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CEE 697K
ENVIRONMENTAL REACTION KINETICS

Lecture #16

Kinetic Modeling: Computer Models
Case Study: Chloramination I
Brezonik, pp.

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Kinetic Modeling

- Multiple & complex kinetic rate laws are what nature has given us
- Lack of easy analytical solutions
  - Therefore, need for computer modeling
- Options
  - Scientist
  - Mat Lab
  - Aquasim (EAWAG)

Chloramines

Inorganic chloramines are formed by the reaction of free chlorine with ammonia. The reaction is stepwise, giving monochloramine (equation 1) followed by dichloramine (equation 2).

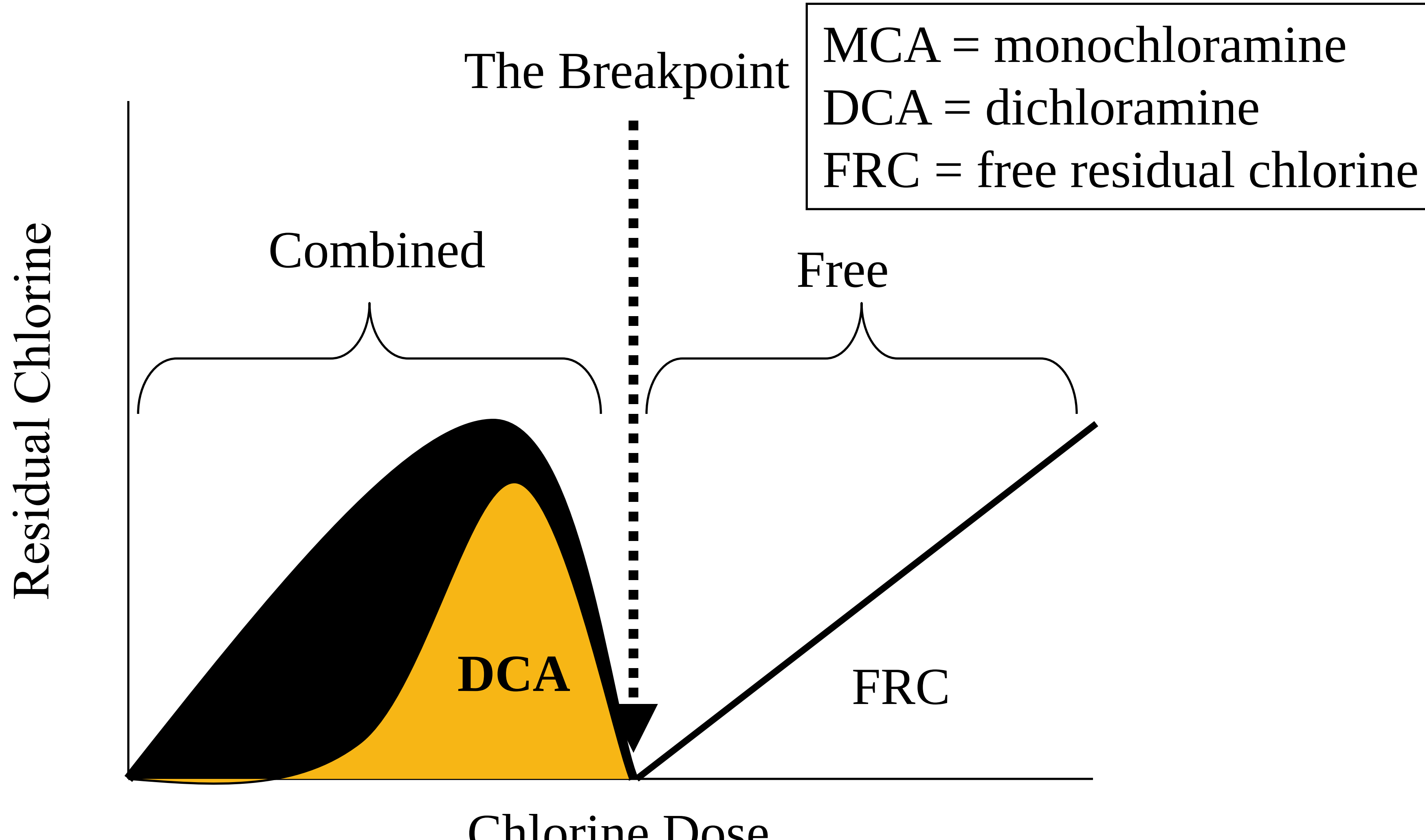
The dichloramine is quite unstable, forming nitrogen gas (equation 3) and some nitrate. This decomposition is responsible for the classic breakpoint chlorination phenomenon.

$$NH_3 + HOCl \text{ --------> } NH_2Cl + H_2O \qquad (1)$$

$$NH_2Cl + HOCl \text{ --------> } NHCl_2 + H_2O \qquad (2)$$

$$NHCl_2 + NHCl_2 + H_2O \text{ --------> } HOCl + 3H^+ + 3Cl^- + N_2 \qquad (3)$$

Chloramines: Breakpoint Curve



Chloramination and regulated DBPs

- Preponderance of DHAAs; very little THM, TCAA
  - Cowman & Singer, 1996
    - EST 30:1:16
  - Zhang et al., 2000
    - In Natural Organic Matter and Disinfection Byproducts, ACS Symp #761, Barrett, Krasner & Amy, eds.
- HAAs decrease substantially
  - 5-20% of that observed from chlorination (no ammonia addition)
    - Review by Speitel, 1999
- DBP formation increases with decreasing pH; possibly the role of dichloramine
  - Speitel, 1999
    - In Formation and Control of Disinfection Byproducts in Drinking Water, P.C.Singer, ed.
  - Symons et al., 1998
    - AWWARF report

- To next lecture