Transfers and reactions modelling of aroma compounds in coffee beans during fermentation

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The aroma quality of coffee is strongly related to the chemical composition of the beans. This depends on the production conditions, the coffee variety and the post-harvest treatment applied. When wet post-harvest treatment is used, the quality of the coffee is often inscreased. Wet processing combines several unit operations: depulping, fermentation and drying. It is known that the fermentation process improves the quality of coffee drink. However, the mechanisms of aroma transfer and reactions involved in fermentation are not yet established.
Therefore, the objective of this study is to use a modelling strategy to characterise the mechanisms involved. To this end, kinetic models of increasing complexity were deployed to identify the mechanisms affecting the evolution of the concentration of three aroma compounds (isoamyl acetate, 2-phenylethanol and butanal) classically produced by yeasts and found in coffee beans. Simulations of the wet treatment were used to identify the parameters of the models by comparing them with the experimental kinetics carried out for four media (M1: dehulled beans, M2: demucilaginated beans, M3: depulped beans, M4: depulped beans with yeast), at 25 °C using labeled aroma compounds. The transfer of 2-phenylethanol was well represented by a model taking into account an evolving resistance of the periphery of the seed (R^2 = 0.98). The more complex evolution of the isoamyl acetate and butanal contents required the use of a model combining two first-order reactions in parallel (R^2= 0.87-0.66 and R^2= 0.80-0.67, respectively). These models provide insight into the mechanisms involved during fermentation. In the futur, coupling these models with kinetic models of yeast aroma production should allow a better definition of optimal fermentation conditions.