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Wine fermentation kinetic model verification and simulation of refrigeration malfunction during wine fermentation

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Abstract: This paper deals with influence of nitrogen compound content on wine fermentation kinetics. It also deals with simulation of refrigeration failure during fermentation. Mathematical model of wine fermentation was adapted. Model is based on kinetics of heat removal, kinetics of fermentation, production of carbon dioxide and ethanol. Ethanol and carbon dioxide concentration profiles during fermentation were obtained as a result. Then the model was used to simulate refrigeration malfunction of a fermentation tank. This might lead to higher energy efficiency and lower cost of winemaking process.

Keywords: fermentation, material balance, energy balance

Introduction

Wine fermentations are often carried out empirically. However there is an effort to develop a reliable model of fermentation in order to obtain better prediction of the process as well as lower energy cost. Various models describe the influence of temperature on fermentation process (Colombié, 2007; Zenteno, 2010). There are also models that include other factors such as assimilable nitrogen (Malherbe, 2004; Coleman, 2007; Cramer, 2002) or yeast dying phase (Borzí, 2014). There are also efforts to develop simulation and optimization software for wine fermentation (Goelzer, 2009). In this paper material and energy analysis of wine fermentation and simulation of refrigeration malfunction is presented focusing on the production of Pinot gris organic white wine from grapes collected in the central Slovak wine region.

Fermentation process

The wine fermentation model includes a mass and an energy balance. Fermentation was simulated in conditions of 10 m^3 fermenter filled up to 88 % of its total capacity. Ambient temperature was 15 °C and desired fermentation temperature was 16 ± 1 °C. The initial sugar concentration was 210 g/l and the initial nitrogen concentration was approximately 190 mg/l. The first ten days of the fermentation process were simulated closely studying the possibility of refrigeration malfunction.
The following assumptions were used in the model:

- bubbles cause ideal stirring – must is homogeneous during most of the fermentation process;
- fermentation tank is situated in a closed room and heat transfer between environment and the outside surface of the bioreactor involves a combination of radiation and convection, while temperature in the environment was constant during the whole fermentation process with no air convection;
- temperature of the outer surface was identical with the must temperature; resistance to heat flow through the tank wall and between the must and the wall was assumed to be negligible;
- effect of total acidity on the fermentation process is negligible;
- nitrogen is the limiting substrate;
- although fructose is used concomitantly with glucose, yeasts prefer glucose over fructose (ratio of glucose/fructose is 1/1);
- ethanol inhibits sugar consumption;
- CO_2 accumulation in the gas phase is negligible;
- biomass viability depends on the combined effect of ethanol and temperature.

Fermentation takes place in an open fermentation vessel. When the previous assumptions are considered, fermentation is described by the following main equations (Zenteno *et al.*, 2010; Carroll *et al.*, 1991):

$$\frac{d\left(X_V \cdot H\right)}{d\tau} = (\mu - k_d)\cdot\left(X_V \cdot H\right) \tag{1}$$

$$\frac{d(N \cdot H)}{d\tau} = -\frac{\mu}{Y_{X/N}}\cdot\left(X_V \cdot H\right) \tag{2}$$

$$\frac{d(G \cdot H)}{d\tau} = -\left(\frac{\mu}{Y_{X/G}} + \frac{\beta_G}{Y_{E/G}} + m\cdot\frac{G}{G+F}\right)\cdot\left(X_V \cdot H\right) \tag{3}$$

$$\frac{d(F \cdot H)}{d\tau} = -\left(\frac{\mu}{Y_{X/F}} + \frac{\beta_F}{Y_{E/F}} + m\cdot\frac{F}{G+F}\right)\cdot\left(X_V \cdot H\right) \tag{4}$$

$$\frac{d(E \cdot H)}{d\tau} = (\beta_G + \beta_F) \cdot (X_V \cdot H) \tag{5}$$

$$F_{CO_2} = \left[\left(\frac{\mu}{Y_{x/CO_2}} + \frac{\beta_G + \beta_F}{Y_{E/CO_2}} + m \right) \cdot X_V \cdot H \cdot A_F \right] - \\ - \left[k_L a_{TF} \cdot H \cdot \left(c_{sat} - c_{CO_2 L} \right) \cdot A_F \right] \tag{6}$$

$$A_F \frac{d(\rho \cdot H)}{d\tau} = -F_{CO_2} \tag{7}$$

$$\frac{d(\rho \cdot H \cdot T)}{d\tau} = \left(1 - x_{Q_{evaporation}}\right) \frac{\Delta H}{c_p} \cdot \frac{d(S \cdot H)}{d\tau} - \\ - \frac{A_{ef}.U.(T - T_{amb}) + Q_{cool}}{c_p A_F} \tag{8}$$

Tab. 1. Constants and parameters used in the model.

Parameter/ Constant	Description	Value/Equation/ Function of
X_V	biomass concentration, kg Bio/m^3	eq. (1)
N	nitrogen compounds concentration, kg N/m^3	eq. (2)
G	glucose concentration, kg G/m^3	eq. (3)
F	fructose concentration, kg F/m^3	eq. (4)
S	total sugar concentration, kg S/m^3	F + G
E	ethanol concentration, kg E/m^3	eq. (5)
H	height of the must, m	
μ	specific growth rate, 1/s	$\mu(T, N)$
k_d	specific death rate, 1/s	$k_d(E, T)$
τ	time, s	
t	must temperature, °C	
T	must temperature, K	eq. (8)
T_{amb}	ambient temperature, K	288 K
ρ	must density, kg/m^3	eq. (7)
c_{CO_2L}	dissolved CO_2, kg CO_2/m^3	$c_{CO_2L}(T)$
c_{sat}	saturation of dissolved CO_2, kg CO_2/m^3	$c_{sat}(T)$
k_L	CO_2 mass transfer coefficient, kg CO_2/(sm^{2}kg CO_2/m^3)	$k_L\ a_{TF}$ = 0.07 1/h
a_{TF}	specific mass transfer area, m^2/m^3	$k_L\ a_{TF}$ = 0.07 1/h
F_{CO_2}	mass flow of liberated CO_2 , kg CO_2/s	eq. (6)
A_F	fermentation tank base area, m^2	3,02 m^2
$x_{Q_{evaporation}}$	term representing heat removal by evaporation	$x_{Q_{evaporation}}(T)$
ΔH	specific metabolic heat, J/kg S	556,74 kJ/kg
c_p	must specific heat capacity, J/kg/K	$c_p(S, E)$
A_{ef}	effective heat transfer area of the fermentation tank, m^2	$A_{ef}(H)$
U	heat transfer coefficient between must and ambient environment, W/(m^2 K)	$U(T)$
Q_{cool}	refrigeration required to cool the fermenter, W	
Q_{ferm}	heat released during fermentation, W	
β_G	specific production rate of ethanol, kg E/kg Bio/s	$\beta_G(G, E, T)$
β_F	specific production rate of ethanol, kg E/kg Bio/s	$\beta_F(F, E, T)$
$Y_{X/N}$	biomass/nitrogen yield coefficient, kg Bio/kg N	$Y_{X/N}(N_{initial})$
$Y_{X/G}$	biomass/glucose yield coefficient, kg Bio/kg G	1,60 kg Bio/kg G
$Y_{X/F}$	biomass/fructose yield coefficient, kg Bio/kg F	1,60 kg Bio/kg F
$Y_{E/G}$	ethanol/glucose yield coefficient, kg E/kg G	0,49 kg E/kg G
$Y_{E/F}$	ethanol/fructose yield coefficient, kg E/kg F	0,49 kg E/kg F
Y_{X/CO_2}	biomass/ CO_2 yield coefficient, kg Bio/kg CO_2	12,72 kg Bio/kg CO_2
Y_{E/CO_2}	ethanol/ CO_2 yield coefficient, kg E/kg CO_2	1,05 kg E/kg CO_2
m	maintenance coefficient, kg S/ kg Bio/s	$m(T)$

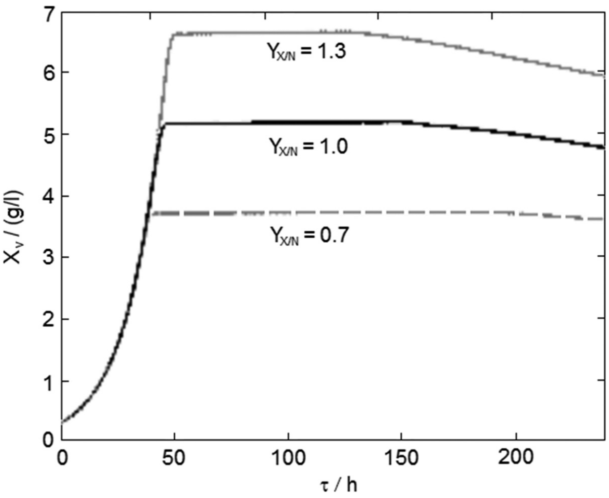

Fig. 1. Concentration of active biomass during fermentation using different biomass/nitrogen yield coefficients.

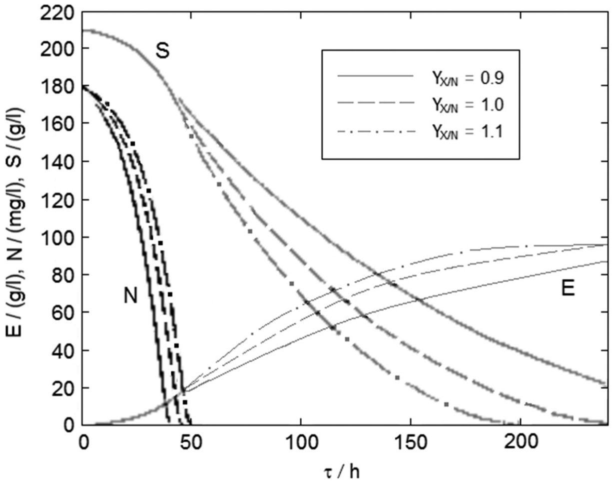

Fig. 2. Concentration of nitrogen, sugar, and ethanol during fermentation using different biomass/nitrogen yield coefficients.

$$Q_{ferm} = \Delta H \cdot A_F \cdot \frac{d(S \cdot H)}{dt} \tag{9}$$

The biomass/nitrogen yield coefficient ($Y_{X/N}$) is strongly dependent on the initial nitrogen compounds concentration. An increase in the initial concentration of nitrogen compounds can cause other nutrients to become growth limiting factors, which explains the observed dependence.

In Figure 1 and 2, three different biomass/nitrogen yield coefficients are compared. Fermentation ends when the residual sugar level of 5 g/l is reached. Fermentation carried out with the original yield coefficient took 221 hours. In order to determine the sensitivity to the biomass/nitrogen yield coefficient, the initial value was both decreased and increased by 30 % while keeping all other values and conditions constant. The reduction led to a prolongation of the fermentation process to 297 hours, while the increase led to a faster fermentation of only 180 hours.

Model was also used for modeling temperature increase in fermentation tank during refrigeration malfunction (for 6 hours at the 50 hour time-point, followed by 2 hours of cooling). If cooling breaks down, the temperature increases up to 17.25 °C (from 16 °C) and when the malfunction is removed, refrigeration capacity at least 8 kW is required to cool down the fermentation vessel within 2 hours as shown in Figure 3 and 4. Figure 5 shows production of CO_2 as a consequence of the consumption of glucose and fructose for ethanol production and biomass growth and maintenance. Before saturation CO_2 dissolves in must and when saturation is reached carbon dioxide is released to atmosphere.

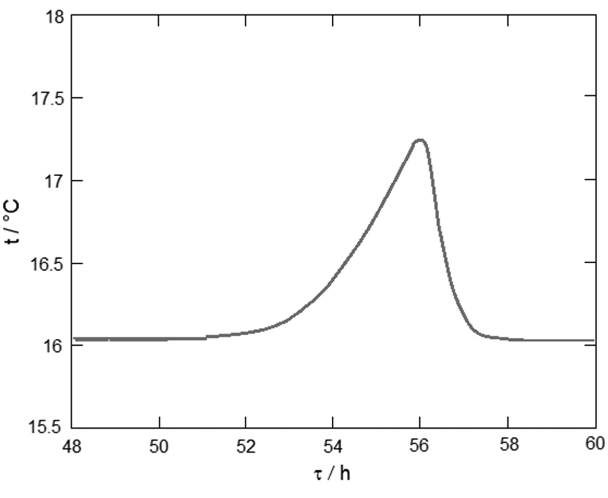

Fig. 3. Temperature increase during fermentation refrigeration malfunction.

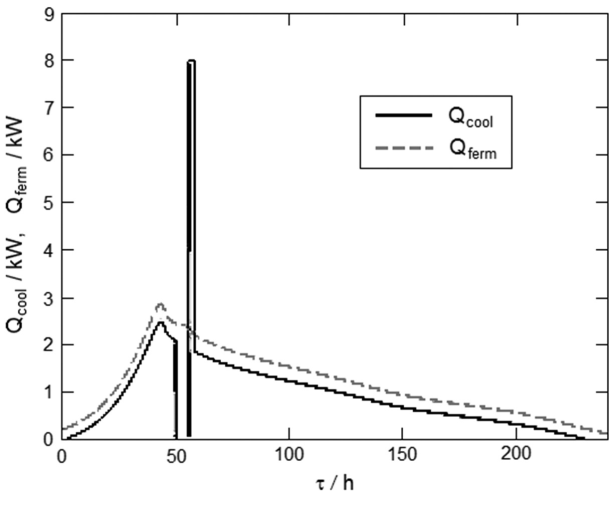

Fig. 4. Refrigeration and fermentation heat during fermentation.

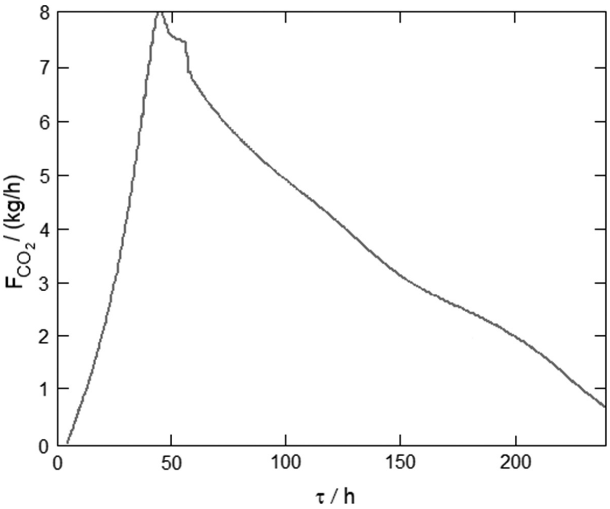

Fig. 5. CO_2 leakage rate from the fermenter.

Conclusion

In this paper, white wine fermentation is described from the point of view of mass and energy balances. Significant impact of the biomass/nitrogen yield coefficient was proved. Also, in case of a refrigeration malfunction of 6 hours, the resulting temperature increase had no significant impact on the fermentation process.

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