PRELIMINARY RESULTS ON QUANTITATIVE GC-IMS ANALYSIS OF ARABICA AND ROBUSTA COFFEES IN MIXES

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Introduction

EU consumption of coffee in the year 2019 was about 45 million bags (one bag = 60kg)

Coffee market revenue (in million U.S. dollars) [2]**:**
(1) Germany 22457.52; (2) France 13198.85; (3) Italy 11831.6; (4) Spain 11635.26; (5) Austria 4268.42.

Nowadays so-called "third wave" of coffee culture is observed.

Coffee is transformed from a regular commodity to a valuable handicraft product.

There are two main groups of factors that can imply on coffee consumption and purchase:[3]

"sensory qualities"

- smell;
- taste;

are caused by:

- aroma of volatile organic compounds;
- substances that are extracted with boiling water.

"functional motives"

- positive emotions;
- feeling of being aroused;
- focused mental state;

are caused by:

- caffeine (quantity and bioavailability)

Dependence between composition and quality

Despite habit changes, general consumer behavior remains the same: the most important demand is to get a high-quality product.

Fraud in coffee mixes is a widespread problem. In the most often case Arabica is replaced with more cheap Robusta species.

Due to the huge difference in compounds, a poor mix affects beverage quality, alters its taste and aroma.

Coffee as an analytic object

Coffee quality can be assessed with modern analytical techniques:
laser-induced-breakdown spectroscopy, high-performance liquid chromatography, gas chromatography **and Ion Mobility Spectrometry (IMS).**

Arabica species

Pirydine
2,5-Dimethylpyrazine
2,6-Dimethylpyrazine
2-Ethylpyrazine
2-Ethyl-6 -methypyrazine
2-Ethyl-5 -methylpyrazine

2-Oxopropanal
Methyl-D3 1-diderterio-2-propenyl ether
2-furanccarboxaldehyde
2-furanmethanol
Butan-2-one
Acetalaldehyde
2-Methylpirimidine
Acetic acid ethenyl ester

Caffeine content is 0.90 – 1.3%

Robusta species

Pyridine
2,5-Dimethylpyrazine
2,6-Dimethylpyrazine
2-Ethylpyrazine
2-Ethyl-6 -methypyrazine
2-Ethyl-5 -methylpyrazine

2-Methylpyrazine
2 -Acetylfuran
Furfuryl acetate
5-Methyl-2-furancarboxaldehyde
2-Furanmethanol
3-Methylbutyric acid
2,3-Dimethylpyrazine

Caffeine content is 1.51 – 3.3%

Problem statement

Small enterprises can not utilize laboratory-grade techniques due to the high cost of equipment and highly-qualified personnel.

The ion mobility spectrometry (IMS) method is successfully used for VOCs identification.

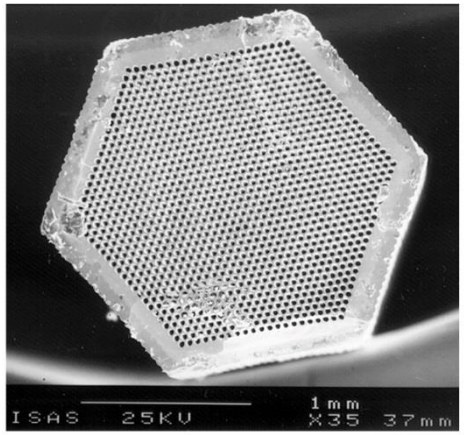
Software based on ML approach may be able to determine the quantitative composition of the coffee mix.

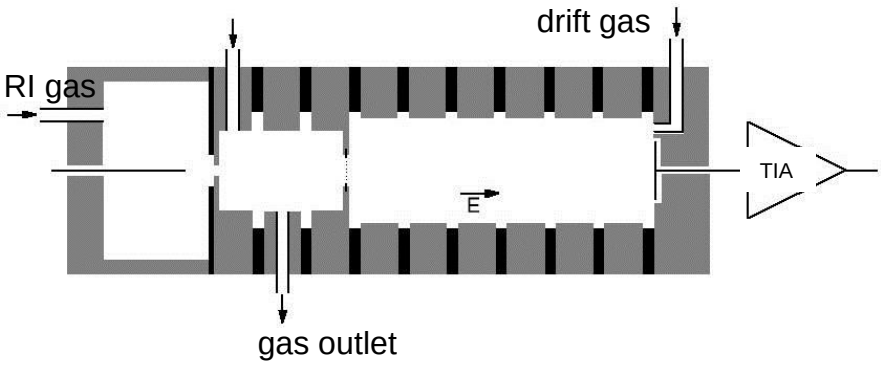
IMS analysis of coffee mixes with ML-based software may become attractive for small coffee-focused enterprises.

MCC-GC-IMS

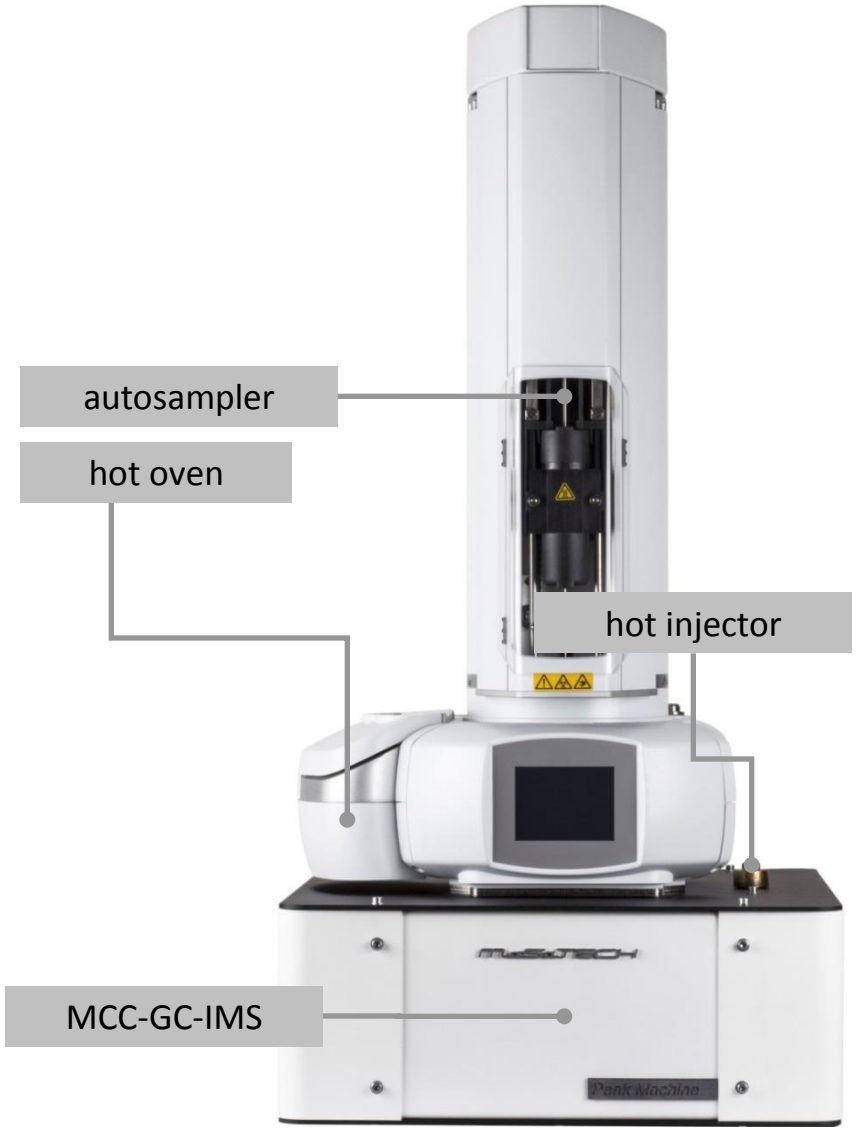
General principle

MCC – multicapillary column;
GC – gas chromatography;
IMS – ion mobility spectrometry.



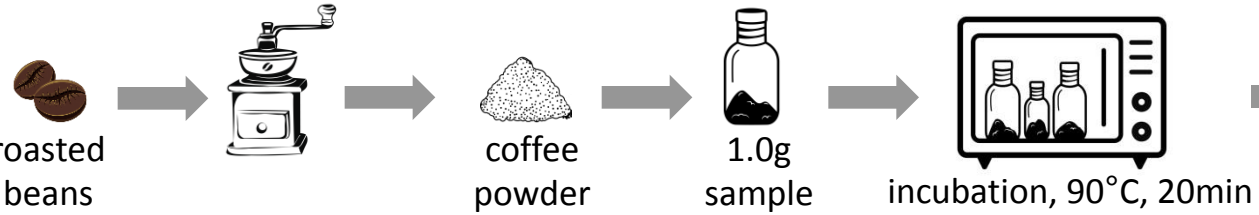


Peakmachine (MaSaTECH, SK)



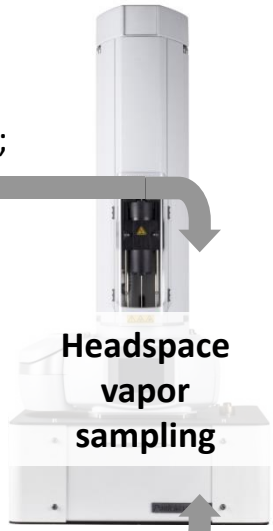
Sample preparation

Pure Robusta or Arabica

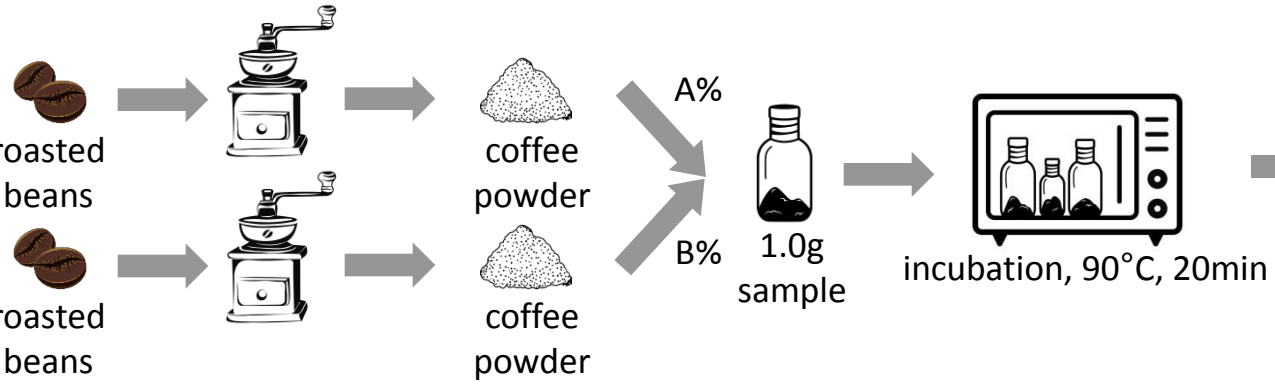


22 Arabica samples;

8 Robusta samples



Mix

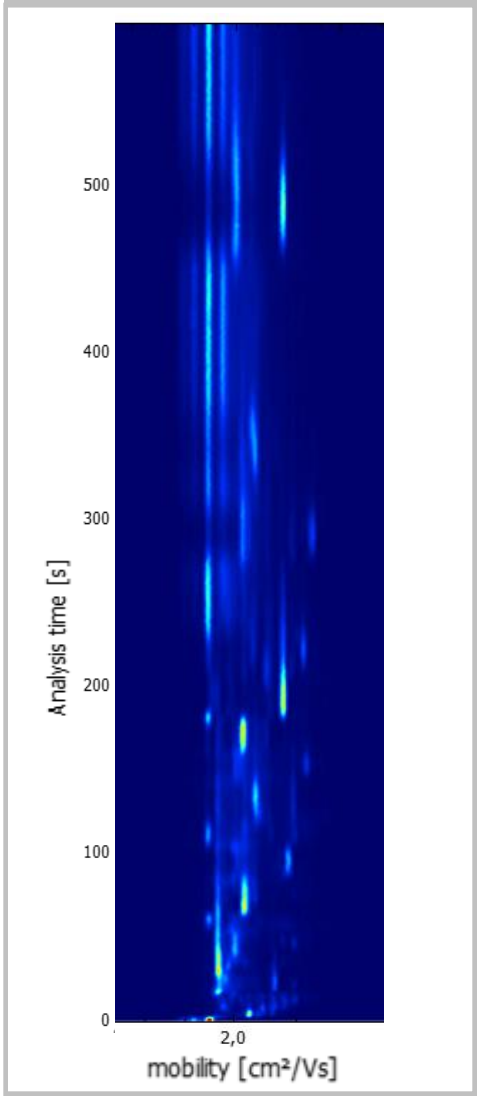


11 mix samples;

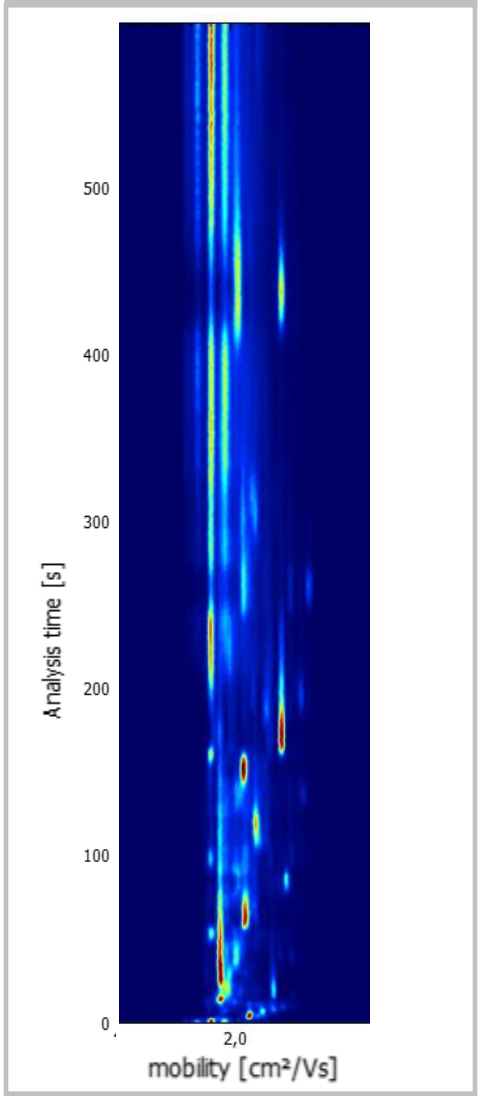
90% Arabica B B 10% Robusta CG I	90% Arabica BE 10% Robusta CG I	80% Arabica B I 20% Robusta H 3c	80% Arabica B G 20% Robusta T	70% Arabica B C 30% Robusta H 3c	20% Arabica T 80% Robusta CP G	20% Arabica C R 80% Robusta SP	20% Arabica T 80% Robusta CPG	20% Arabica B I 80% Robusta CG I	10% Arabica CDC Bol 90% Robusta Caf I	10% Arabica CDC P 90% Robusta CDC M

2D IMS spectra

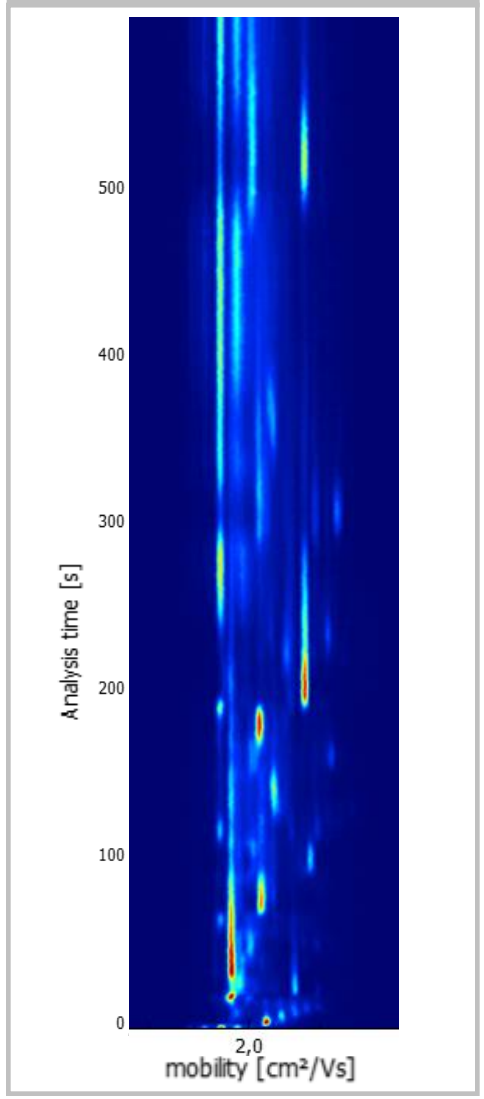
Pure Arabica



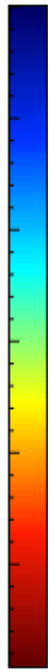
Pure Robusta



Mix (80% A + 20% R)[1]



Peak intensity [a. u.]



[1] 80% Arabica Bozin India with 20% Robusta Hardy 3 countries.

Results

Analysis of obtained 2D spectra with Chemometrics software allowed to achieve 96.6% accuracy.

Mix 1	Mix 2	Mix 3	Mix 4	Mix 5	Mix 6	Mix 7	Mix 8	Mix 9	Mix 10	Mix 11
90% Arabica B B 10% Robusta CG I	90% Arabica B E 10% Robusta CG I	80% Arabica B I 20% Robusta H 3c	80% Arabica B G 20% Robusta T	70% Arabica B C 30% Robusta H 3c	20% Arabica T 80% Robusta CP G	20% Arabica C R 80% Robusta SP	20% Arabica T 80% Robusta CPG	20% Arabica B I 80% Robusta CG I	10% Arabica CDC Bol 90% Robusta Caf I	10% Arabica CDC P 90% Robusta CDC M
89,9% Arabica B B 10,1% Robusta CG I	70,4% Arabica B E 29,6% Robusta CG I	83,3% Arabica B I 16,7% Robusta H 3c	85% Arabica B G 15% Robusta T	68,5% Arabica B C 31,5% Robusta H 3c	14,4% Arabica T 85,6% Robusta CP G	17,6% Arabica C R 82,4% Robusta SP	19,8% Arabica T 80,2% Robusta CP G	21,1% Arabica B I 78,9% Robusta CG I	9,6% Arabica CDC Bol 90,4% Robusta Caf I	8,8% Arabica CDC P 91,2% Robusta CDC M

Conclusion

- Meaningful IMS spectra can be obtained by the sampling of VOCs from the vial headspace.
- Application of Chemometrics software featured with ML algorithms allowed obtaining average accuracy of 96% in the determination of Arabica-Robusta composition in ground coffee mixes.
- Inclusion of this kind of software to IMS device software bundle could eliminate the need for the employment of skilled professional for the analysis results interpretation.
- IMS method may become easy-to-use and cost-effective thus attractive to small coffee-related enterprises.

Acknowledgments

I would like to express sincere gratitude

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RNDr. Ladislav Moravský

Q & A

Thank you for attention!

Now questions are welcome