

A novel engineering tool for ozonation -Unprecedented process insights



Info@AM-TEAM.com

LIVE WEBINAR – June 23rd, 2020 - slides



Today's objectives



Context

AM-TEAM has developed a novel simulation model for ozonation. Already available today through services. The simulation tool will become available soon.

Objectives

••• You get new, detailed process insights

I You learn the basics of ozonation process simulation

••• You understand the practical application and potential of process simulation for process optimisation, design and monitoring

Format

Questions: '<u>Q&A</u>' (not the chat)

I Short questionnaire after webinar



Outline



Intro

Personal introduction

Ozonation and simulation basics

- --- Virtual experimenting and virtual piloting
 - From batch to full-scale
 - **I** Drinking water and wastewater





Personal introduction

We help process technologists getting the processes they desire using very realistic computer simulations

Process simulation services for

- Process optimisation (energy saving, performance increase, ...)
- Process design (optimal mixing, smaller footprint, CapEx saving, ...)
- Process scale-up (lower time to market, significant piloting cost saving, ...)
- II Highly specialised in CFD and kinetic modelling
- Global reach
- Our clients
 - Technology vendors
 - End users and utilities
 - Consulting & Engineering firms
- Exclusive focus on processes

Extensive case studies and blogs: <u>AM-TEAM.com</u>



This is AM-TEAM







3 fundamental ozone facts

FACT #1 OZONE DECAY KNOWS 2 PHASES



FACT #2 TARGET POLLUTANTS ARE REMOVED BY **BOTH O₃ AND HO* RADICALS**



FACT #2 TARGET POLLUTANTS ARE REMOVED BY **BOTH O₃ AND HO* RADICALS**



Target pollutants are removed by both O₃ and HO*





Target pollutants are removed by both O₃ and HO*





Target pollutants are removed by both O₃ and HO*





O₃ DOSED IN A SIMPLE BENDED PIPE – CFD-kinetic simulation including HO*



FACT #3 Bromate is formed by **both O₃ and HO* radicals**



Buffle, M., Galli, S., von Gunten, U. 2004. Enhanced bromate control during ozonation: the chlorine-ammonia process



Batch demonstration

Conclusions



In order to have a valuable simulation model, these facts have to be considered:

- Ozone decay in 'real water' (Fact #1)
- $\square O_3$ and HO* based target pollutant removal (Fact #2)

■ O₃ and HO* based BrO₃ formation (Fact #3)





What is a process simulation model?

What is a process simulation model?





A simulation model for ozonation



Water matrix data

- DOC, COD, UV_{254}
- Conductivity
- Target pollutants
- Br-
- Carbonates

Process model

 $dC_{1,4}$ –dioxane dt $\frac{dC_{BrO_3}}{dt} =$

Prediction of

- Ozone decay
- Target pollutant
 - removal
- Bromate

. . .

• Disinfection

- **Process settings**
- O₃ dose
- Chemical dose
- Volume and flow rates

Prediction examples







What would be the practical value of a process simulation tool for O_3 ??? LIVE DEMO

Different categories of applications (apart from 'process understanding')



II TECHNOLOGY SELECTION

- I How suitable would O_3 be for a specific matrix?
- **..** What would be the specific removal of target pollutants at a certain O₃ dose?
- I Can bromate be suppressed, and what is impact on target pollutant removal?
- Increase the value of real-life piloting efforts (eg complement data; learning)

PROCESS DESIGN

■ What will be the O₃ residual throughout the train? (eg sensor location)

- ••• What is the optimal sizing in view of current and future water characteristics?
- Selection of injection technology (FBD, SSI) what's happening?
- Ozonation runs at Plant A. How would it perform at Plant B?

PROCESS OPERATION

- Real-time monitoring (i.e. 'digital twin')
- New operational strategies (e.g. smart dosing; testing of control strategies)





Conclusion



Conclusion



Status of model application

- I The model is currently being applied at plants in Europe and the US (wastewater effluent and drinking water ozonation)
- Services and support available through AM-TEAM
 - If you have a case: email info@am-team.com)
- I The simulation tool will become available soon
 - No in-house simulation expertise required
- ••• We expect to remove significant practical, regulatory and financial barriers with regard to the application of ozonation
- In Special acknowledgements: Dynamita (FR) and HRSD (US), Dunea (NL)



FULL WEBINAR RECORDING





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APPENDIX: live demo slides

Case 1 – batch reactor Batch reactor **I** Fitting real batch data O3 reacts with water matrix **II** BrO3 formed by complex chain of reactions Value Aqueous ozone (Batch reactor) (mg O3/L) \checkmark Bromate (Batch reactor) (µg BrO3/L) \checkmark 15- Total UVA absorbance at 254nm (Batch reactor) (m-1) \checkmark Bentazone (Batch reactor) (µg Bentazone/L) Atrazine (Batch reactor) (µq Atrazine/L) Hydroxyl radical (Batch reactor) (mol/L) 11- – 1,4 Dioxane (Batch reactor) (µg 1,4 Dioxane/L) measured O3 resid \sim 7.5-UV254

14

12

9.0

6.0-



1-4Dioxane

Case 1 – batch reactor



HO* concentrationpredicted in real time













Case 2 – Dynamic influent





Case 3 – Full scale plant (SSI VS bubble column)

Bubble column treatment train profile



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Case 3 – Full scale plant (SSI VS bubble column)









Case 3 – Full scale plant (SSI VS bubble column)

Advanced Modelling for process optimisation

1,4 Dioxane (µg 1,4 Dioxane/L)

An unlimited amount of target pollutants can be monitored throughout the whole treatment train



- **SSI** configuration
- Available data (for 270 days!!)
 - Influent UVA254 sensor data
 - Effluent UVA254 sensor data



Based on the influent water matrix is possible to predict HO* concentration and therefore MPs removal

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IN Nonetheless, BrO3 formation for the whole period of 270days



Effluent UVA254 sensor data and modelled data for all 270 days



Using a single parameter set calibrated on a plant in US treating secondary effluent