Thoughts on Steady State for Oxidation of a Small Alkane

Fill in the blanks and answer the *questions* below

1) Consider the mechanism below from Homework #5

$C_2H_6 + OH \rightarrow \bullet C_2H_5 + HOH$	k_1
$\bullet C_2H_5 + O_2 \rightarrow C_2H_5OO\bullet$	k_2
$C_2H_5OO\bullet + NO \rightarrow C_2H_5O\bullet + NO_2$	k_3
$C_2H_5O\bullet + O_2 \rightarrow CH_3CH{=}O + HOO\bullet$	k_4

Define L_{C2H6} as the rate of loss of C_2H_6 = Rate of reaction 1 (R_1)

Define P_{C2H5} as the rate of production of C_2H_5 = Rate of Reaction _____

Consider similar definitions of L_{C2H5}, L_{C2H5OO}, and L_{C2H5O}. Consider similar definitions of P_{C2H5OO} and P_{C2H5O}.

At steady state, $d([C_2H_5]/dt = P_{C2H5} - L_{C2H6}$ = _____ *(Enter a number. No calculators!)*

<u>At steady state</u>:

What is the relationship between P_{C2H5} and L_{C2H6} ?

What is the relationship between P_{C2H5} and L_{C2H5}

What is the relationship between P_{C2H5OO} and L_{C2H5OO} ?

What is the relationship between P_{C2H5O} and L_{C2H5O} ?

What is the relationship between $P_{\mathbf{C2H5O}}$, $L_{\mathbf{C2H6}}$, R_1, R_2, R_3, and R_4?

$$[C_2H_5O\bullet]_{ss} = \frac{P_{C2H5O}}{k'_{\text{loss of C2H5O}}} = \frac{\text{Rate of reaction } \mathbf{N}}{k'_{\text{loss of C2H5O}}}$$ *Why can we use N=1 here?*

2) To the mechanism above, add the reaction below, as in Homework #6.

$C_2H_5O_2 + HOO \rightarrow C_2H_5OOH + O_2$ k_5

Q2 What Rates are equal to each other, if any, once we add reaction 5?