Indexes of tobacco smoke contribution to environmental particulates based on molecular fingerprints of alkanes

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Abstract
Tobacco smoking is the source of a number of toxicants globally affecting the air and posing a concern also for no smokers. Hence, chemical, physical and toxicological features of exhausts (i.e., vapours as well as mainstream, sidestream and third hand smoke) have been extensively investigated. Apart from a handful of macro-components of combustion (e.g., CO, tar, fine and ultrafine particles, nitrogen oxides), some hundreds of organic substances have been identified in smoke. Some of these chemicals, individually or as groups, give raise to peculiar molecular fingerprints and look potentially suitable to act as "chemical signature" of tobacco smoke (TS). Nevertheless, except for nicotelline [1] no indexes have been identified until now as suitable to draw (semi)quantitative estimates of the contribution of TS to environmental pollution, e.g. the TS percentage in particulate matters (carbonaceous aerosol and settled dust), nor in the respective organic fractions. Among TS costituents, long-chain *normal-*, *iso-* and *anteiso-* alkanes (C_{29}-C_{34}) show special percent distributions and molecular signatures [2]. Besides, thanks to low volatility and high persistence in the atmosphere, the evaluation of these chemicals is less prone to artifacts than nicotinoids and organic vapours. This contribution describes the results of an extensive investigation conducted on non-polar lipid fraction of particulates collected in interiors and outdoors. Among various potential parameters associated to long-chain alkane fingerprints, the three most promising ones were selected and finally a cumulative index (TSI) was defined through averaging them, suitable to estimate the TS percentage in organic particulates. Besides, the exceedance of normal C_{31} alkane with respect to average of *n*-C_{29} and *n*-C_{33} homologues was identified as a further index, and the two indexes were plotted vs. each other, revealing a link in the case of airborne particulates but not of dusts. According to back analysis carried out on several sets of particulates, TS seemed to affect even rural areas, while inside non smokers' homes the contributions of TS to PM could account for up to ca. 4.9% and 3.2%, respectively, in airborne particulates and dusts. The TSI% index seemed to run well in locations forbidden to smoking and fail in very polluted locations (e.g. smoking rooms), where other molecular markers, e.g. nicotine and cotinine, are expected to work better.

[1] N.J. Aquilina, C.M. Havel, P. Cheung, R.M. Harrison, K.F. Ho, N.L. Benowitz, P. Jacob III, *Environ. Int*., 2021, **150**, 106417. DOI: 10.1016/j.envint.2021.106417.
[2] I.G. Kavouras, N. Stratigakis, E.G. Stephanou, *Environ. Sci. Technol.,* 1998, **32**, 1369-1377. DOI: 2481/10.1021/es970634e