One of the main technical challenges associated with the modular multilevel converter (MMC) for any application is the optimal control of its states. Optimal control of the MMC requires determination of the following: 1) an accurate MMC model, 2) the MMC states to be controlled and their corresponding reference trajectories, and 3) an appropriate controller type/form and its parameters. The aforementioned tasks lead to the formulation of a multistate control optimization problem, which is tackled in this paper. This paper enhances the accuracy of the existing MMC state-space model by including the following: 1) a piecewise affine insulated-gate bipolar transistor/diode model and 2) the impact of dead time. This paper also proposes a simulation-based gradient-descent optimization algorithm (cosimulation) to optimize the controller gains, given the controller type/form and the reference state trajectory. The theoretical proofs of the gradients required in the optimization algorithm are also provided. The aforementioned optimization algorithm is applied to a variable-frequency MMC-based drive system. Experimental results on a scaled-down prototype and simulation results on a real-world application are provided to validate the accuracy of the proposed MMC model and to show the effectiveness of the proposed optimization algorithm.