

# Physics-Based Dynamic Estimation of NO<sub>2</sub> and H<sub>2</sub>O Concentrations with CNT-FETs and Extended Kalman Filter

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## Summary:

We present a Langmuir-based Extended Kalman Filter (EKF) framework for real-time estimation of NO<sub>2</sub> at ppb-level concentrations in humid air at room temperature. Two CNT-FETs gas sensors were exposed to a gas-mixture experiment involving different NO<sub>2</sub> and humidity (H<sub>2</sub>O) concentrations, with threshold voltages ( $V_T$ ) extracted from sensors transfer characteristics over time. The  $V_T$  signals were first fitted using a two-gas Langmuir isotherm-based model; next, an Extended Kalman Filter (EKF) enabled dynamic NO<sub>2</sub> and H<sub>2</sub>O simultaneous estimation.

**Keywords:** Carbon Nanotube Gas Sensor, Signal Processing, Dynamic Modeling, Real-time Prediction, Extended Kalman Filter (EKF).

## Background, Motivation and Objective

Carbon nanotubes (CNTs) are 1D materials known for their gas sensing capabilities and high sensitivity to nitrogen dioxide (NO<sub>2</sub>). In this work, we fabricate NO<sub>2</sub> gas sensors based on CNT field-effect transistors (CNT-FETs), where a pristine CNT is suspended between platinum source and drain electrodes, with the gate located beneath the channel (Fig. 1a). The device is a p-type transistor, in which NO<sub>2</sub> adsorbed onto the CNT p-dopes the channel through electron withdrawal. This effect is visible in the transfer characteristics (i.e., drain current  $I_D$  as a function of gate voltage  $V_{GS}$  at fixed  $V_{DS}$ ), where NO<sub>2</sub> adsorption on the CNT induces a threshold voltage  $V_T$  shift [1]. Humidity (H<sub>2</sub>O) produces an

opposite, though weaker, effect (Fig. 1b). The objective of this work is to estimate NO<sub>2</sub> and H<sub>2</sub>O concentrations dynamically over time. In previous works, we extracted multiple features from transfer characteristics [2] and used quasi-steady-state data to predict gas concentrations via machine learning [3]. Here, we move from a static to a dynamic approach by modeling the temporal evolution of  $V_T$  induced by gas adsorption/desorption, using a two-gas Langmuir model applied to two CNT-FETs [4]. Following a calibration phase in which the model parameters are fitted, NO<sub>2</sub> and H<sub>2</sub>O concentrations are estimated online using an Extended Kalman Filter (EKF) [5]. With respect to our most recent work [6], the present study introduces the following novelties. First, two devices are used, demonstrating that the Langmuir based-model is reproducible across different CNT-FETs. Second, the experimental dataset is split into a calibration subset (phase I) for model fitting and a subsequent test subset (phase II), designed to mimic a realistic gas exposure scenario, for gas concentrations estimation; previously, the EKF was validated on the same data used for model fitting, while real-scenario testing was limited to synthetic data. Finally, whereas H<sub>2</sub>O was assumed known, here we simultaneously estimate both NO<sub>2</sub> and H<sub>2</sub>O concentrations.

## Gas Experiment

Two CNT-FETs devices (devA and devB) were exposed to the same gas experiment at room temperature, as shown in Fig. 2a. The experiment can be divided into two phases. In phase I, NO<sub>2</sub> and H<sub>2</sub>O concentrations were changed

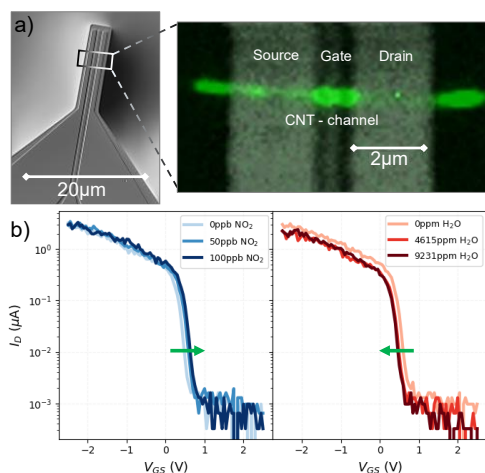


Fig. 1. a) CNT-FET, with CNT identified by Raman spectroscopy (representative). b) Transfer characteristics for different NO<sub>2</sub> and H<sub>2</sub>O at  $V_{DS}=0.1$  V (devA). Each curve was subtracted by its minimum value.

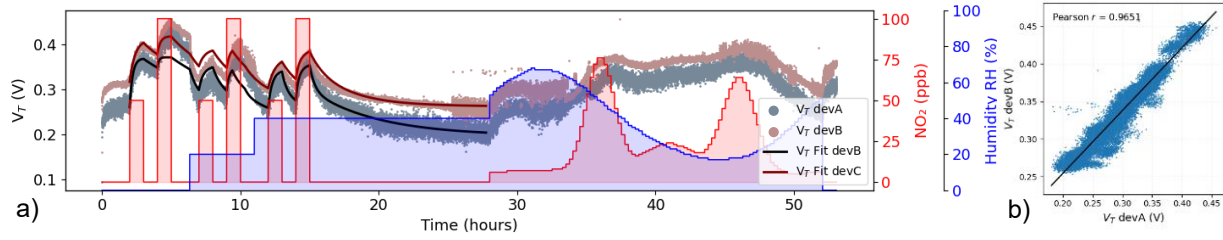


Fig. 2. a) Gas experiment: threshold voltage ( $V_T$ ) and dynamic model fit (phase I). b) Scatter plot of  $V_T$ (devA) vs.  $V_T$ (devB) and Pearson correlation coefficient.

stepwise. In phase II, the gas profiles were designed to mimic a realistic 24-hour scenario: H<sub>2</sub>O follows a sinusoidal-like variation, higher during the night and early morning and lower during the day, while NO<sub>2</sub> exhibits two peaks corresponding to high-traffic times and lower levels at night. During the experiment, transfer characteristics were acquired every 5 s.

### Methods: Dynamic-model-based Prediction

The threshold voltage  $V_T$  signals were fitted over time for devA and devB using the following model, assuming that  $V_T$  is proportional to the surface coverage  $\theta$  of the two gases, and that the steady-state  $\theta$  follows a bi-component Langmuir isotherm [4]:

$$V_T(t) = \alpha_1 \theta_1(t) + \alpha_2 \theta_2(t) + \beta; \quad 1: \text{NO}_2, \quad 2: \text{H}_2\text{O}$$

$$K_{1,2} = \frac{K_{a1,2}}{K_{d1,2}}; \theta_{ss1,2} = \frac{K_{1,2} p_{1,2}}{1 + K_{1,2} p_{1,2} + K_{2,1} p_{2,1}}; \theta_{01,2} = \theta_{1,2} \Big|_{t=0}$$

$$\theta_{1,2}(t) = (\theta_{ss1,2} - \theta_{01,2}) \left( 1 - e^{-(K_{a1,2} p_{1,2} + K_{d1,2})t} \right) + \theta_{01,2}$$

where  $p_1$  and  $p_2$  are NO<sub>2</sub> and H<sub>2</sub>O concentrations, respectively. The fitted parameters include the conversion coefficients  $\alpha_{1,2}$ , the adsorption constants  $K_{a1,2}$  and the desorption constants  $K_{d1,2}$ . The fitting results are illustrated in Fig. 2a. Continuous-time NO<sub>2</sub> estimation is achieved using an Extended Kalman Filter (EKF), that estimates the state of a dynamic system by optimally combining noisy measurements with a predictive model, with covariance matrices tuned empirically [5]. Here, the system state is defined as:  $\hat{x} = [\theta_1, \theta_2, p_1, p_2]$ , and the continuous-time EKF

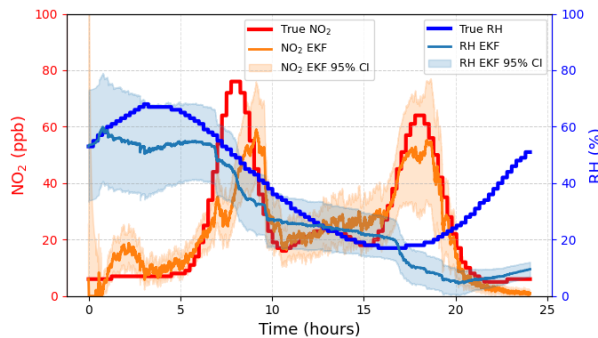


Fig. 3. EKF NO<sub>2</sub> and H<sub>2</sub>O predictions. Mean Absolute Error (MAE) is 6.81 ppb for NO<sub>2</sub> and 2604 ppm (~11% RH: Relative Humidity at 20°C) for H<sub>2</sub>O.

correction equation is given by:  $\hat{x}(t) = f(\hat{x}(t)) + K(t)(V_T(t) - h(\hat{x}(t)))$ , where  $K$  is the Kalman gain,  $f()$  describes the state dynamics and  $h()$  maps the state to the  $V_T$  signals.

### Results and Discussion

NO<sub>2</sub> and H<sub>2</sub>O estimations obtained through EKF are shown in Fig. 3. The dynamic modeling-based prediction approach represents a realistic framework for continuous NO<sub>2</sub> and H<sub>2</sub>O tracking. It should be noted that CNT-FETs exhibit higher sensitivity to NO<sub>2</sub> than to H<sub>2</sub>O, and that the  $V_T$  signals of the two devices are strongly correlated (Fig. 2b). Ideally, improved selectivity could be achieved by using devices with different sensitivities to the two gases. Nevertheless, the proposed method enables ppb-level NO<sub>2</sub> estimation in the presence of unknown humidity, representing a promising approach for real-world gas sensing applications.

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