrium properties of the system. For many-particle systems, the number of degrees of freedom prohibit a direct solution of the underlying stochastic equations and a reduced model is necessary. Under minimal assumptions, we derive a dynamical density functional theory (DDFT), i.e. a reduction to the dynamics of the reduced one-body distribution. Via computations based on spectral methods extended to integral operators, we demonstrate the excellent agreement between this DDFT and the full Langevin equations for a range of multi-species systems. In suitable limits we recover existing DDFTs (which neglect inertia and/or hydrodynamic interactions) and we investigate the resulting corrections to these DDFTs.

> Serafim Kalliadasis Department of Chemical Engineering, Imperial College London

Date submitted: 01 Aug 2012

Electronic form version 1.4