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N-hexane abatement using a non-thermal plasma

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Abstract: This work is part of a collaborative research project to evaluate the relevance of combining an oxidation technique to a complementary process for the treatment of VOCs in air. VOCs are volatile organic molecules that are among the main atmospheric pollutants. They have several uses in different industry sectors, in particular as solvents, but they have harmful effects on health and the environment. Conventional VOC treatment methods (adsorption, oxidation...) are not always sufficient. The use of non-thermal plasmas can be a solution. The present study is done with the purpose of evaluating and understanding the effect of a dielectric barrier discharge (DBD) on a heavy hydrocarbon in terms of removal efficiency in dry air as well as by-product formation, in view of further coupling to a complementary process. The chosen molecule, n-hexane, C₆H₁₄, is a VOC found in different types of industries, its treatment is likely to generate numerous by-products. This aim of this study is to understand the physicochemical processes involved in the abatement of n-hexane in air by non thermal plasma,

EXPERIMENTAL SET-UP

DBD reactor:

Reactor volume = 3.9 cm³
Flow rate : Q = [0,5, 1] L/min

Electrical Parameters :

ND 23 kV
V_c = 11,5 kV
E_{pulse} = 3,8 mJ

- Frequencies : f = [500, 1000, 1500] Hz.
- Energy E_{pulse} (J) deposited in the plasma per pulse:
E_{pulse} = ∫ I(t)·V(t)dt
- Specific energy density(J/L):
SED = E·f/Q

Mesures effectu es avec un oscilloscope LeCroy 204MXi-A (0.5 L/min, 500 Hz)

Detectors at the reactor outlet:

- Real-time ozone (UV 254 nm) and CO₂ (IR)
- Detection et quantification of n-hexane, H₂, CO, formaldehyde using gas-phase chromatography (Micro-GC Fusion).
- Detection of remaining by-products (ppb) using high-resolution mass spectrometry.

BTrap : The high mass resolution allows to separate quasi-isobaric compounds and to follow their evolution in the discharge. The chemical ionization can be done with two different precursors: either O₂⁺ (to follow the n-hexane) or H₃O⁺ (to follow the by-products)

RESULTS AND DISCUSSION

Ozone production:

Effect of n-hexane on ozone production (500 Hz, 150 J/L, 500 mL/min)

Δ(Ozone)_{air} = 30 ppm
Δ(Ozone)_{hexane} = 10 ppm

- Ozone production: [2,3]
 - O₂ + e → O(³P) + O(³P) + e
 - O₂ + e → O(¹D) + O(³P) + e
 - O(¹D) + M → O(³P) + M
 - O₂ + O(³P) + M → O₃ + M
- Ozone destruction: [2,3]
 - O₃ + NO → NO₂ + O₂
 - O₃ + O₂(¹Δ) → O₂ + O₂ + O(³P)
 - O(³P) + O₃ → O₂ + O₂
 - O(³D) + O₃ → O₂ + O₂(¹Δ)

Thermal effect in an air discharge (1000 Hz, 660 J/L, 500 mL/min)

In the presence of C₆H₁₄ in the gas stream, in addition to the previous reactions, an atomic oxygen O or a hydroxyl radical HO[•] can break a C-H bond on the n-hexane molecule.

$$C_6H_{14} + O(^3P) \rightarrow HO^\bullet + C_6H_{13}$$

$$C_6H_{14} + HO^\bullet \rightarrow H_2O + C_6H_{13}$$

O and especially OH are also involved in other reactions with by-products.
This explains the lower ozone detection when n-hexane is introduced into the discharge.

There are three possibilities for initiation reactions with breaking on : C₁(C₆), C₂(C₅) or C₃(C₄) in n-hexane molecule

Q = 0.5 L/min and f = 500 Hz

β = 350 J/L

N-hexane abatement:

- Results were obtained at the exit of the reactor using the micro -GC Fusion (black points) and the BTrap (hollow points).
- Exponential decay:

$$[COV] = [COV]_0 \exp(-SED)/\beta$$

- [COV]₀: inlet concentration of n-hexane
- β: characteristic energy
- n-hexane : [5-500] ppm

Q = 0.5 L/min and f = 500 Hz

Q = 1 L/min and f = 500 Hz

Complete conversion:

- at 930 J/L (5 ppm)
- at 1350 J/L (11 ppm)

Effect of total gas flow rate:

Residual C₆H₁₄ measured at the reactor exit as a function of the SED for an inlet concentration of 50 ppm of C₆H₁₄ at 500 Hz and 0.5 L/min and 1 L/min).

In our case: no critical influence of the gas flow rate on the abatement of C₆H₁₄

Removal efficiency:

$$\text{Efficiency } \chi = \frac{[COV]_0 - [COV]}{[COV]_0} * 100$$

- Results obtained at the exit of the reactor using the BTrap, and the Micro-GC Fusion.
- SED = 250 J/L, f = 500 Hz.
- Applied voltage 25 kV, Q = 0,5 L/min

The less polluted the air stream, the easier is the treatment

By-product formation:

By-products detected using the Btrap (210 J/L, 500 Hz, 0.5 L/min).

Evolution of the main by-products in the discharge in air with and without n-hexane (100 ppm) (210 J/L, 500 Hz, 0.5 L/min)

Main by-products: formaldehyde, acetaldehyde, propanal, carbon dioxide

Detection of by-products that aren't issued from the oxidation of n-hexane: H₂ (13 ppm for 500 ppm of n-hexane) and HCN.

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