Flow and polymerization in small cracks with application to self-healing composites

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Sandia National Labs — The flow of a fluid undergoing a ring opening metathesis polymerization has been used for autonomic healing of cracks in self-healing materials under development. A monomer healing agent flows into a crack bringing it into contact with a healing agent catalyst which induces polymerization. Under the right conditions this has been demonstrated to heal the material. We have designed a simulation tool to investigate the coupled micro-fluid mechanics, the advection-diffusion of the healing agent, and the solidification in the crack. The polymerization is approximated by a large increase in the viscosity of the fluid. Lagrangian particles within the finite-element mesh are used to track the contact of monomer with the local catalyst concentration and integrate the rate equation for polymerization. The simulation tool is used to construct “phase diagrams” which identify the regimes in which healing occurs for various ranges of parameters of the system. These are useful for assessing the robustness of designs and optimizing the healing system.

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