On the stochastic modelling of surface reactions through reflected chemical Langevin equations

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Highlights

- Modeling heterogeneous catalytic systems with traditional Langevin equations can lead to species coverages that exceed the physically realistic bounds of 0 and 1
- Adding reflection terms to these equations ensures physically realistic solutions
- Numerical implementations of reflection reproduce the analytical steady-state solutions for the probability of the coverage in a simple system
- The computational cost of the Langevin equations with reflections is constant, making this approach highly efficient for the modelling of mesoscale systems