Modelling of the production kinetics of the main fermentative aromas in winemaking fermentation

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Modeling of the production kinetics of the fermentative aromas in winemaking conditions
Introduction

Alcoholic fermentation in winemaking

- Objective: better control of this major step of the winemaking process to act on the wine characteristics

- Possibility to on-line monitor and control the main reaction (bioconversion of sugar into ethanol and CO₂) by using current devices based on the measurement of density, CO₂ production…

- Dynamic models available to predict the main reaction … but no consideration of fermentative aromas

→ Needs for new approaches:

  Online monitoring of higher alcohols and esters

  Dynamic modeling of the synthesis of these volatile compounds
Online monitoring of fermentative aromas

- Heated transfer lines
- Valve selector

Cold trap - GC

- 16 carbon compounds analysed
- Maximum analysis frequency: 1h (with 1 tank)

(Morakul et al., 2011, 2013)
(Mouret et al., 2012, 2014)
Online monitoring of fermentative aromas

Compounds measured online (once hourly):

- **Higher alcohols**: propanol, isobutanol, isoamyl alcohol, phenyl ethanol
- **Acetate esters**: ethyl acetate, isoamyl acetate, isobutyl acetate, phenyl ethyl acetate
- **Ethyl esters**: ethyl butyrate, ethyl hexanoate, ethyl octanoate, ethyl decanoate, ethyl dodecanoate
- **H₂S**
Experimental plan
Impact of $T^\circ$ and initial nitrogen content

- Focus on 5 volatile compounds, in synthetic medium:
  - 2 higher alcohols: propanol, isobutanol, isoamyl alcohol
  - 1 acetate ester: isoamyl acetate
  - 2 ethyl esters: ethyl hexanoate, ethyl octanoate
Yields of production from sugar

(Yield = f(T°, initial nitrogen) )

(Mouret et al., 2014)

- 2 successive production phases from sugar for the 5 aromas
  - Transition when nitrogen = 0 for higher alcohols and acetate ester
  - Transition at fixed consumed sugar C° for ethyl esters
Modeling of the production yields

\[ Isoamyleacl = Y_{Isoamylealc\ 1} \times S_{conso\ 1} + Y_{Isoamylealc\ 2}(N0, T) \times S_{conso\ 2} \]

\[ Y_1 = \exp(p_1 + p_2 N_0 + p_3 T + p_4 N_0^2 + p_5 T^2 + p_6 N_0 T) \]

\[ Y_2 = \exp(p_7 + p_8 N_0 + p_9 T + p_{10} N_0^2 + p_{11} T^2 + p_{12} N_0 T) \]

(Mouret et al., 2015)
Modeling of the kinetic of the main reaction of the fermentation: MOMAF

- MOMAF (MOdeling of the Main reaction of Alcoholic Fermentation)
- Input values
  - Initial sugar and nitrogen content
  - T° profile (including anisotherm)
- Prediction of
  - Sugar and nitrogen consumption
  - Biomass, ethanol and CO₂ production
  - CO₂ production rate
  - Fermentation duration

(Malherbe et al., 2004)
Modeling of the kinetics of production of fermentative aromas

✓ To predict the kinetics of production of volatile compounds, modeling of the production yields from sugar must be coupled to the MOMAF model

\[ Isoamyleacl = Y_{Isoamylealc\ 1} \times S_{conso\ 1} + Y_{Isoamylealc\ 2}(N0, T) \times S_{conso\ 2} \]

✓ To use the production yields, the key point is to determine the consumed sugar C° corresponding to the transition between the 2 phases of linear production: ‘S_transition’

✓ S_transition is
  - constant in all conditions for ethyl esters
  - dependent on the initial nitrogen C° for the higher alcohols and the acetate ester
  - Independent of T° for all compounds
Modeling of the kinetics of production of fermentative aromas

MODAPEC (MODeling of Aroma Production in Enological Conditions)

Deviation less than 7% between experimental and calculated values for both the fermentations used to build the model and those used for validation
Conclusions and perspectives

✓ Main results:

- Identification of two linear production phases from sugar for the 5 studied fermentative aromas
- Possibility to simulate, for the first time, the production kinetics of these fermentative aromas from the 2 main factors affecting the fermentation process: nitrogen content and T°

✓ Next steps:

- Modeling of the production kinetics of other aromas
- Effects of other parameters: lipids, O₂ and nitrogen addition
- Genericity of the results: natural must, other strains?
- Development of innovative strategies aiming to maximize or minimize the synthesis of fermentative aromas, by controlling fermentation parameters
Thank you for your attention

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It’s not so simple !!!!