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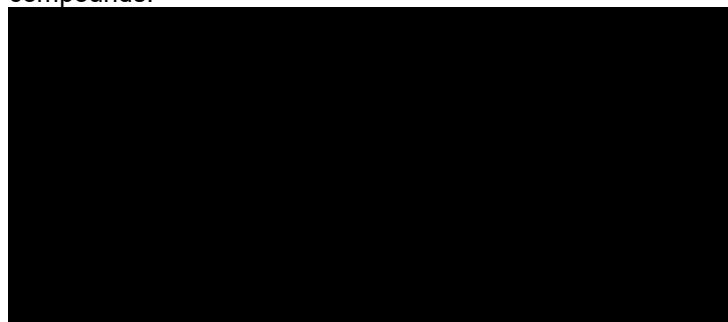
hydrogen peroxide production kinetics-

Aim

Understanding the kinetics of hydrogen peroxide production, including the factors determining the side product formation.

Justification

Hydrogen peroxide is a chemical compound which is used as an oxidizer, bleaching agent, and antiseptic, usually as a dilute solution (3–6% by weight) in water for consumer use, and in higher concentrations for industrial use. Concentrated hydrogen peroxide, or "high-test peroxide", decomposes explosively when heated and has been used as a propellant in rocketry. Hydrogen peroxide is a reactive oxygen species and the simplest peroxide, a compound having an oxygen–oxygen single bond. It decomposes slowly when exposed to light, and rapidly in the presence of organic or reactive compounds.



Hydrogen peroxide is manufactured almost exclusively by the anthraquinone process, which was originally developed by BASF in 1939. It begins with the reduction of an anthraquinone (such as 2-ethylanthraquinone or the 2-amyl derivative) to the corresponding anthrahydroquinone, typically by hydrogenation on a palladium catalyst. In the presence of oxygen, the anthrahydroquinone then undergoes autoxidation: the labile hydrogen atoms of the hydroxy groups transfer to the oxygen molecule, to give hydrogen peroxide and regenerating the anthraquinone. Most commercial processes achieve oxidation by bubbling compressed air through a solution of the anthrahydroquinone, with the hydrogen peroxide then extracted from the solution and the anthraquinone recycled back for successive cycles of hydrogenation and oxidation.

Program

- Analysis of a kinetics data set provided by the industrial project partner.
- Construction of a kinetic model for the main reaction and for the side reactions, including the definition of the corresponding elementary steps.
- Regression of the model to the experimental data to determine the best fitting model parameters.
- Suggestion of operating conditions for further kinetics assessment of the main reactions as well as of the side reactions.