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Rate-equation modelling and ensemble approach to extraction of parameters for viral infection-induced cell apoptosis and necrosis. SERGII DOMANSKYI, JOSHUA SCHILLING, Clarkson University, VYACHESLAV GORSHKOV, National Technical University of Ukraine KPI, SERGIY LIBERT, Cornell University, VLADIMIR PRIVMAN, Clarkson University — We develop a theoretical approach that uses physiochemical kinetics modelling to describe cell population dynamics upon progression of viral infection in cell culture, which results in cell apoptosis (programmed cell death) and necrosis (direct cell death). Several model parameters necessary for computer simulation were determined by reviewing and analyzing available published experimental data. By comparing experimental data to computer modelling results, we identify the parameters that are the most sensitive to the measured system properties and allow for the best data fitting. Our model allows extraction of parameters from experimental data and also has predictive power. Using the model we describe interesting time-dependent quantities that were not directly measured in the experiment and identify correlations among the fitted parameter values. Numerical simulation of viral infection progression is done by a rate-equation approach resulting in a system of "stiff" equations, which are solved by using a novel variant of the stochastic ensemble modelling approach. The latter was originally developed for coupled chemical reactions.

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