Langmuir-Hinshelwood Mechanism

Many chemical reactions are catalyzed on surfaces. In particular, suppose we have two gases A and B, where the free energy barrier to their joining

$$\mathrm{A} + \mathrm{B} \to \mathrm{C}$$

is simply too high for the reaction to reasonably proceed in air. Nonetheless, suppose both A and B can attach to a surface. An unoccupied site S on the surface can then be treated as an effective chemical reacting in the system:

$$\mathrm{S} + \mathrm{A} \underset{\alpha_2}{\overset{\alpha_1}{\rightleftharpoons}} \mathrm{AS}$$

$$\mathrm{S} + \mathrm{B} \underset{\beta_2}{\overset{\beta_1}{\rightleftharpoons}} \mathrm{BS}$$

We then assume that the following reaction only proceeds forwards:

$$\mathrm{AS} + \mathrm{BS} \xrightarrow{\lambda} \mathrm{S} + \mathrm{C}$$

Suppose that the total number of possible reaction sites on the surface is S_0. Let A denote the concentration of A and B the concentration of B.

(a) Suppose that the intermediate binding steps of A and B are in equilibrium. What does this imply about time scales in the problem?

(b) Let $\alpha_2/\alpha_1 = A_0$ and $\beta_2/\beta_1 = B_0$; let $a = A/A_0$ and $b = B/B_0$. Show that the rate R of production of C is given by

$$R = \lambda S_0^2 \frac{ab}{(1+a+b)^2}.$$

(c) Suppose that we hold a fixed. Sketch $R(b)$, and comment on the physics at play in any interesting region of the sketch.

(d) How should one maximize the rate R?