I. INTRODUCTION

Crude oil and its derivatives are compounds that have deep practical and industrial significance. Although of varying composition, even from the same source, crude oils have distribution spectra of predominantly n-alkanes (abbreviated C_n), which are straight-chained hydrocarbons having the general formula C_nH_{2n+2}. Natural gas is comprised of C_1–C_5 molecules in varying ratios (1) and crude oil is generally from C_6–C_{30} (2–7). Some basic practical information about alkanes can be found in Table 1.

Because alkanes comprise a family of compounds, they lend themselves quite nicely to comparative studies in theoretical, computational, and experimental arenas. Because of the wide distribution of alkane chain lengths in crude oils, they make ideal systems for the study of comparisons and contrasts within the alkane family. Computer simulations can give much insight into the behavior of physical systems from both supplementary and predictive standpoints and can shed light on system dynamics not readily accessible in experiments. The studies that exist involving natural gas and crude oil are macroscopic in nature and, although very useful, do not address nanoscale dynamics and processes inside transport pipes and on surfaces. Such an understanding could prove very useful in helping delineate the effects and possible repair of pipe breaks, in facilitating an understanding of new methods of fractionating crude oil and in characterizing the alkane layers adsorbed onto transport pipes that need remediation. In many cases, it then becomes relevant to study the atomistic behavior of alkane mixtures in confined geometries.

The behavior of atomic and molecular systems in confined geometries has been widely studied (8). Generally, a confined liquid tends to organize into lamellae, or layers. Moreover, there are density and solvation force oscillations perpendicular to the boundary whose wavelength is on the order of the dynamic radius of the confined molecule. Such effects have been studied in confined alkanes (8–16). For organic molecules, branching can disrupt the spatial periodicity of density and solvation force oscillations (17). Another intriguing result is that a confined liquid system can possess a distinctly solidlike character: shear stress (18). Confinement can also slow down the dynamics of a system and, in particular, longer molecules of a given family can be affected more than shorter ones (18, 19). In addition to the wealth of studies on confined organic systems, computer