# Future Design Techniques for Chemical Disinfection

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## Introduction

Water and wastewater disinfection has been practiced in the US for more than 175 years. This is particularly noteworthy since the understanding that infectious diseases are transmitted by microorganisms only dates back about 120 years following the important work of Pasteur and Koch. Over the years of practice in disinfection, there has been an evolution in the techniques used for design of disinfection processes. This paper will provide a historical summary of these methods, and present an approach for the next stage in process design.

## Historical Evolution

The earliest disinfection "design" guidelines were based on dosing for the purpose of deodorization (in accordance with the miasmatic theory of disease). Following the understanding of bacteria as pathogenic agents, and experiments in the first decades of the twentieth century, it was recognized that dose and time were required to achieve bacterial kill in accord with the quality of the water or wastewater (demand) being disinfected.

During the 1930-1970 period, there was increasing development of rate expressions for disinfection, and recognition that the disinfectant residual combined with the contact time (also as functions of pH and temperature) were crucial predictors of disinfection efficiency. The work of Fair et al. was particularly noteworthy in calling attention by careful kinetic analysis to the direct relationship between the acid dissociation of HOCl and the efficacy of free chlorine as a function of pH.

In the late 1970's, with the development of the US EPA Surface Water Treatment Rule, it was recognized that the non-ideal hydraulics particularly during disinfectant contacting needed to be incorporated into design and compliance calculations. The empirical use of the $t_{10}$ (time for most rapid 10% of water to pass through a system) was an attempt to correct for this. However many have recognized that this has severe limitations, as opposed to a fuller consideration of the overall residence time distribution (originally set forth by Trussell and Chao).

Even the use of the full RTD in a design approach (generally termed the Integrated Disinfection Design Framework) suffers from oversimplification of mixing conditions – and further, if a system has not been built, the RTD cannot be experimentally determined. In addition, there has been a greater understanding that as yet incompletely understood aspects of water quality can influence inactivation kinetics. Therefore, a more detailed design approach is called for.

## Proposed Approach

The vision for a framework for modern predictive chemical disinfection system design has the following elements:

- Predictive model of inactivation kinetics incorporating water quality factors
- Predictive model of continuous flow reactor (contactor) performance using computational fluid dynamics (CFD) to directly describe disinfectant concentration and microbial decay
- Predictive model of disinfectant demand
- Predictive model of disinfection byproduct formation kinetics

In the presentation, progress towards the first two bullets will be discussed, including a proof of concept that CFD methods can be directly applied to full scale disinfectant contactor simulation. It will also be shown that neural network models can be used to describe multivariate water quality effects on disinfection. This provides encouragement that it will be possible to develop optimal designs by computational efforts, given the (necessary development) of more robust data sets on inactivation, disinfection decay, and DBP formation in a variety of water matrices.

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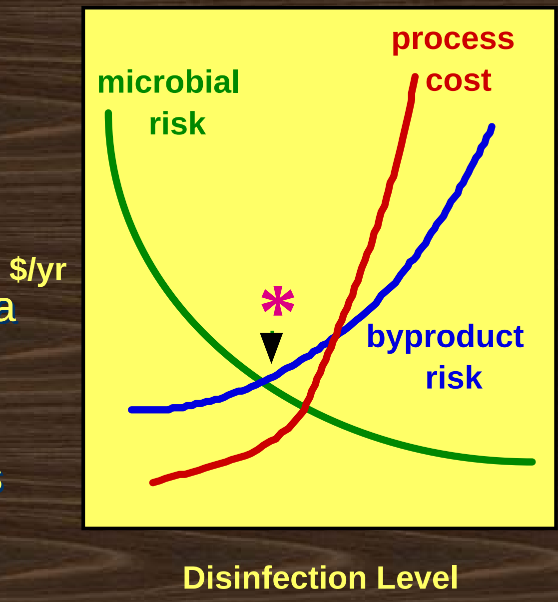
## Outline

- Continuing motivation for better methods for design
- Historical evolution of design methods
- Vision for future framework
- What we have and what we need

2

# Motivation

- DBP/Recalcitrant pathogens (water)
  - Balancing for competing risks
  - Rational design to meet multiple criteria
- Wastewater
  - Balancing for ecological effects (as well as DBPs)



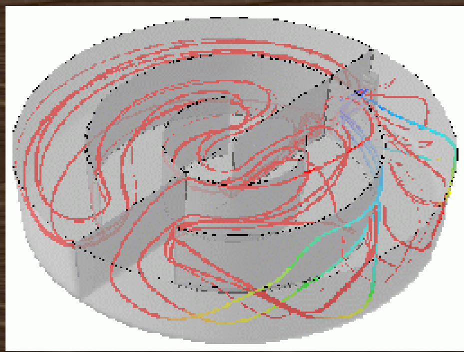

# Early History of Design Methods

- Miasmatic theory (1820's-1900)
- Dose only (recognizing bacteria) (1900-1930's)
- Importance of residual, time (pH...) leading to "ct" concept (1930's-1970's)
  - EPA SWTR

4

# Recognition of a Problem

- Full Scale Disinfection Contactors have non-ideal flow



5

# Disinfection 2.5 (1980, SWTR)

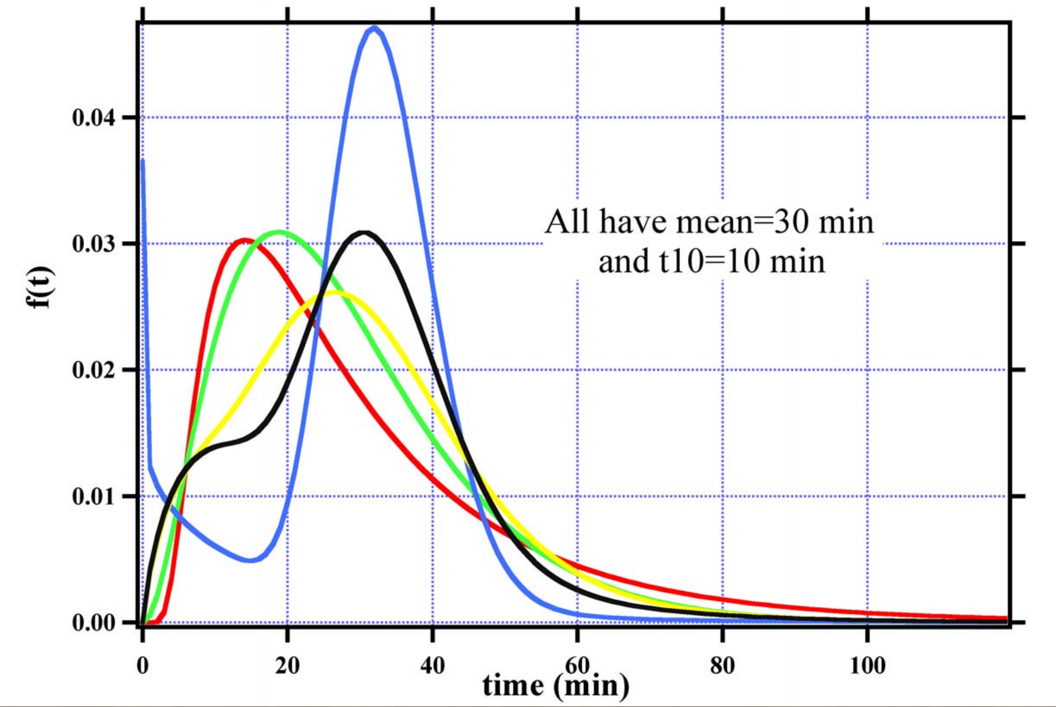
- Approximate contact time by $t_{10}$ and use $c*t = f(pH, temperature)$

TABLE 1
CT Values for Disinfectants to Inactivate 99.99% of Giardia Lamblia Cysts
USEPA Guidance Manual to the SWTR[2]

| Disinfectant | pH | <1°C | 5°C | 10°C | 20°C | 25°C |
|---|---|---|---|---|---|---|
| Free Chlorine at 2 mg/l[3] | 6 | 165 | 116 | 87 | 44 | 29 |
| | 7 | 236 | 165 | 124 | 62 | 41 |
| | 8 | 346 | 243 | 182 | 91 | 61 |
| | 9 | 500 | 353 | 265 | 132 | 88 |
| Ozone | 6-9 | 2.9 | 1.9 | 1.43 | 0.72 | 0.48 |
| Chlorine Dioxide | 6-9 | 63 | 26 | 23 | 15 | 11 |
| Chloramine (performed[4]) | 6-9 | 3800 | 2200 | 1850 | 1100 | 750 |

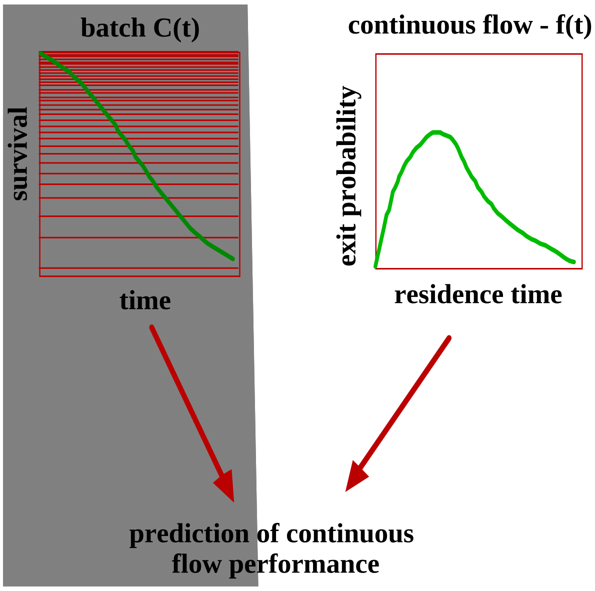
6

# Problems with 2.5

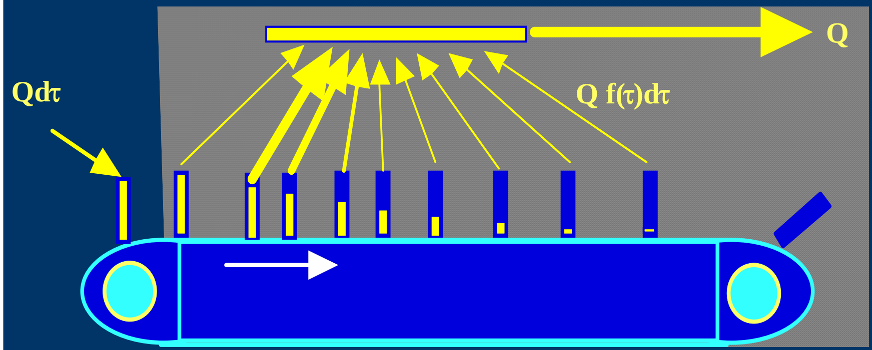



# Disinfection 3 - Integrated Disinfection Design Framework (1977-current)

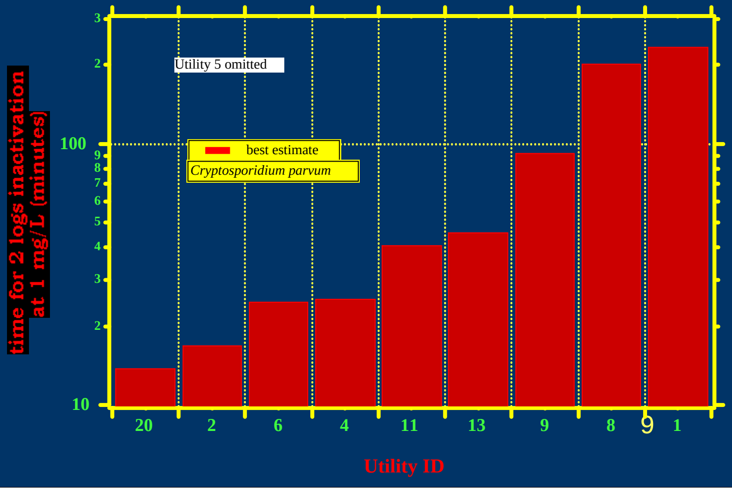
- Trussell & Chao
  - Application of chemical reaction engineering theory
  - Assumption of complete segregated flow
- Major improvement over 2/2.5
- But there are still problems



# Problems with 3




Also, need RTD to design - which may not be available if system is not built




# Disinfection 4 - Vision

- Given
  - Water quality information
  - Design dose
  - Contactor geometry and flow
- Predict a priori
  - Inactivation performance
  - DBP production
- Optimize geometry, dose, point(s) of application
  - That minimize cost &
  - Satisfy the multiple (and increasing) regulatory concerns

- We need
  - Predictive model of inactivation kinetics
  - Predictive model of disinfectant demand
  - Predictive model of DBP formation kinetics
  - Predictive model of continuous flow reactor performance (hydraulics and concentrations)

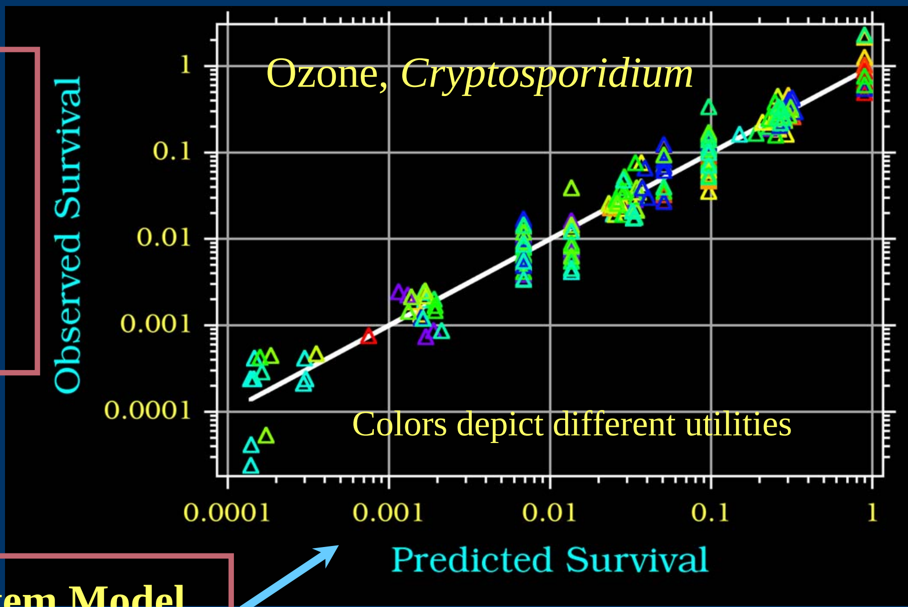
10

Remainder of presentation

# Inactivation Model Incorporating Water Quality

**Time, residual, temperature, pH, alkalinity**

**Calibrated System Model**




Neural Network Model (in progresss)

# Direct CFD Model - Chlorination

- Direct CFD solution
  - Eulerian-Eulerian disinfection model
  - Simultaneous solution of continuity, momentum and mass transfer equations
    - *Accounting for reaction terms of disinfectant (1st order with immediate demand) and inactivation (Hom)*
  - Use of k-ε model for turbulence closure (small Reynolds number option)
  - Use of commercial package (CFX)

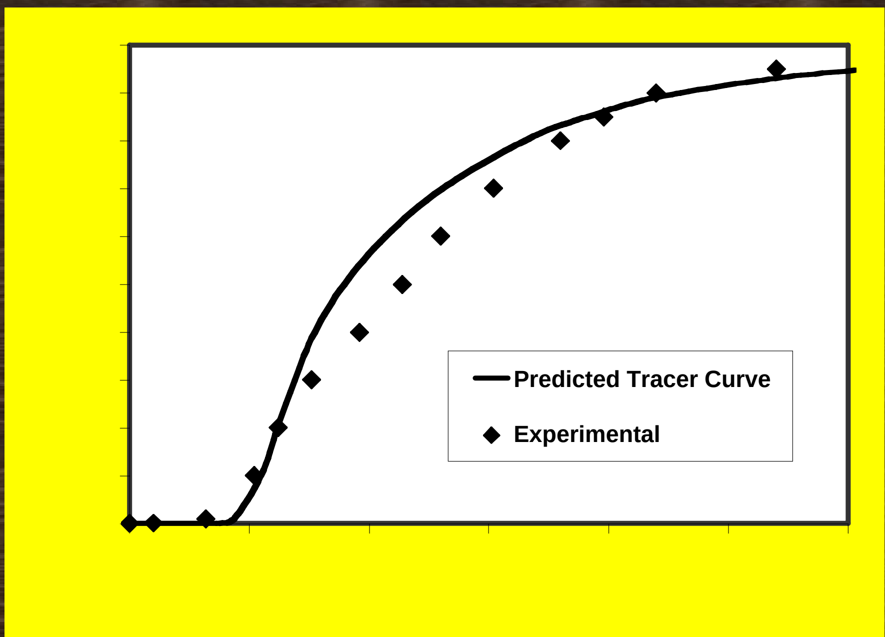
## Pilot Chlorine Contactor

- <u>Three-pass serpentine reactor</u>
  - 3 gpm (11.4 liter/min)
  - theoretical hydraulic detention time=3hr
  - NaOCl was added to the contactor through an in-line static mixer
  - 8 intermediate taps

Funding - AWWARF, Collaborators - Montgomery-Watson

13

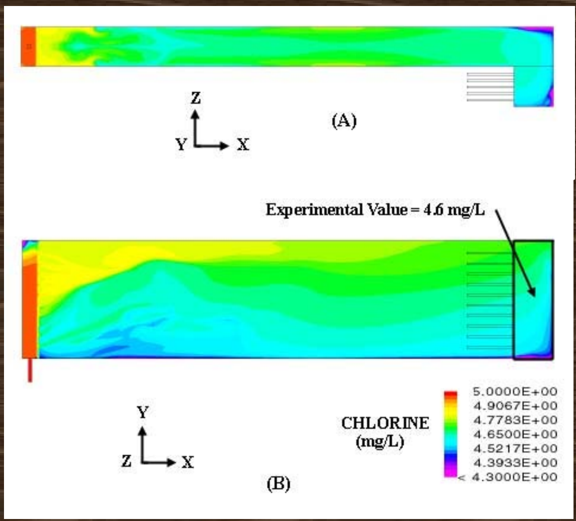
## RTD Prediction (not fitting)

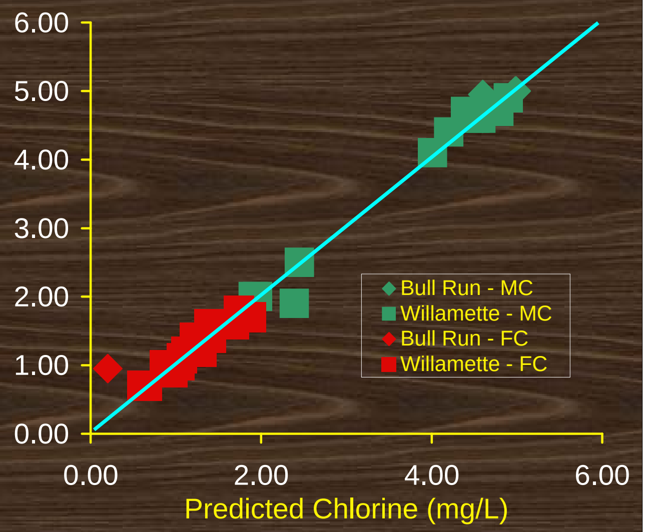



Experimental and Predicted Tracer Curves for Pass 1 Monitor Location

# Residual Prediction (not fitting)

Representative Chlorine Concentration Plot for Reactor - Run R1 (a) Plan at Mid-Depth; (b) Profile at Mid-Width.




# Inactivation Prediction (not fitting)

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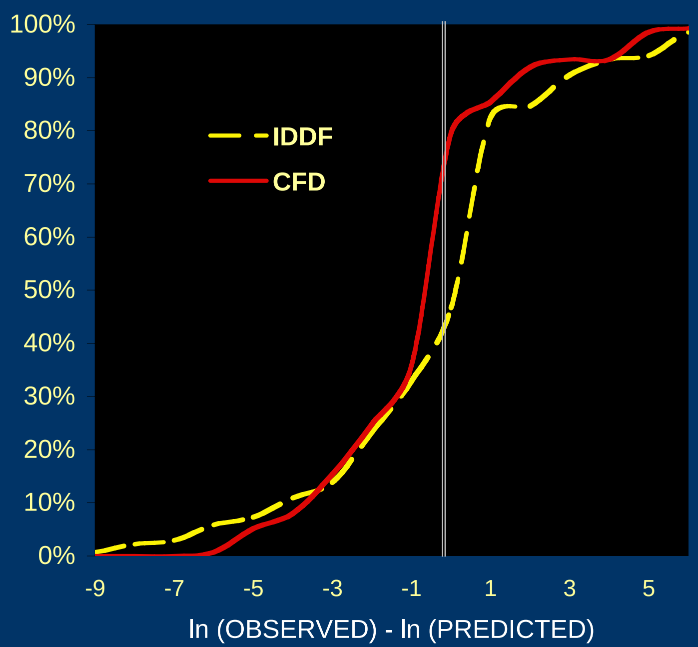
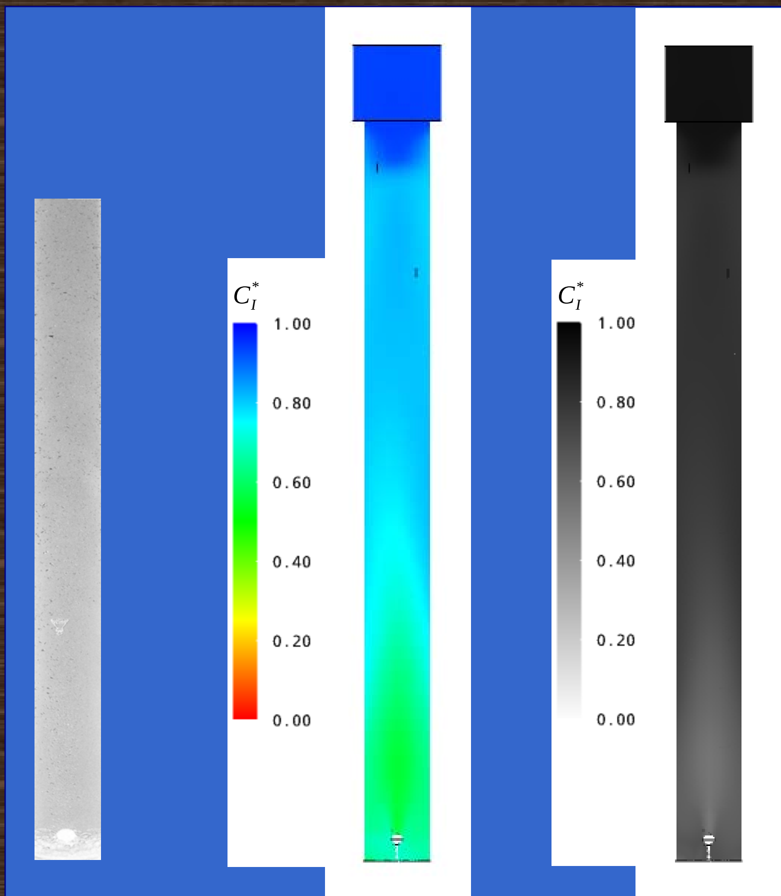
Representative Viable Microorganism Density Plot for Reactor – Run R1, (a) Plan at Mid-Depth; (b) Profile at Mid-Width



# Countercurrent Pilot $O_3$ Column

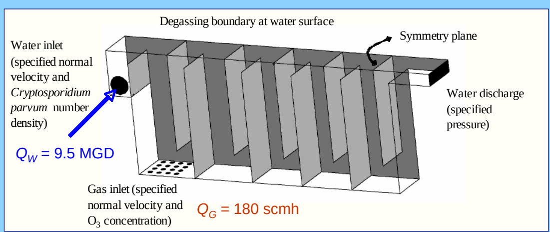
- $Q_{gas}$ = 0.4 slpm,
- $Q_L$ = 7 lpm
  - CFD captures gradual consumption of indigo
  - CFD images provide greater resolution of bubble plume than photographs (averaging)

Bartrand, 2006




(a) Experiment (b) CFD, Color Contours (c) CFD, Grayscale

## Full scale reactor - Alameda County Water District (ACWD) (Tang et al. 2006)



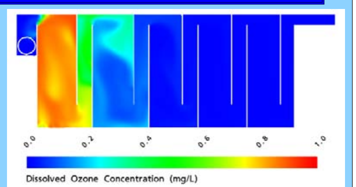

- "Rough " grid (700,000 elements)
- First order ozone decay
- First order *Cryptosporidium parvum* inactivation
- First order bromate formation

52

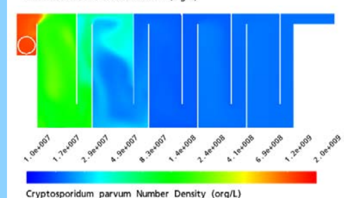
# Demonstration of Full Scale Feasibility (Bartrand, 2006)

## Dissolved ozone concentration

Ozone decays rapidly; almost no residual when water reaches the third chamber



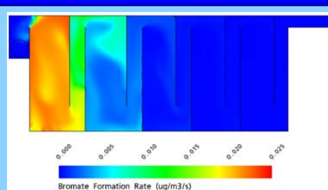

Predicted inactivation matches gross measurements made in full scale contactors



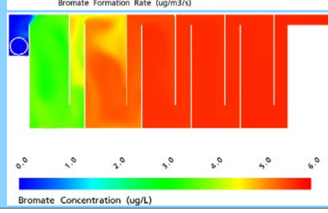

56

## Bromate formation rate

Bromate formation hot spots coincide with regions of high ozone concentration




Predicted bromate concentration matches gross measurements made in full scale contactors

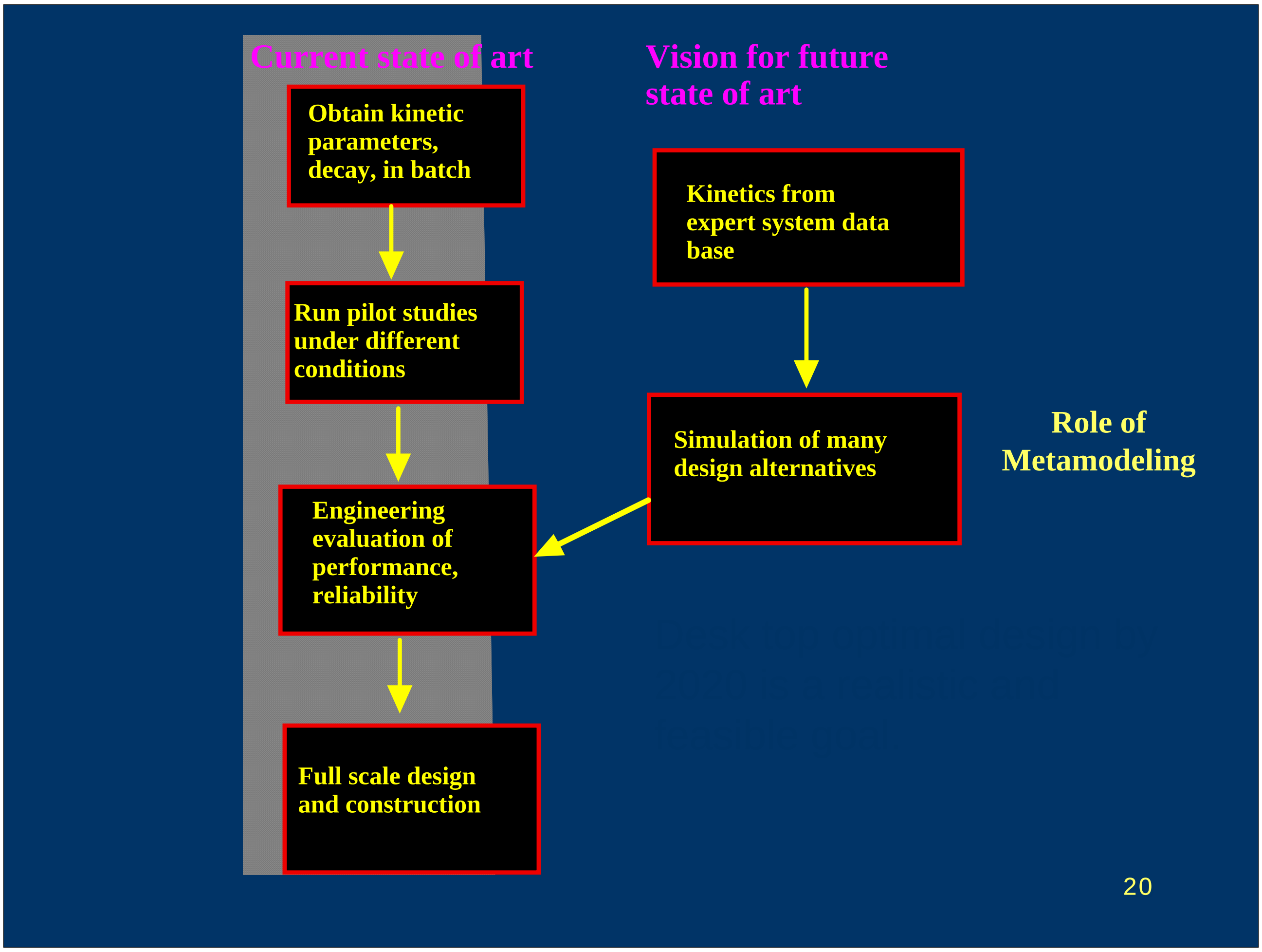



57

# Needs for Future R&D

- More extensive tests of NN kinetic model fitting
  - Data gathering to fill in gaps (rich spectrum of water characteristics)
- Exploration of NN for predictive DBP and demand models
- Validation of CFD approaches in full scale

19



# Oh and by the way

- If we can do this for disinfection …
  - Why not for
    - *Coagulation/flocculation*
    - *Filter performance …*
- And we can build self-learning treatment plants

21

# Acknowledgements (partial)

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22