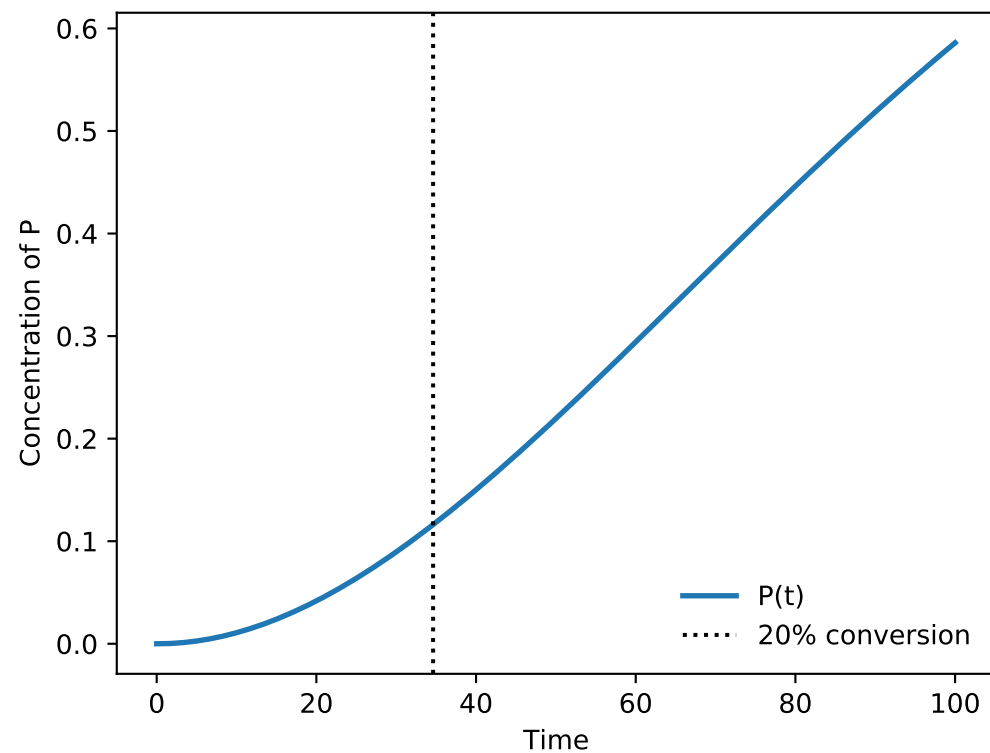


Mechanism M6 parameter set:  $k_1 = 1$ ,  $k_{-1} = 0.5$ ,  $k_2 = 5$ ,  $k_{-2} = 0.1$ ,  $k_3 = 0.01$   $[\text{cat}]_0 = 0.030$

Product concentration over time



Active catalyst fraction ( $\text{cat}^* + \text{cat}^* \text{S}$ ) at 20% conversion

