Abstract Submitted
for the DFD15 Meeting of
The American Physical Society

Non-equilibrium molecular dynamics simulation of the unstirred layer in the osmotically driven flow KEITO KONNO, TOMOAKI ITANO, MASAKO SEKI, Kansai Univ — We studied the solvent flows driven by the osmotic pressure difference across the semi-permeable membrane. The flow penetrating from the low concentration side transports away solutes adjacent of the membrane, so that the concentration is reduced significantly only at the vicinity of the membrane. It is expected that the relatively low solute concentration develops into a thin boundary layer in the vicinity of the membrane in the case of absence of external stirring process, which is termed as un-stirred layer (USL). To investigate concentration distribution in USL, we carried out non-equilibrium molecular dynamics simulations. The flows driven by th osmotic pressure are idealized as 2 dimensional hard disk model, which is composed of solvent and solute molecules. The membrane is modeled as a medium composed of stationary parallel rods distributed by a spatial interval, which is less than the diameter of the solute molecules. The following results were obtained from the numerical simulation. First, the thickness of USL, which was estimated from the obtained concentration distribution, is on the order of a length determined by mean free path. Second, USL was semicircle the center of which is on the end of pore of membrane.

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Date submitted: 01 Aug 2015 Electronic form version 1.4