

Example of four simulated kinetic profiles (Sample Index: 2132102)

Mechanism: M9

Initial catalyst concentrations (x1): [0.034, 0.096, 0.100, 0.034]

Mechanism one-hot label (y): [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

Parameter vector (theta): [1.93 , 0.328, 2.18 , 0.826, 0.032, nan]

