

Update: Nov 01 2019

Students research topics in theoretical and computational data analysis.

Requirement:

1. Computational physics with Python
2. Differential equations.

* No experiment is required. Students will focus on theoretical modeling and computational data analysis.

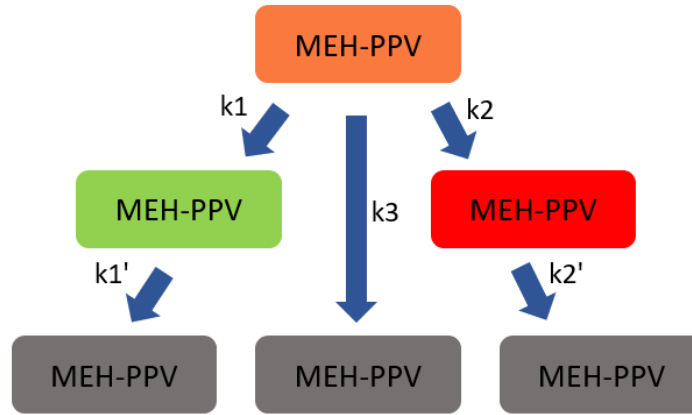


Fig. 1. Schematic decay diagram of MEH-PPV polymer with two intermediate states of green and red emission colors. They decay into optically inactive dark states (grey).

Since PPV polymers are generally unstable under normal device operation conditions. It is important to understand the dynamic mechanism of the optical degradation processes. The polymers decay into optically inactive states through several intermediate states. If two intermediate states are considered, their dynamic decay in the photochemical degradation can be described by a decay diagram (Fig. 1). An intermediate state population is given by a set of rate equations (Eq-1).

$$\begin{aligned}\frac{dN_0}{dt} &= C_0 e^{-k_0 t} \\ \frac{dN_1}{dt} &= k_1 N_0 - k'_1 N_1\end{aligned}\quad (\text{Eq-1})$$

, where N_0 : population of pristine state, N_1 : population of green intermediate state, C_0 : initial population of pristine state. For example, the decay channel of the green emission state is simply described by two rate constants. Once we can determine the total decay rate from the pristine orange as $k_{\text{total}} = k_1 + k_2 + k_3$. The population (N_1) of the green state is given by Bateman equation:

$$N_1 = \frac{k_1}{k'_1 - k_1} C_0 (e^{-k_1 t} - e^{-k'_1 t}) \quad (\text{Eq-2})$$

The general form of Bateman equation is

$$N_n(t) = \frac{N_0(t)}{k_n} \sum_{i=0}^n k_i \alpha_i e^{-k_i t}$$

$$\alpha_i = \prod_{j \neq i, j=0}^n \frac{k_j}{k_j - k_i}$$
(Eq-3)

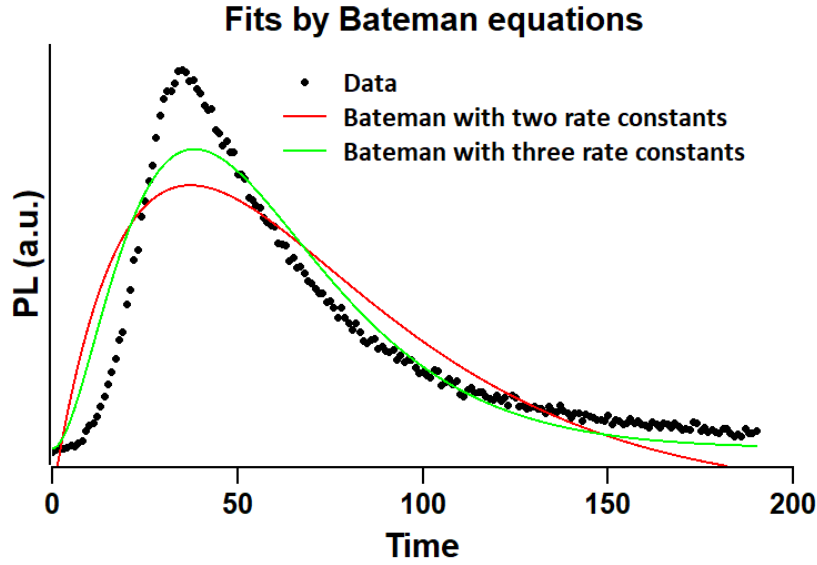


Fig. 2. Experimental data of the PL at 500 nm in Fig. 6, and fits by Bateman equations with two and three rate constants. A preliminary data set from the PI's group.

However, this model cannot fit the experimental data for the green emission (Fig. 2). The degradation decay is not a simple process and involves several intermediate states. As a trial rate equation (Eq-4), we may consider a nonlinear decay in which the population of the intermediate state is concentration dependent.

$$\begin{aligned} \frac{dN_0}{dt} &= C_0 e^{-k_0 t} \\ \frac{dN_1}{dt} &= C_1 e^{-k_1 t} - C_2 \frac{N_{2\max} - N_2}{N_{2\max}} N_1 \\ \frac{dN_2}{dt} &= C_2 \frac{N_{2\max} - N_2}{N_{2\max}} N_1 - C_3 N_2 \end{aligned}$$
(Eq-4)

Students will investigate these theoretical decay models to explain the dynamics of the degradation decay including computational numerical calculation.