Supplemental Data for:

Miller KV, Oberholster A and Block DE. 2020.
Predicting the impact of fermentor geometry and cap management on phenolic profile using a reactor engineering model. Am J Enol Vitic 71:44-51. doi: 10.5344/ajev.2019.19051.

Supplemental Material

Reactor engineering governing equations, as derived elsewhere (Miller et al. 2019a).

$$\frac{dX_A}{dt} = \mu X_A - k_d X_A;\ where\ \mu = \frac{\mu_{max} N}{K_N + N}\ \ and\ k_d = k'_d E$$

$$\frac{dN}{dt} = -\frac{\mu}{Y_{X/_N}} X_A$$

$$\frac{dS}{dt} = -\frac{\beta}{Y_{E/_S}} X_A;\ where\ \beta = \frac{\beta_{max} S}{K_S + S}$$

$$\frac{dE}{dt} = \beta X_A$$

Equation 1: Fermentation model

$$\rho c_v \frac{DT}{Dt} = \nabla \cdot (k \nabla T) + \dot{Q}$$

Equation 2: Heat transfer within the fermentor

$$\frac{Dc_i}{Dt} = \nabla \cdot (D_i \nabla c_i) + R_i$$

Equation 3: Mass transfer material balance

$$\rho \frac{D\vec{v}}{Dt} = \rho g + \nabla \cdot \left(\eta (\nabla \vec{v} + \ (\nabla \vec{v})^T) - \frac{2}{3} \eta (\nabla \cdot \vec{v}) \boldsymbol{I} \right) \ - \ \nabla P$$

Equation 4: Navier-Stokes for compressible flow with gravity

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Reactor engineering table of parameters.	
Symbol	**Description**
X_A	Active biomass concentration
μ	Specific growth rate
k_d	Combined temperature/ethanol death constant
μ_{max}	Maximum specific growth rate
N	Yeast assimilable nitrogen (YAN) concentration
K_N	Monod constant for YAN consumption
k_d'	Temperature portion of inactivation constant
E	Ethanol concentration
S	Sugar concentration
$Y_{X/_N}$	Yield coefficient of YAN to biomass
β	Specific sugar consumption rate
β_{max}	Maximum specific ethanol production rate
K_S	Monod constant for sugar consumption
ρ	Density
T	Temperature
c_v	Heat capacity
k	Thermal conductivity
$\dot{Q}$	Heat generation rate
c_i	Concentration of species i
D	Diffusion coefficient
R_i	Rate of generation of species i
g	Gravitational acceleration constant
v	Liquid velocity
η	Viscosity
P	Pressure
$\boldsymbol{I}$	Identity matrix

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Extraction model parameters as a function of temperature and ethanol, as derived elsewhere (Miller et al. 2019d).

Parameter	Symbol (unit)	Fit as a function of T (°C)
Skin–tannin release constant	$k_{G,Tan,Skin}$ (1/h)	$y = -0.000014T^2 + 0.001554T - 0.019916$
Skin–anthocyanin release constant	$k_{G,Anth,Skin}$ (1/h)	$y = -0.0000081T^2 + 0.0011173T - 0.0095045$
Seed–tannin release constant	$k_{G,Tan,Seed}$ (mg/L/h)	$y = 0.00089T^2 - 0.00703T + 0.19030$
Unavailable anthocyanin concentration	$C_{Anth,U}$ (mg/L)	$y = -0.53615T^2 + 16.57825T + 75.70350$
Unavailable skin–tannin concentration	$C_{Tan,U}$ (mg/L)	$y = -25.1835T + 1{,}080.7055$
Anthocyanin reaction rate	$k_{R,Anth}$ (mg/L/h)	See Arrhenius parameters

Anthocyanin reaction rate Arrhenius parameters:

Pre-exponential constant = 1.38×10^{18} mg/L/hr

Activation energy = 107.3 kJ/mol

Langmuir adsorption parameters

T = temperature (K)

E = ethanol concentration (% v/v)

$$K_{eq,Tannin} = (1.21 \cdot 10^{-3}) + \frac{(-2.69 \cdot 10^{-3} \cdot T)}{(-9.01 \cdot T) + (-1.25 \cdot 10^{2} \cdot E) + (T \cdot E)}$$ [=] L/mg

$$q_{Tannin} = (4.57 \cdot 10^{-1}) + \frac{(2.04 \cdot 10^{1} \cdot E)}{(-6.69 \cdot E) + (4.57 \cdot 10^{-1} \cdot T) + (T \cdot E)}$$ [=] mg/mg

$$K_{eq,Anthocyanin} = -18.0 + 1.26 \cdot E + 6.26 \cdot 10^{-2} \cdot T - 4.17 \cdot 10^{-3} \cdot T \cdot E$$ [=] L/mg

$$q_{Anthocyanin} = 0.715 - 0.337 \cdot E - 2.07 \cdot 10^{-3} \cdot T + 1.16 \cdot 10^{-3} \cdot T \cdot E$$ [=] mg/mg