PHOTOCATALYTIC DEGRADATION OF NITRIC OXIDE IN AN ANNULAR REACTOR: EXPERIMENTAL STUDY AND CFD MODELING

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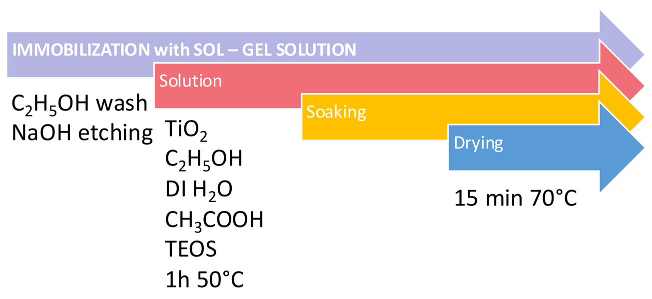
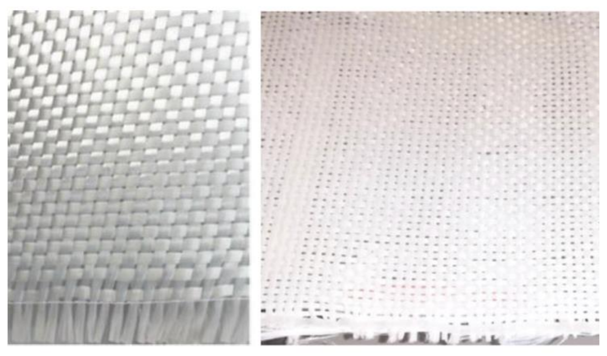
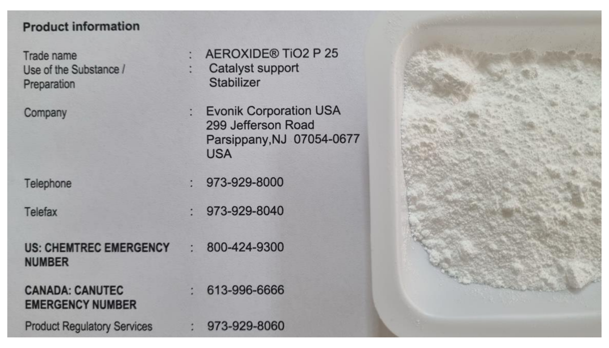
Nitrogen oxides (NO_x) are major air pollutants associated with combustion processes and urban air pollution. Semiconductor photocatalysis using titanium dioxide (TiO_2) represents a promising approach for passive and active air purification. However, transferring laboratory-scale photocatalytic performance to larger systems requires an understanding of reaction kinetics, mass transfer, fluid flow and radiation distribution. This study investigated the degradation of nitric oxide (NO) using TiO_2 immobilized on glass fiber mesh in an an annular reactor under simulated solar irradiation. Experimental results were used for the development of a CFD model applicable to photocatalytic reactor scale-up.

PHOTOCATALYTIC MATERIAL





Comparison of the glass fiber mesh and the photocatalytic film mounted on a glass fiber mesh



TiO_2 powder and product information sheet

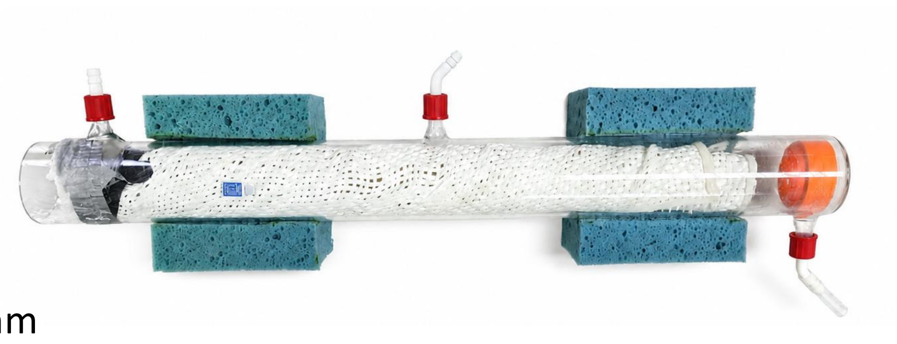
75% anatase : 25% rutile
primary particle size: 30 nm

BET surface area: 56 m^2g^{-1}

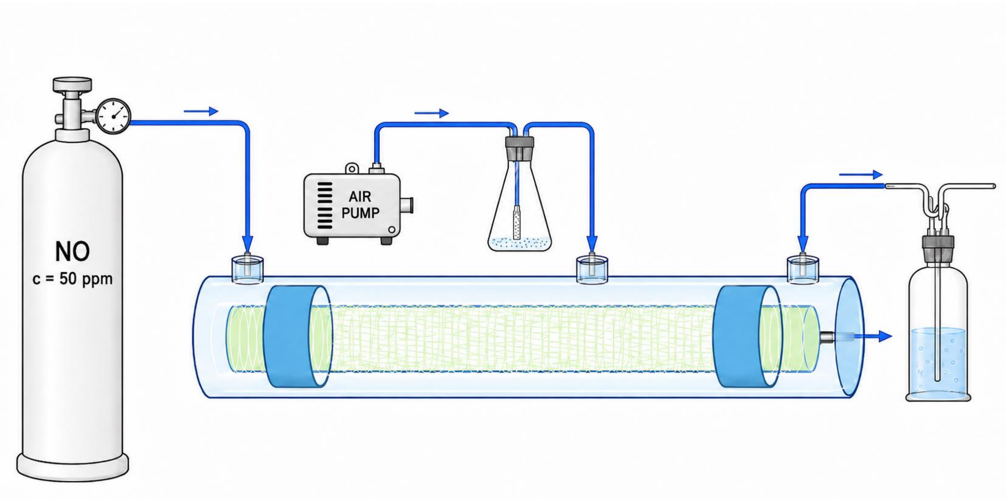
GM + TiO_2 layer thickness:
3.4 ± 0.2 mm

TiO_2 loading on GM:
0.0017 ± 0.0001 g/cm^2

EXPERIMENTAL SETUP

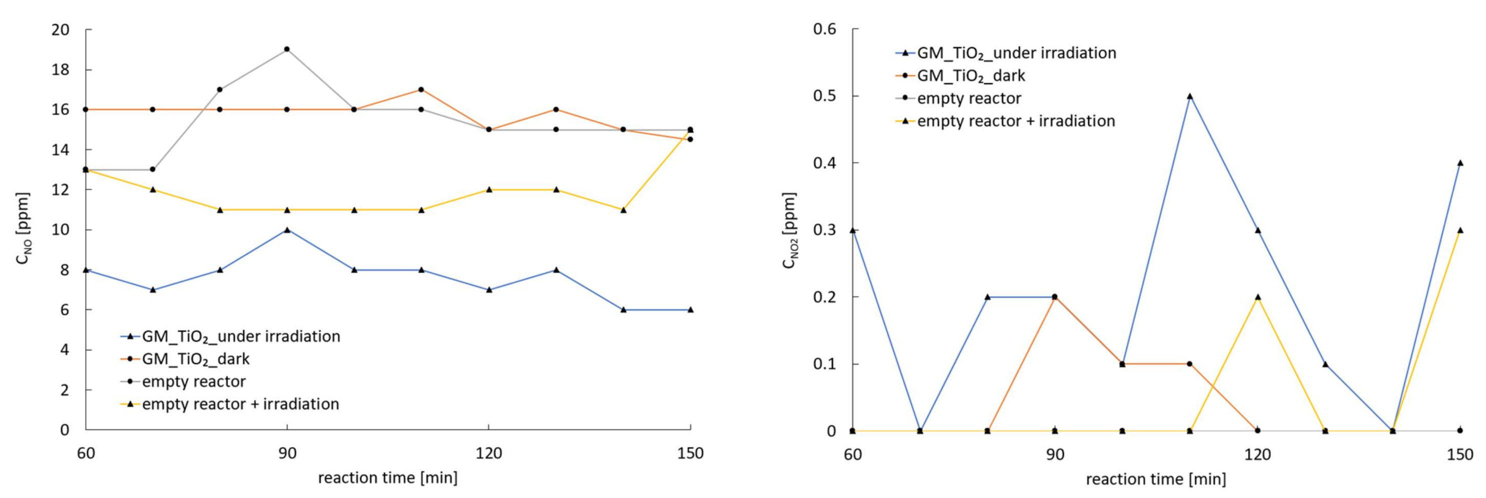


Annular reactor with TiO_2 immobilized on glass fiber mesh

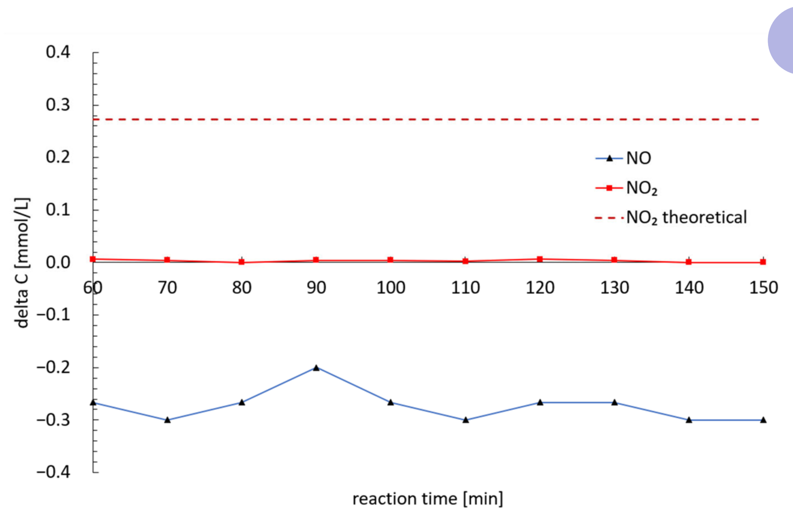


Shematic of annular reactor setup

PHOTOCATALYTIC TRANSFORMATION OF NO



Measured NO and NO_2 concentration at the outlet: comparison in an empty reactor with and without irradiation and during the adsorption experiments (GM_TiO$_2$_dark) and photocatalytic experiments (GM_TiO$_2$_under irradiation)

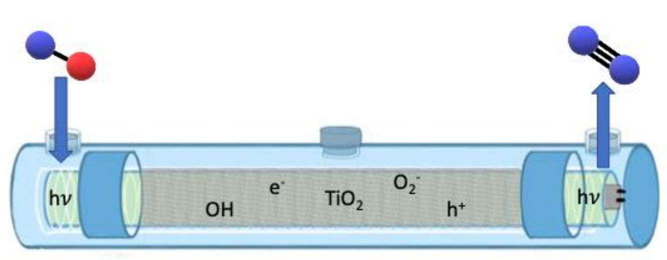


Relative changes in NO and NO_2 concentration during photocatalytic transformations in an annular reactor

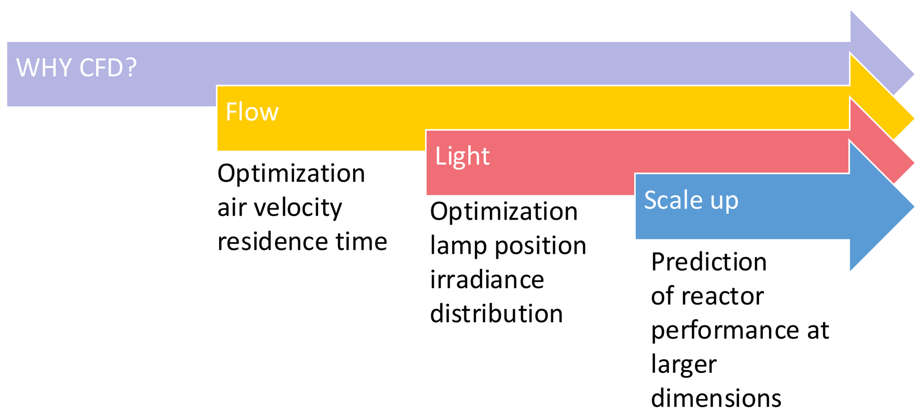
Two principal photocatalytic pathways were identified: reduction of NO to molecular nitrogen and oxidation to nitrate species

The photocatalytic transformation of NO followed mass-transfer-controlled first order kinetics

$k = 0.0984\ min^{-1}$

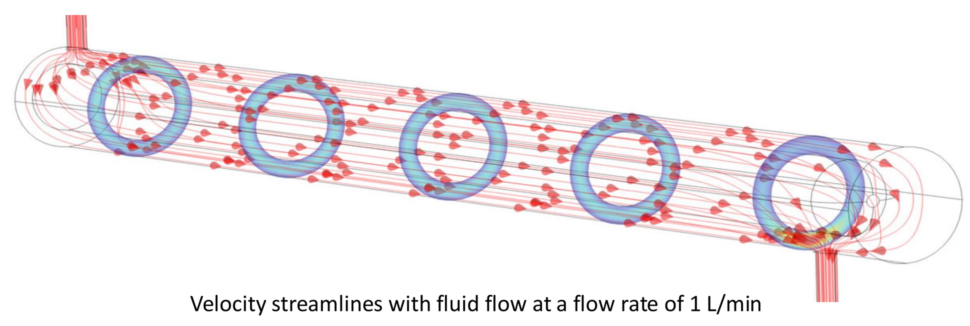


CFD MODEL

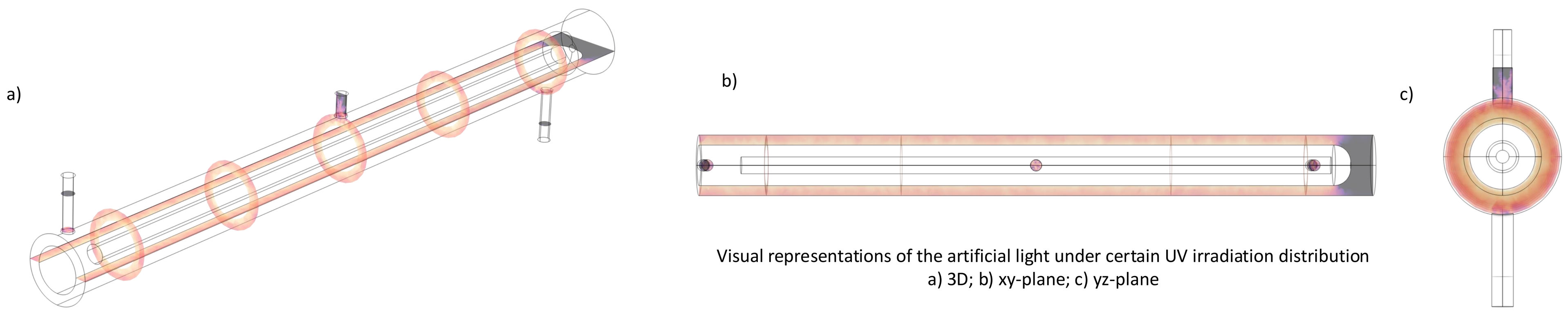


The highest gas velocities were observed at the reactor inlet and outlet, while laminar flow was maintained along the reactor length

Experimental data were implemented in COMSOL Multiphysics 6.2 to model reactor geometry, fluid flow, irradiation, species transport and chemical reactions



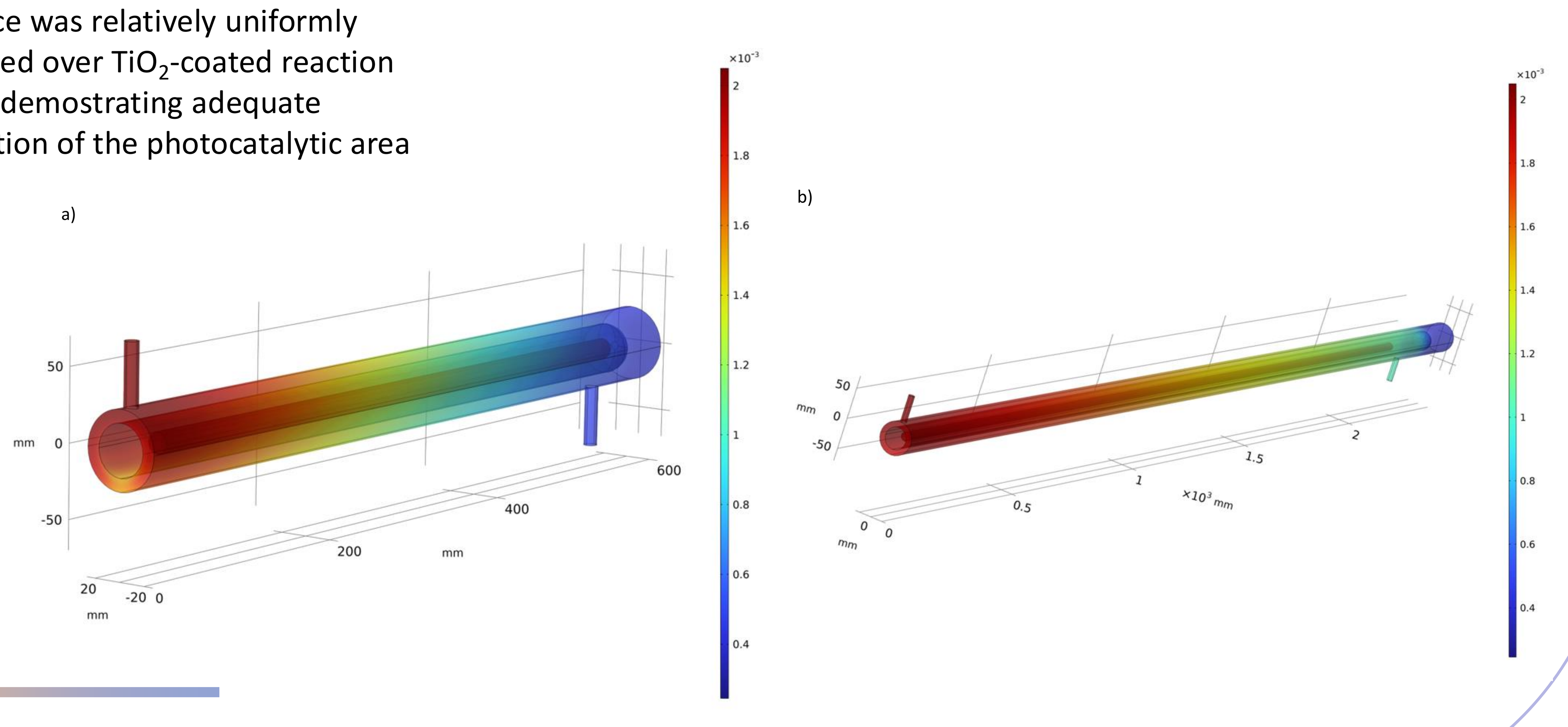
Velocity streamlines with fluid flow at a flow rate of 1 L/min



Visual representations of the artificial light under certain UV irradiation distribution
a) 3D; b) xy-plane; c) yz-plane

Irradiance was relatively uniformly distributed over TiO_2-coated reaction surface, demostrating adequate illumination of the photocatalytic area

Provided results successfully replicate the test results following the Langmuir-Hinshelwood mechanism



Simulated concentration profile of NO at time step t = 9000 s at inlet concentration of 2.045*10^{-6} mol/L in
a) annular reactor L = 600 mm; b) prolongated reactor L = 2400 mm

The results of this study demonstrate that the photocatalytic transformation of NO under humid air conditions proceeds predominantly through two reaction pathways, namely reduction to N_2 and oxidation to nitrate species. A detailed understanding of the governing reaction kinetics is essential for the reliable interpretation of photocatalytic performance, the optimization of operating parameters, and the rational design of reactors intended for larger-scale applications. While annular reactors are intrinsically constrained by their limited air throughput and are therefore not directly applicable to large-scale outdoor air purification, computational fluid dynamics (CFD) provides a powerful approach for evaluating reactor performance, optimizing geometrical and operational parameters, and identifying design modifications that may facilitate the development and scale-up of photocatalytic air treatment systems.

From laboratory kinetics to real-scale air purification

Coupling experimental photocatalysis with CFD modeling provides a pathway toward the rational design and scale-up of photocatalytic air treatment reactors

RECYCLING RUBBER &
SOLAR PHOTOCATALYSIS
ecological innovation for passive air and health protection
KK.01.1.1.07.0058

Gumiimpex - GRP

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