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Investigation of Nucleation and Thermal Conductivity of Waxy Crude Oil on Pipe Wall via Particle Dynamics

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Abstract : As waxy crude oil is easy to crystallization and deposition in the pipeline wall, it causes pipeline clogging and leads to the reduction of oil and gas gathering and transmission efficiency. In this paper, a mesoscopic scale dissipative particle dynamics method is employed, and constructed four pipe wall models, including smooth wall (SW), hydroxylated wall (HW), rough wall (RW), and single-layer graphene wall (GW). Snapshots of the simulation output trajectories show that paraffin molecules interact with each other to form a network structure that constrains water molecules as their nucleation sites. Meanwhile, it is observed that the paraffin molecules on the near-wall side are adsorbed horizontally between inter-lattice gaps of the solid wall. In the pressure range of 0 - 50 MPa, the pressure change has less effect on the affinity properties of SS, HS, and GS walls, but for RS walls, the contact angle between paraffin wax and water molecules was found to decrease with the increase in pressure, while the water molecules showed the opposite trend, the phenomenon is due to the change in pressure, leading to the transition of paraffin wax molecules from amorphous to crystalline state. Meanwhile, the minimum crystalline phase pressure (MCPP) was proposed to describe the lowest pressure at which crystallization of paraffin molecules occurs. The maximum number of crystalline clusters formed by paraffin molecules at MCPP in the system showed NSS (0.52 MPa) > NHS (0.55 MPa) > NRS (0.62 MPa) > NGS (0.75 MPa). The MCPP on the graphene surface, with the least number of clusters formed, indicates that the addition of graphene inhibited the crystallization process of paraffin deposition on the wall surface. Finally, the thermal conductivity was calculated, and the results show that on the near-wall side, the thermal conductivity changes drastically due to the occurrence of adsorption crystallization of paraffin waxes; on the fluid side the thermal conductivity gradually tends to stabilize, and the average thermal conductivity shows: κRS(0.254W/(m·K)) > κRS(0.249W/(m·K)) > κRS(0.218W/(m·K)) > κRS(0.188W/(m·K)).This study provides a theoretical basis for improving the transport efficiency and heat transfer characteristics of waxy crude oil in terms of wall type, wall roughness, and MCPP.

Keywords : waxy crude oil, thermal conductivity, crystallization, dissipative particle dynamics, MCPP
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