Lattice Monte Carlo modeling of solid particle erosion

Erosion caused by repeated impact of solid particles entrained in a moving fluid is relevant for many technical applications, for example, resulting wear and reduced service life of turbine blades, propellers, valves, etc. The ductile and brittle fracture mechanisms that emerge in solid particle erosion are complex and range from atomic to macroscopic scales. Those mechanisms are strongly dependent on the material properties of impinging particles and the target surface. Finite element method simulations can provide important information but only for the impact of a relatively few particles, due to current computational limitations.



The main goal is to develop a general and flexible modeling framework based on a novel application of the Monte Carlo method in order to simulate readily the effect of diverse fracture mechanisms. The lattice Monte Carlo Model of Solid Particle Erosion (LMC-SPE model) is based on a three dimensional representation of the target surface by a cubic lattice, where each cell embodies a small portion of the material susceptible to ductile or brittle fracture and subsequent removal. This is a coarse grained description where a real variable accounts for the fracture advancement within each lattice cell. The fracture mechanisms are represented as a coordinated action of simple micro-events, namely, rearrangement, internal fracture propagation, and detachment of lattice cells. The simulation is driven by a kinetic Monte-Carlo method where the rate at which the microevents are applied is given by an erosion probability distribution that depends on time and represents the dynamical transfer of impact energy. Hardness, toughness, and other material properties as well as velocity, size, and impinging angle of the particles can be incorporated as simulation parameters in a probabilistic sense. Those parameters have to be adjusted for each specific problem comparing the simulations with corresponding constitutive laws, detailed finite element method simulations, and experimental data.



We claim that in spite of its simplicity and low level of detail, the LMC-SPE model can simulate the main topographic features of individual impacts and reproduce correctly dependencies of the erosion rate on velocity, size, and impact angle of the particles. Because the micro-events depend only on the local topography of the surface, the simulation of subsequent impacts on an already eroded surface is straightforward. Then roughening regimes due to the accumulative effect of thousands of individual impacts acting on relatively large areas can be simulated within reasonable computational times. We propose to develop LMC-SPE models for three specific systems: (i) A class of glass subjected to impact of alumina particles (brittle fracture), (ii) a surface of a titanium-alloy impacted by steel particles (ductile fracture), and (iii) a ceramic coating on a metallic substrate where both brittle and ductile fracture can occur simultaneously.

Acknowlegment

The research will be sponsored by the Deutschen Forschungsgemeinschaft (DFG) under the number 746/135-1. We are grateful to the DFG for the financial support.

Project start:	01.01.2014
Project end:	31.12.2016

Contact Person

Dr. rer. nat. Alejandro Mora Tel.: +49 / 711 685 - 62701 e-mail: alejandro.mora@imwf.uni-stuttgart.de