Multi-phase and multi-scale wear model using phonon, quantum chemical molecular dynamics and machine learning

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ABSTRACT

Nearly one-third of the energy supplied by fossil fuel in automotive vehicles is spent to overcome various forms of wear and friction while the life of an automotive engine is often limited by the ability of its components to resist wear, therefore, reducing wear and friction can meet sustainable development goals, in particular carbon peak and carbon neutral needs. The ability to predict wear would greatly aid the development process of both tribopairs and lubricants. This work addresses a theoretical framework of the multi-phase and multiscale wear modelling, involving adhesive wear, abrasive wear, delamination wear, tribocorrosion, tribofilm formation and evolution, phonon energy dissipation etc. Spatial and temporal sub-partition of each reactor volume are based on the continuity equations of the mass flow and the conservation of mass momentumto to account for interactions from the numerous mechanical, material, thermal, and chemical variables over a multiscale range of time and length. The deep convolutional generative adversarial networks (DCGANs) in machine learning (ML) techniques as general image representations are employed by using huge data from experiments, analysis instruments, and computer simulation etc. High-throughput reactive molecular dynamics (RMD) with ReaxFF reaction force field sampling and simulations are performed via LAMMPS software package. The results (such as the reaction rate constants, chemical composition of adsorbed layer, probability of a bond forming between the lubricant additive molecules and slab surface, depth profiles of atomic distribution in the system, the friction coefficient, coordination number contribution, evolution of structural properties of the friction interface with size and content of the additives, bond dissociation energies, binding energies, valence angle energy, heats of formation, energy barrier and reaction energies, product distributions, number of chemisorbed atoms, radicals and molecules, coverage of atoms, radicals and molecules on the slab surface, number of worn atoms, snapshots of wear and friction morphology, tribocorrosion rate, mechanical wear rate, wear volume) are treated using Naive Bayesian classifier with a Laplacian correction (a simple and effective classification techniques that is used in ML to help build a prediction or classification model)'s unsupervised learning with the expectation maximization algorithm to accomplish the selection of which sampling and reasonable relevant reaction pathways. A conditional probability independent of each other in Naive Bayesian classifier has three distributions: multi-variate Gauss, multi-variate Bernoulli, and multinomial. The accumulated energy method is used in RMD simulations to consider effect of phonon energy dissipation. According to the assumption that all the reactive reactions are first order irreversible, the kinetic analysis of complex mechanochemical reaction networks corresponding to the reasonable reaction pathways from the obtained best sample and RMD simulations by ignoring minor reactions and retaining key reactions based on the tribofilm formation and tribocorrosion progress is carried out by solving the relevant kinetic differential equations with the classical fourth-and fifth-order Runge-Kutta method in order to verify and modify the method for the above high-throughput RMD sampling and simulations until convergence in all the molecule concentrations. The key concepts behind the theoretical model will be introduced. Two extreme pressure additives, Di-tert-butyl Disulfide and Zinc dialkyl-dithiophosphate (ZDDP), and an friction modifier additive, Mo-DTC, are, respectively, confined between two Fe(100) slabs moving laterally in opposite directions at the same speed. Effects of the initial molecular position and concentration, heat, load, and shear on wear are theoretically and experimentally studied to verify the proposed approach. Preliminary results show that when the entire validation of the model and refinement are complete, it may be a useful tool at the design stage of tribopairs, the operating dynamics of a system, or the formulation of lubricants and additives.