Machine learning based determination of photoacoustic signal parameters for different gas mixtures

Lukić M(1)*, Ćojbašić Ž(2), Markushev D(3)

(1) Faculty of Occupational Safety, University of Nis, Carnojevica 10a, Nis 18000, Serbia
(2) Mechanical Engineering Faculty, University of Nis, Aleksandra Medvedeva 14, Nis 18000, Serbia
(3) Institute of Physics, University of Belgrade, Pregrevica 118, Belgrade-Zemun 11080, Serbia

* Corresponding author's email: mladenalukic@gmail.com

Detection of different trace gases with the same instrument is one of the important requirements for in situ measurement. Benefits of computational intelligence (CI) implementation in photoacoustic spectroscopy (PAS) such as real-time operation and accuracy are confirmed [1], but whether intelligent PAS method can provide high selectivity in the detection of different trace gases? In this paper pulsed PAS is used to study C_2H_4+Ar gas mixture. Experimental signals are generated in the C_2H_4+Ar gas mixture, at absorber pressures $p_{(C2H4)} = 0.47$ mbar, total mixture pressure $p_{tot} = 100$ mbar, and laser fluence $\Phi = 1\ \mathrm{Jcm^{-2}}$ [2]. Although multilayer perceptron network (MLPN) determines parameters of PA signal (spatial laser beam radius and vibrational-to-translational relaxation time) successful, selection of optimal MLPN architecture through a trial-and-error process, can be computational cost. To overcome problems related to network architecture Generalized Regression Neural Network (GRNN) is used to estimates PA signal parameters [3]. GRNN has some advantages such as fixed structure (there is no requirements for overall network optimization to select parameters of hidden neurons), and fast training (without an iterative procedure). Networks were trained in an off-line regime. Theoretical PA signals (1) as the solution of the nonhomogeneous linearized wave equation, are calculated by the Fourier method [4] for top-hat spatial laser beam profile and different values of parameter ε (relaxation time) $\in$ [0.5-4] and parameter r^* (laser beam radius) $\in$ (39, 39.5, 40, 40.5).

$$\delta p(r^*, t^*) = \frac{RE_0}{C_v V} \int_0^\infty (l^2 + \varepsilon^2)^{-1} [-\varepsilon exp(-\varepsilon t^*) + lsinlt^* + \varepsilon coslt^*] J_0(lr^*) h(l) l dl. \quad \text{Eqn. 1}$$

where ε related with relaxation time τ_{V-T} ($\varepsilon = \tau_p/\tau_{V-T}$) and r^* related to the radius of the laser beam r_L ($r^* = r/r_L$). GRNN was trained with 284 theoretical PA signals (Fig. 1). Several network structures were designed with different numbers of neurons in input layers (21 to 50) to test network prediction under different numbers of neurons in the input layer. To compare the efficiency and effectiveness of MLPN prediction for SF_6+Ar gas mixture and GRNN prediction for C_2H_4+Ar, a regression network was designed with 21 input neurons (as well as the MLPN). GRNN with 50 input neurons (Fig. 2) estimated parameters ε and r^* with errors 0.79%, and 0,02% respectively. GRNN with 21 input neurons provides better prediction in

comparison with MLPN primary for parameters ε. Molecules SF_6 and C_2H_4, are medium-sized polyatomic molecules with common relaxation characteristics, so possible limitations for in situ measurement are discussed.

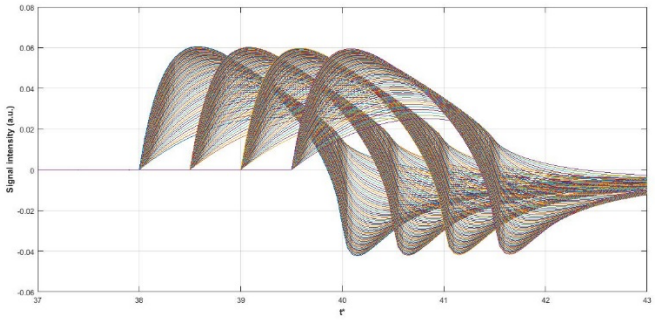

Fig. 1. Training set of 284 PA signals calculated by the Fourier method for top hat spatial laser beam profile and ε ∈ [0.5-4] and r^*∈ (39, 39.5, 40, 40.5).

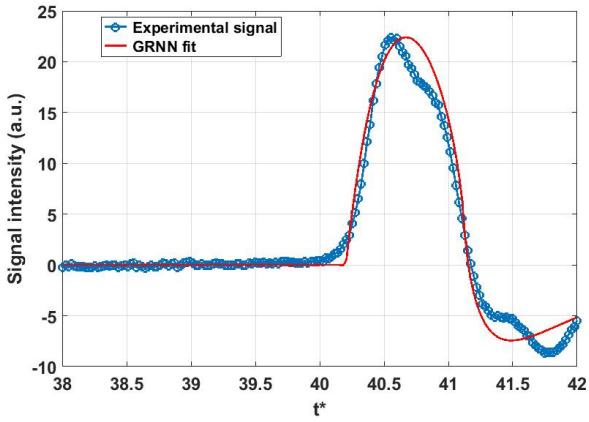

Fig. 2. Comparison between experimental PA signal and PA signal estimated by GRNN with 50 input neurons.

References

[1] M. Lukić, Ž. Ćojbašić, M.D. Rabasović, D.D. Markushev, Computationally intelligent pulsed photoacoustics, Meas. Sci. Technol. 25 (2014) 125203 (9pp). https://doi.org/10.1088/0957-0233/25/12/125203.

[2] Rabasović, M.D., Nikolić, J.D. & Markushev, D.D. (2006b) Pulsed photoacoustic system calibration for highly excited molecules: II. Influence of the laser beam profile and the excitation energy decay. Meas. Sci. Technol. 17 (2006) 1826–1837. https://doi.org/10.1088/0957-0233/17/7/022.

[3] D.F. Specht, A General Regression Neural Network, IEEE Trans. Neural Netw. 2 (1991) 568-576. https://doi.org/10.1109/72.97934.

[4] K.M. Beck, A. Ringwelski, R.J. Gordon, Time-resolved optoacoustic measurements of vibrational relaxation rates, Chem. Phys. Lett. 121 (1985) 529 – 534. https://doi.org/10.1016/0009-2614(85)87134-7.