A Lennard-Jones Van Der Waals Type Equation of State

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In a previous work, simulation data for the Lennard-Jones 12-6 (LJ) fluid have been analysed in a way such that the repulsive and attractive contributions to the total virial pressure were separated. This led to the development of an accurate semi-empirical van der Waals type equation of state (EoS) for the LJ fluid based on a balance between separated repulsive and attractive contributions. In a recent development, however, the friction theory (FT) has been extended to the estimation of the fluid interfacial tension. The relevance of the recent development is that, through the FT interfacial tension approach, a connection between the interfacial density profile and the EoS interfacial van der Waals loop (including the unstable region) can be established. This may allow for the use of interfacial tension estimations, in combination with simulation results for the interfacial density profile and the FT interfacial tension approach, in the development of accurate EoS having stable van der Waals loops. The approach is illustrated by reviewing the previously developed LJ EoS showing how the EoS interfacial van der Waals loops can be tuned against interfacial simulation results for the LJ fluid.