Application Of A Global Airborne Pollutant Indicator To Quantify The Danger Of Air Pollution

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Abstract

Many researches on air analysis have been carried out for many years. But air analysis reports are sometimes difficult to understand by non-scientific people. That's why a global airborne pollutant indicator (GAPI) to quickly determine the level of pollution was built. Such an indicator used relative impact weights of the different molecules to quantify a pollution based on one or several criteria. These impact weights could take into account several characteristics of the pollutant molecules (toxicity, ability to produce ozone, molecular volume and its impact on microelectronic process…). A combination of factors could also be used in order to be as close as possible to the reality. So, it could be used in different ways: controlling air toxicity, determining the level of pollution in the controlled environment, for example in microelectronics that require less and less contaminants in cleanrooms. GAPI can be adapted to a large range of situations and give a more precise quantification of pollution depending on the selected criteria to be followed.

Examples of utilisation of this indicator are shown in this study. An analysis of an industrial pollution is used as an example for report. Then GAPI is calculated with an MIR indicator as impact factor to calculate the ability of global exhaust to produce ozone. Comparison between GAPI and the classical sum of concentration can give an overview of the impact of pollution in the production of ozone. Then, an example of GAPI utilisation in indoor air is given for an irritant atmosphere.

Keywords: air quality, VOC, measurement, pollutant impact.

1 Introduction

Nowadays, volatile organic compounds (VOCs) are known to be an important air pollution factor for both human health and environmental impact. However having a rapid idea of the pollution level and the danger of this air for human is difficult. The evaluation of VOC pollution might be very important in some industrial production for the process made in the fab.

Actually, when an analytical report gives a sum of VOC concentrations that can be obtained directly by a flame ionisation detector, it does not represent a real impact of the pollution but just estimation.

For example in microelectronic cleanrooms, VOCs become a very important problem to solve before the decrease of the device geometries based on silicon wafers. Organic contaminants can be adsorbed on the silicon surfaces and had an important effect on breakdown charge yield (Mendicino *et al.* [1]). In this case, molecule size is considered as a problem, so it has to be considered as an impact factor and the concentration of each pollutant must be corrected by this impact. Such correction to precise the impact of pollution is included in proposed Global Airborn Pollutant Indicator (GAPI).

Creation of ozone from VOCs has been a big problem for several years. Tsai *et al.* [2] investigate the relationship between VOC profiles and emission sources. They concluded that aromatics and paraffins were the dominant species which contributed to the ozone formation. That's why the control of exhaust fumes potentiality to create ozone might be important.

So building an indicator that takes account of the real impact of pollutant can clearly show the level of pollution in the considered atmosphere because everybody, particularly non-scientific people, can not easily understand a detailed report of analysis but can follow the evolution of an indicator that gives just one value based on several ponderated concentrations.

Moreover, comparison between air qualities in several atmospheres can be done if the same compound is taken as reference in GAPI calculation and if the same pollution criteria are considered.

2 Definition of the indicator

The indicator (GAPI) includes all the concentrations found in the analysis report and associates an impact weight for each concentration. The methodology to build the indicator was previously described by Cariou *et al.* [3]. The GAPI is defined by eqn. (1).

$$GAPI = \sum_i W_i C_i \tag{1}$$

with C_i the concentration of pollutant i and W_i the impact weight of the contaminant i.

The impact weight W_i is defined as a characteristic or a combination of molecule parameters. These molecules are potentially dangerous for humans, for a process or for other objective and the potentiality is expressed by the impact weight. For example, MIR index might be taken as impact factor.

W_i can also be a combination of several impact factors. In this case, it is calculated as shown in eqn. (2) with two factors X_i and Y_i.

$$W_i = \sqrt[2]{X_i Y_i} \qquad (2)$$

Each impact factor X_i or Y_i is defined as the chosen parameter ratio between each molecule and reference.

3 Examples of utilisation

3.1 Materials and methods

A complete identification and quantification of pollutants in air is required to build the GAPI. This can be obtained by analysis based on air sampling, gas chromatography to separate pollutants and mass spectrometry to identify and quantify the different species. Of course, if levels of pollution are too low, a preconcentration step might be used before GC/MS.

In our studies, glass tubes packed with Tenax TA (0.17 g) and Carboxen 564 (0.17 g) were used for air sampling by Fernandez [4]. Air was pumped for 4h at 200 mL/min. Sorbent tubes were thermally desorbed by a Perkin Elmer ATD 400 at 250°C for 5 min. The desorb analytes were trapped at –30°C and then the trap was flash-heated to 250°C at 40°C/s for 2min.

The analytical column was a BPX-5 capillary column of 60 m × 0.32 mm I.D. with 3 µm film thickness. Oven temperature was programmed as follows: start at 35°C for 5 min followed by a temperature increase at 10°C/min to reach 300°C held for 5 min. Detection was made by a Perkin Elmer Q-mass 910 detector. Quantification of aromatic compounds was done with toluene as reference, for C-6 alkanes, chlorine compounds and sulphur compounds, references were hexane, tetrachloroethylene and dimethylsulphide respectively.

3.2 Air pollution in a dump of a glass fiber fab

A first example is a fab that uses solvents to impregnate glass fibers. So, VOCs could be found in air of the dump. These reactive VOCs must be considered as potentially sources of ozone production. That is the reason why the MIR index that corresponds to this potentiality was retained as impact factor. All MIR indexes were extracted from Carter tables [5]. MIR value of toluene is taken as reference to calculate the impact weight. This choice is based on the fact that toluene is a major compound and the main aromatic one.

Results of the analysis and ponderation coefficient are shown in table 1.

In this example, toluene is taken as reference for the MIR index based on the formation of ozone, so W_i for toluene is fixed at 1. The other factors W_i are calculated relatively to toluene.

Table 1: Example of GAPI calculation based on MIR index.

Compound	W_i	Concentration ($\mu g/m^3$)	C_iW_i
1,1,1-Trichloroethane	0.0009	50	0.045
Tetrachloroethylene	0.01	1080	10.8
Concentration of chlorinated derivatives		1130	
GAPI (eq $\mu g/m^3$)			**10.845**
Toluene	1	150	150
Ethylbenzene	0.70	40	28
p-Xylene	1.07	110	117.7
o,m-Xylene	2.28	40	91.2
1-Methyl-4-ethylbenzene	1.54	80	123.2
Phenol	0.46	60	27.6
Trimethylbenzene	2.82	40	112.8
2-Ethyl-1-hexanol	0.55	40	22
Concentration of hydrocarbons		**560**	
GAPI (eq $\mu g/m^3$)			**672.5**

Original total concentrations are 1130 $\mu g/m^3$ equivalent tetrachloroethylene for chlorinated compounds and 560 $\mu g/m^3$ equivalent toluene for hydrocarbons. When corrections are calculated by the ozone formation potentiality, GAPI for chlorinated compounds strongly decreases to 10.845 $\mu g/m^3$ and for other compounds GAPI reaches up to 672.5 $\mu g/m^3$.

Comparison between these results shows that a high level of tetrachloroethylene (1080 $\mu g/m^3$) has the same impact than a smaller concentration of ethylbenzene (approximately 15 $\mu g/m^3$) when toluene is chosen as reference. So, to prevent an ozone peak formation, it is better to decrease the level of ethylbenzene than tetrachloroethylene's one. The relative impact on ozone production is clearly shown by W_i values. Obviously, if ozone production is the only factor, ethylbenzene is a stronger pollutant than tetrachloroethylene but if other environmental or health criteria are considered, results can be different. That is why GAPI can be built to combine impacts in order to give the more global impact of air pollutants.

3.3 Fruit and vegetable packaging plant

In this second example, the considered impact of air pollution was the irritation problem due to VOCs into indoor air of a food packaging plant. The annoyance and potential risk were simply estimated considering risk sentences as quality parameter for impact factor. These sentences that characterise the selected compound are R36, R37 or R38 and correspond to irritation as illustrated in table 2.

The GAPI impact factor is fixed arbitrarily. The coefficient 1 is affected to compounds with no risk sentence and 2 is put when the molecule has an irritant property as shown by table 2 and of course the combination of n risks leads to an impact factor given by 2^n. Organic compounds with no irritant property are taken as reference.

Table 2: Impact factor for irritation.

Compounds	Irritation			
	Eye (R36)	Respiratory tract (R37)	Skin (R38)	**X_i**
Hexane	1	1	1	**1**
Butanone	2	2	2	**8**
Methylcyclopentane	1	1	1	**1**
Propionitrile	1	1	1	**1**
Toluene	1	1	1	**1**
Limonene	1	1	2	**2**
Propyldisulfide	2	2	2	**8**

These coefficients show that two compounds are strong irritants (butanone and propyldisulphide) and that limonene presents also an impact.
The real concentrations and the GAPI calculation with Xi given in table 2 are shown in table 3. In this study, we have only one impact factor, so W_i equals X_i.

Table 3: Calculation of GAPI for the packaging plant.

Compound	W_i	Real concentration (mg/m^3)	W_iC_i
Hexane	1	1.22	1.22
Butanone	8	3.44	27.52
Methylcyclopentane	1	0.64	0.64
Propionitrile	1	0.94	0.94
Toluene	1	0.78	0.78
Limonene	2	19.80	39.60
Propyldisulphide	8	0.97	7.76
Total concentration		**27.79**	
GAPI (eq mg/m^3)			**78.46**

GAPI, in this case, gives a rapid indication of the irritant potential of the atmosphere in the packaging plant. The comparison of the sum of the real concentration and the GAPI shows that the atmosphere can be considered as three times more irritant than a similar atmosphere with no irritant compound. The indoor air quality of this packaging plant could be increased by a rapid decrease of VOC concentrations especially butanone, propyldisulphide and limonene.

4 Conclusion

These examples prove the importance of this indicator in the real knowledge of the danger of atmosphere in indoor air or the potentiality to reduce VOC emissions to avoid ozone formation. When a scale is built, well adapted to demand, it will be easier to see if the air is clean or not. The real impact is always difficult to quantify but GAPI can give a better estimation of this impact. One of the main advantages is that GAPI gives only an adapted value to follow air quality in all situations that need this kind of information.

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