Kinetics & Reactor Design I: Kinetics

Continuing Ed workshop by Richard Skeirik, PE

Reversible Reactions & Reaction Networks Exercise

Terathane goes into making great Spandex. It's an oligomer of THF. The polymerization is unusual: it is reversible. It gets started when a proton attacks the electrons in the THF oxygen atom. Then that positively charged O (called an oxonium ion) keeps attracting more THF: oxonium ion groundhog day.

Free Proton THF Protonated THF Secondary Oxonium Ion

$$H^{+} + THF \rightarrow THF_{n}^{+}$$

$$K_{2f} \rightarrow K_{2r} \rightarrow K_{2r}$$

$$THF + THF_{n}^{+} + THF_{n}^{+} \Rightarrow THF_{n}^{+}$$

How does that sit with you? THF_n^+ is both reactant and product? n is the number of THF units in the linear chain tail. It can be zero (as in the product of the first reaction), or greater. Keep in mind, n changes as each THF adds to the chain. Treating all growing chains together is called lumping. It works fine for irreversible chain growth but not so well for reversible, but we don't need to worry about that right now.

Write two rates expressions: for H+ and for THF (Hint, no matter how strange those structures look to you, the technique is just the same. Remember? Model: simplified representation of something complex.)

$$r(H^{+}) =$$

$$r(THF) =$$

How could anyone possible know this chemistry?