UNSW Centre for Transformational Environmental Technologies

Catalytic Ozonation Reactor Design using Computational Fluid Dynamics (CFD) modelling

UNSW Centre for Transformational Environmental Technologies

Our expertise:

Using the state of art technology, CFD coupling with chemical reactions to optimise the **catalytic ozonation reactor design.**

✓ **World-class Modelling** ✓ **High Efficiency** ✓ **High Precision**

Catalytic Ozonation in Full-scale Reactors

A set of **elementary chemical reactions** with constant kinetic rates. ✗

Reactions in full-scale reactors are complicated, involving the **interactions between fluid flow, mass transfer and chemical reactions**.

Similar to the three-dimensional distribution of flow field in the full-scale reactors, the reactants and products are usually **unevenly distributed** in the reactors, leading to the consideration of '**Chemical Reaction Dead Zone**' in addition to '**Flow Dead Zone**' in catalytic ozonation reactor design.

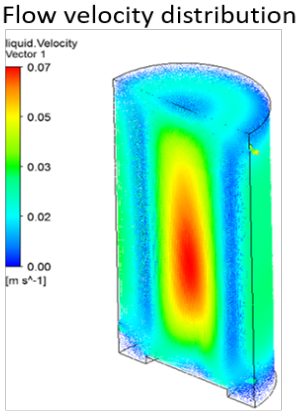
1 Kinetic Modelling of Chemical reactions

Traditional experimental methods was employed to obtain the kinetic models for pure ozonation of formate.

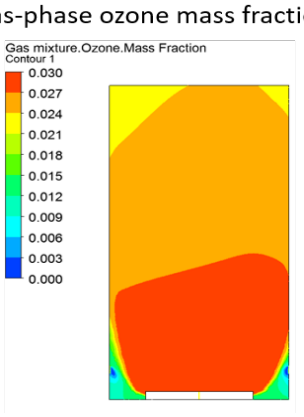
#	Elementary reaction	Reaction rate
1	$O_3 \rightarrow H_2O_2 + O_2$	k_1=2.21e-4 [s^{-1}], R = k_1 [O_3]
2	$O_3 + H_2O_2 \rightarrow OH^* + O_2 + O_2^*$	k_2=97.6 [L/mol/s], R = k_2 [O_3] [H_2O_2]
3	$O_3 + O_2^* \rightarrow OH^* + O_2$	k_3=1.5e+09 [L/mol/s], R = k_3 [O_3] [O_2*]
4	$CO_3^* + O_3 \rightarrow HCO_3^- + O_2$	k_4=1.0e+05 [L/mol/s], R = k_4 [CO_3^{2-}] [O_3]
5	$OH^* + HCO_3^- \rightarrow CO_3^* + OH^-$	k_5=1.22e+07 [L/mol/s], R = k_4 [OH*] [HCO_3^-]
6	$CO_3^* + H_2O_2 \rightarrow HCO_3^- + O_2^*$	k_6=4.30e+05 [L/mol/s], R = k_6 [H_2O_2] [CO_3^{2-}]
7	$HCOOH + O_3 \rightarrow CO_3^* + O_2^*$	k_7=10[L/mol/s], R = k_4 [HCOOH] [O_3]
8	$HCOOH + CO_3^* \rightarrow CO_2^* + HCO_3^-$	k_8=1.5e+05[L/mol/s], R = k_8 [HCOOH] [CO_3*]
9	$HCOOH + OH^* \rightarrow CO_2^* + H_2O$	k_9=3.2e+09[L/mol/s], R = k_9[HCOOH] [OH*]
10	$CO_2^* + O_2 \rightarrow HCO_3^- + O_2^*$	k_{10}=4.2e+09[L/mol/s], R = k_{10}[CO_2*] [O_2]

2 Coupling of Hydrodynamics and reactions

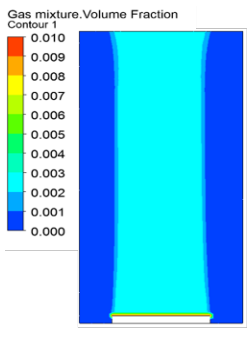
Flow velocity distribution



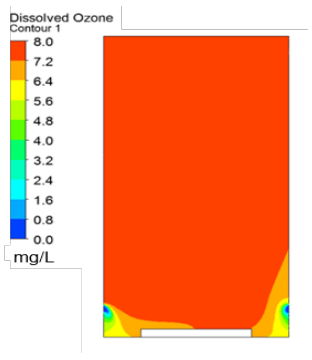
Gas-phase ozone mass fraction



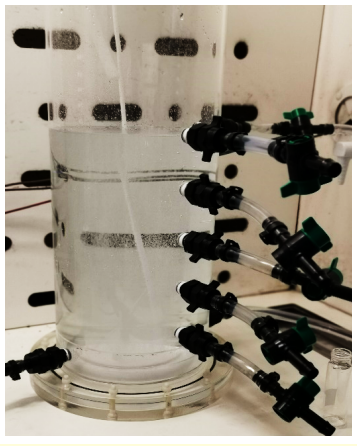
Gas volume fraction

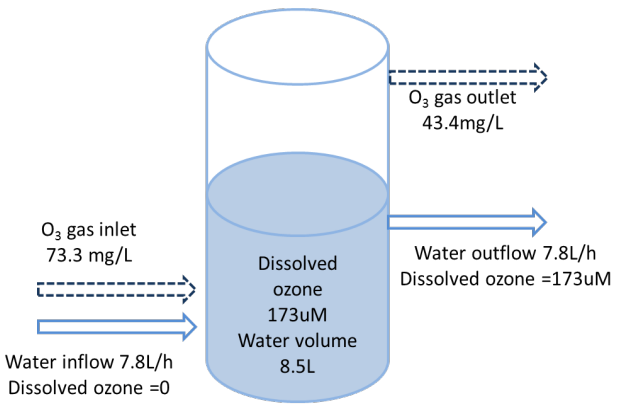


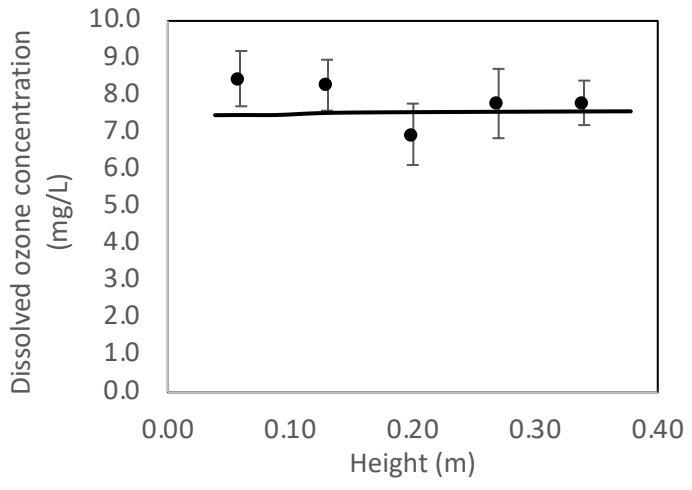
Dissolved ozone concentration



3 Continuous Flow Experiments for Model validation







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