State of the art of aromatic composition of french e-liquids and flavors

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INTRODUCTION

Today, producers of e-liquids offer hundreds of flavors (apple, mint, tobacco, cola, etc). While many studies focus on propylene glycol and vegetable glycerin(1), only few flavors have been looked. The custard ones, "creamy" or "buttered" type, are the subject of very recent studies. The molecules of certain flavor can contain diacetyl which, in large quantities, may have some inhalation toxicity(2).
However other molecules may cause toxicity. It is necessary to identify the molecules present in the aromatic raw materials of e-liquids in order to accede to its toxicological impact. It is therefore necessary to control the chemical and in particular aromatic composition of e-liquids in order to be able to study their toxicity and their degradation products in emission to provide this information to both health authorities and consumers.
The present study shows the results of an analysis campaign of flavors and french e-liquids manufacture in terms of aromatic composition.

Materials & Methods

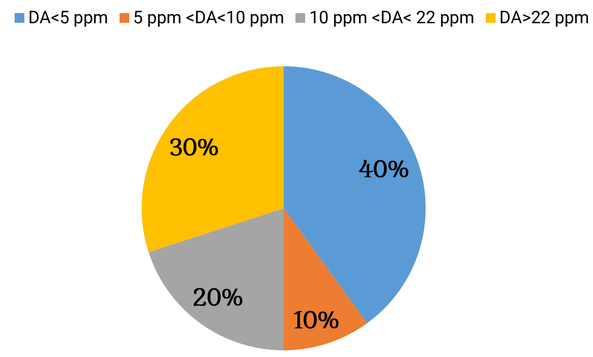
More than 500 french e-liquids with different flavors were analysed :
-350 e-liquids overs 10 brands were analysed for their aromatic composition as part of TPD compliance.
-more than 150 e-liquids overs 6 brands were analysed for the research and quantification of diacetyl.
Moreover flavors from 10 different producers were also tested for diacetyl presence and quantification.
The determination of the aromatic composition of the e-liquids regarding to the molecules above 0,1% of its total mass was performed using a GC-MS-FID system.
The determination of diacetyl is based on their derivatization with 1,2-diaminobenzène to form quinoxalin derivatives. Their determination was done by a GC-MS system using the "single ion monitoring" mode. We focused on the 158 uma ion for the diacetyl derivative determination. Internal calibration was done using 2,3-heptanedione as internal standard.

Results

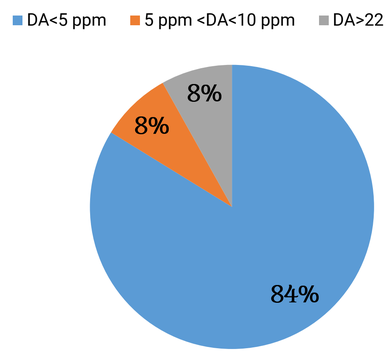
Diacetyl Analysis

Flavors

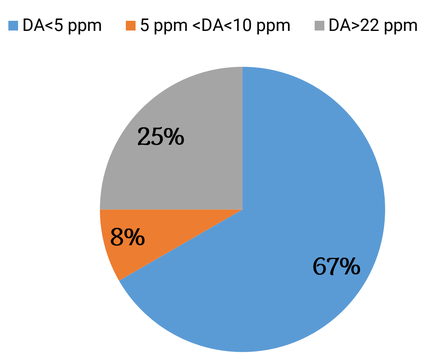
Repartition of Diacetyl Concentration over Synthetic Caramel flavors



Repartition of Diacetyl Concentration over Synthetic Tabac flavors

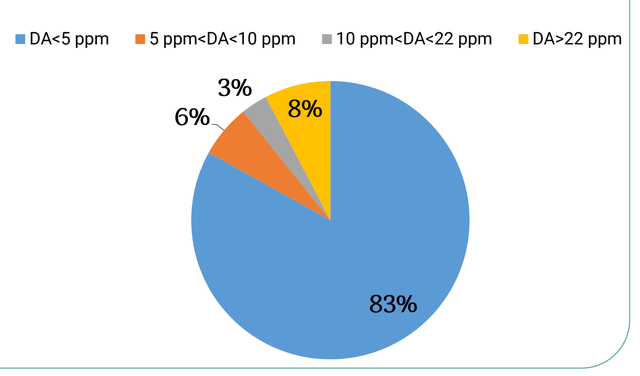


Repartition of Diacetyl Concentration over Synthetic Chocolate flavors



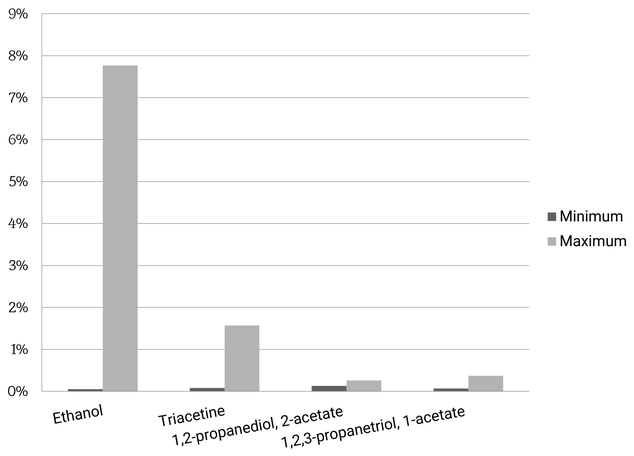
E-liquids

Distribustion of diacetyl concentration over 130 french e-liquids



Solvent composition of french e-liquids

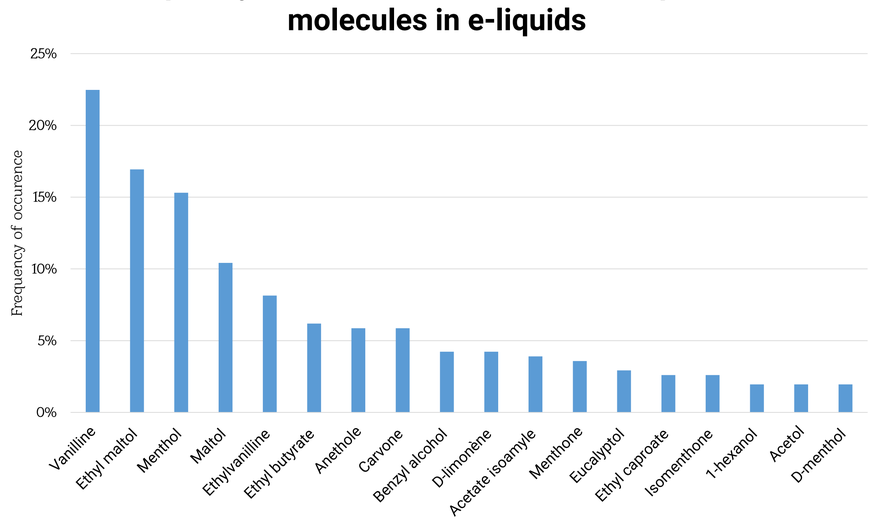
Minimum and maximum concentrations for solvents



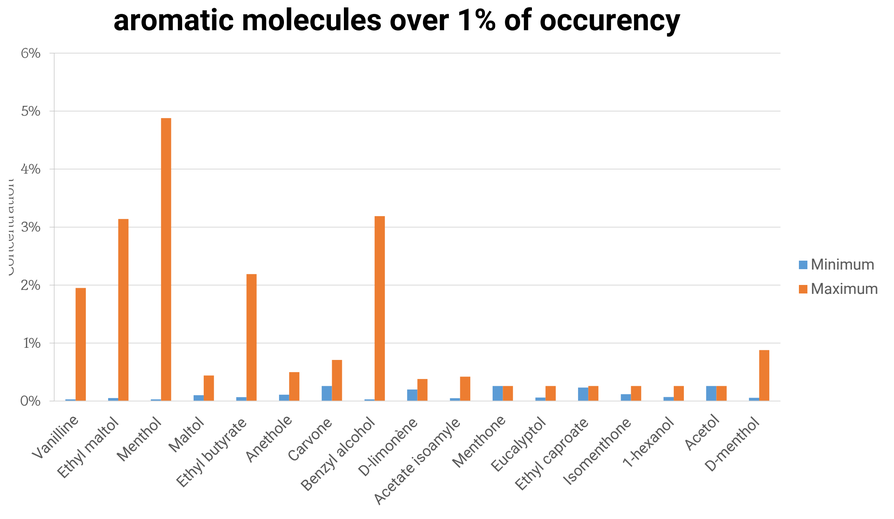
- Maximum concentration in ethanol found in e-liquids: 7.7%
- Most used solvent is ethanol with a frequency of occurrence superior to 50%
- Triacetin is used in less than 10% of e-liquids

Aromatic composition of french e-liquids

Frequency of occurence of the 13 most present molecules in e-liquids



Minimum and maximum concentrations for the aromatic molecules over 1% of occurency



- 100 molecules have been found with a concentration higher than 0.1% w/w
- 12.7% of the liquids did not contain molecules to declare, that is to say concentrations less than 0.1%

CONCLUSION

The present study confirms that some gourmet type flavors such as caramel or chocolate are predisposed to contain diacetyl. Indeed, there is a high variability of concentration of DA in these flavors of which a proportion of 30% exceeds 22ppm (3). A more conventional flavor as tobacco has lower DA concentrations. In the case of the e-liquids tested, 92% of them comply with the limit of 22 ppm with a 83% share which is less than 5 ppm.
Among the solvents contained in the e-liquids, it is noted that the manufacturers use mainly (54%) ethanol, molecule brought by the flavors. When used, ethanol is detected at maximum concentrations of 7.7%.
Concerning the aromatic composition of the e-liquids, among the 100 molecules found at concentrations higher than 0.1% w, only 13 appear at frequencies higher than 1%.
In conclusion, this first study shows that although manufacturers offer a multitude of flavors, the list of molecules of interest is reduced because of their redundancy. Such information is important because it shows that this short list of molecules will lead to less emission / inhalation toxicological research.
The first bibliographic research on these molecules from a toxicological point of view does not reveal molecules dangerous for health in the short term.

BIBLIOGRAPHY

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(2) Leigh N., et al. Flavourings significantly affect inhalation toxicity of aerosol generated from electronic nicotine delivery systems. Tobacco control, 2016 (0), pp 1-7.
(3) AFNOR XP D90-300-2