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This paper presents a novel single-shooting algorithm for gradient-based solution of optimal control problems with vapor-liquid equilibrium constraints. Such optimal control problems are important in several engineering applications, for instance in control of distillation columns, in certain two-phase flow problems, and in operation of oil reservoirs. The single-shooting algorithm uses an adjoint method for the computation of gradients. Furthermore, the algorithm uses either a simultaneous or a nested approach for the numerical solution of the dynamic vapor-liquid equilibrium model equations. Two numerical examples illustrate that the simultaneous approach is faster than the nested approach and that the efficiency of the underlying thermodynamic computations is important for the overall performance of the single-shooting algorithm. We compare the performance of different optimization software as well as the performance of different compilers in a Linux operating system. These tests indicate that real-time nonlinear model predictive control of UV flash processes is computationally feasible.

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