Numerical modeling of wine fermentation based on coupled weakly hyperbolic nonlinear integro-differential equations

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ALGORITHMIC OPTIMIZATION

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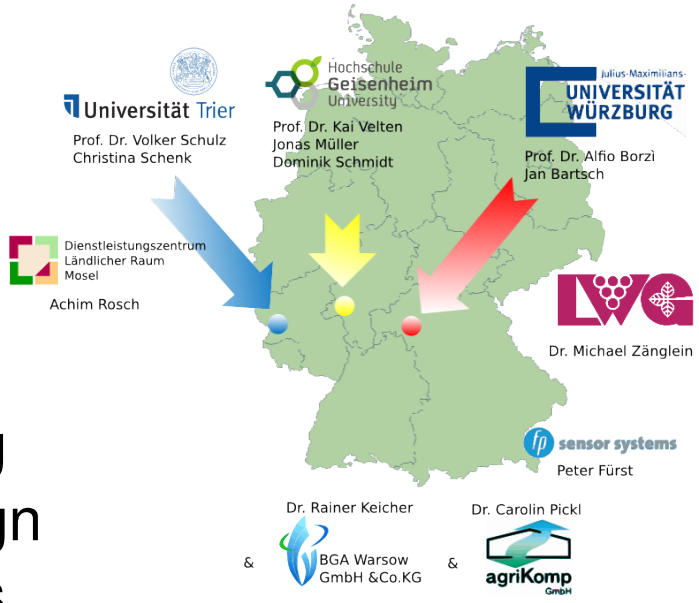
Agenda

The Project RŒNOBIO

Robust Energy-Optimization of Fermentation Processes for the Production of Biogas and Wine

- Modeling:
  Kinetics, Fluid dynamics,
  Yeast cell growth dynamics
- Numerical modeling
- Existence and uniqueness
- Optimal design and placement of cooling element for wine tanks and optimal design of mixer configuration for biogas reactors
- Parameter estimation and optimal control
- Real-time optimization for wine fermentation



Introduction

Mashing of grapes

Wine press

Fermentation

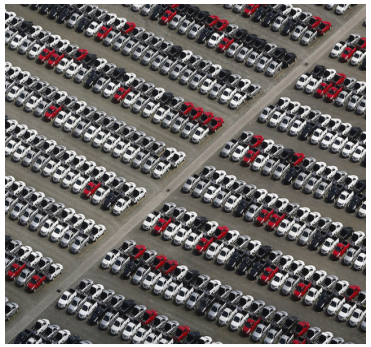
The process of making wine

Addition of yeast and eventually nutrients to must yield:

- Yeast growth by metabolizing sugar and nutrients such as nitrogen
- Conversion of sugar into ethanol usually under anaerobic conditions (exothermic reaction)
- Temperature important factor (too high: death of yeast cells)$\rightarrow$ Cooling

Motivation for Energy Conservation

- 0.08% of global greenhouse gas emissions in 2009 $\approx$1 M cars annually or 2kg/0.75l bottle (Smyth et al., 2011)
- In California second highest energy consumer in food industry (Galitzky et al., 2005)
- High potential for saving energy in the process of making wine $\rightarrow$ control of fermentation temperature significant
- Objective: Minimize cooling energy and maintain wine quality



[Source: tagesanzeiger.ch]

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Yeast Cell Growth Dynamics

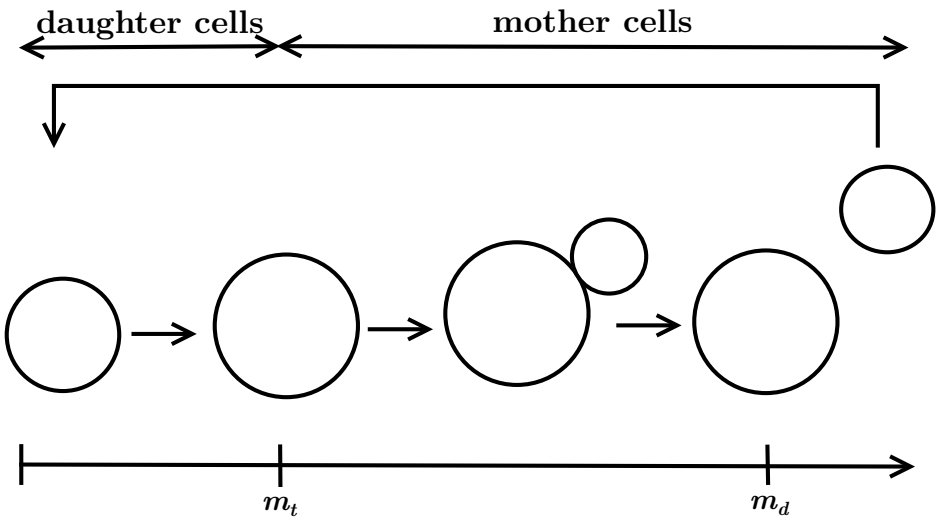


Figure: Simplified cell cycle for budding yeast

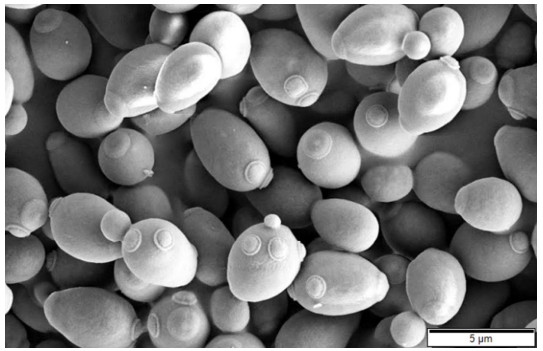


Figure: Visualization of birth-scars and buds for Saccharomyces cerivisiae from Wikipedia (2017)

- Motivation: Open-loop dynamics of yeast are highly dependent on initial cell mass distribution (Zhang et al., 2002)
- Cell-cycle lasts 90 to 120 minutes (Morgan, 2007)

Model Based on Integro-Differential Equations 1/2

- Population balance equation (PBE):

$$\frac{\partial W(m,t)}{\partial t} = -div(r_\epsilon(m,N,S,O)W(m,t)) + 2\int_{m_{min}}^{m_{max}} p(m,m')\Gamma(m')W(m',t)dm' - \Gamma(m)W(m,t) - \Phi(E)W(m,t)m - k_d W(m,t)m$$

Boundary conditions:

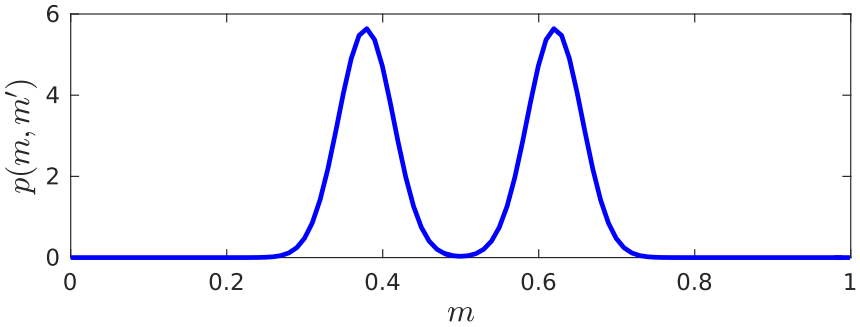
$$r_\epsilon(m_{min},N,S,O)W(m_{min},t) = 0 = r_\epsilon(m_{max},N,S,O)W(m_{max},t)$$

- m cell mass
- S, N, O, E sugar, nitrogen, oxygen, ethanol concentration
- $W(m,t)$ cell number density
- $r_\epsilon(m,N,S,O)$ single-cell growth rate
- $p(m,m')$ partitioning function
- $\Gamma(m)$ division rate
- $\Phi(E)$ death function

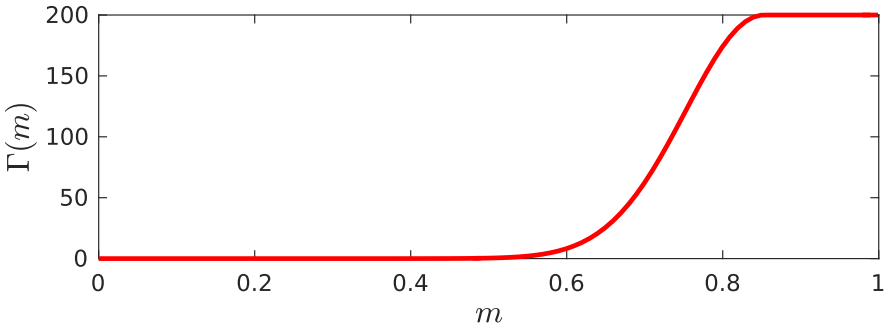
Development of [Daoutidis and Henson (2002); Henson (2003); Mantzaris et al. (2002)]

Partitioning Function, Division Rate, Death Term

$$p(m,m') = \begin{cases} \lambda e^{-\beta(m-m_t)^2} + \lambda e^{-\beta(m-m'+m_t)^2} & , \ m' > m \text{ and } m' > m_t \\ 0 & , \text{ else} \end{cases}$$



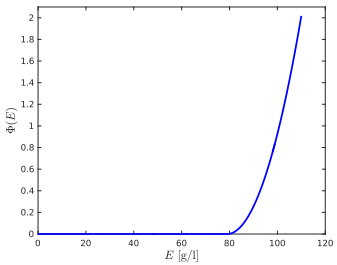
$$\begin{aligned} m_t &= 0.3784, & m' &= 0.999, \\ m_d &= 0.8525, & & \\ \gamma &= 200, & \beta &= 400, \\ \delta &= 50, & \lambda &= 5.6419 \end{aligned}$$



$$\Gamma(m) = \begin{cases} 0 & , \ m \le m_t \\ \gamma e^{-\delta(m-m_d)^2} & , \ m_t < m < m_d \\ \gamma & , \text{ else} \end{cases}$$

$$\Phi(E) = \left(0.5 + \frac{1}{\pi}\arctan(k_{d1}(E - tol))\right) k_{d2}(E - tol)^2,$$

where k_{d1} and k_{d2} ethanol inhibition constants and tol tolerance of ethanol (strong inhibition)



$$\begin{aligned} tol &= 79\text{g/l}, \\ k_{d_1} &= 99.86, \\ k_{d_2} &= 0.0021, \\ E &\in [0, 110] \end{aligned}$$

Model Based on IDEs 2/2

- Nitrogen concentration (oxygen without ϵ):

$$\frac{dN}{dt} = -k_1 \int_{m_{min}}^{m_{max}} r_\epsilon(m, N, S, O) W(m, t) dm$$

- Sugar concentration:

$$\frac{dS}{dt} = - \int_{m_{min}}^{m_{max}} q(m, N, S, E, O) W(m, t) dm$$

- Product / ethanol concentration:

$$\frac{dE}{dt} = \int_{m_{min}}^{m_{max}} q_E(m, S, E) W(m, t) dm$$

- k_1 yield coefficient for nitrogen
- $r_\epsilon(m, N, S, O)$ growth rate
- $q(m, N, S, O)$ consumption rate vector
- $q_E(m, S, E)$ ethanol growth rate vector

Growth, Consumption and Formation Rates

- μ_{max}, β_{max} reaction rates
- K_E growth inhibition by ethanol
- K_N, K_{S_1}, K_{S_2}, K_O Michaelis constants for nitrogen, sugar, oxygen
- k_2, k_3 yield coefficients for sugar

$$r_\epsilon(m, N, S, O) = \mu_{max}(T)\frac{N}{K_N + N}\frac{S}{K_{S_1} + S}\left(\frac{O}{K_O + O} + \epsilon\right)m$$

$$q_E(m, S, E) = \beta_{max}(T)\frac{S}{K_{S_2} + S}\frac{K_E(T)}{K_E(T) + E}m$$

$$q(m, N, S, E, O) = k_2 q_E(m, S, E) + k_3 r_\epsilon(m, N, S, O)$$

where μ_{max}, β_{max} and K_E assumed to be linear dependent on temperature T.

Solution: Existence and Uniqueness

Simplified Case

- Hyperbolic boundary value problem with the velocity term r_ϵ described by a constant **r** (not dependent on the other substrate concentrations and m)
- Existence and uniqueness of the solution shown based on semigroup theory (Idea of proof: Dautray and Lions,1993)

Nonlinear Case

- Local Lipschitz continuity of right hand side
- Rigorous literature study
- Discussion of challenges for strongly nonlinear and weakly hyperbolic properties of the system of P/OIDEs

[Schenk (2018)]

Simplified Case

- Semilinear hyperbolic partial integro-differential equation

$$(\star)\begin{cases} \dfrac{\partial W(m,t)}{\partial t} + \mathbf{r}\cdot \operatorname{div}(W(m,t)) + \Sigma(m)W(m,t) = KW(m,t), \\ \qquad m \in M,\ \mathbf{r} \in \mathbb{R}^+,\ t > 0 \\ W\big|_{\Theta} = 0,\ \Theta = \{m_{min}, m_{max}\} \\ W(m,0) = W_0 \text{ on } M,\ W_0 \text{ given.} \end{cases}$$

Σ positive function of m with

$$\Sigma(m) = \Gamma(m) + \Phi(E)m + k_d m \tag{1}$$

and given operator K

$$(KW)(m) = \int_M f(m,m')W(m',t)dm' \tag{2}$$

with

$$f(m,m') = p(m,m')\Gamma(m') \tag{3}$$

Semigroup Theory Notation I

Definition

Semigroup of class $\mathcal{C}^0$

Let $\{G(t)\}_{t\geq 0}$ be a family of elements $G(t) \in \mathfrak{L}(L^2(M))$ for $t \geq 0$. This family forms a semigroup of class $\mathcal{C}^0$ in $L^2(M)$ if it fulfills these conditions

$$\begin{cases} G(s+t) = G(s)G(t) \quad \forall s,t \geq 0 & (i) \quad \textit{(algebraic property)} \\ G(0) = Id & (ii) \quad \textit{(identity in } \mathfrak{L}(L^2(M))\textit{)} \\ \lim\limits_{t\to+0} \|G(t)m - m\|_{L^2(M)} = 0 \quad \forall m \in L^2(M) & (iii) \quad \textit{(topological property).} \end{cases}$$

Semigroup Theory Notation II

Definition

Set of differentiable vectors

We call $D(A)$ the set of differentiable vectors in $L^2(M)$, i.e. the subset of elements $m \in L^2(M)$ such that the function $t \to G(t)m$ is differentiable for $t \geq 0$. Because of the algebraic property (i), $D(A)$ is represented by

$$D(A) = \{m \in L^2(M); \frac{G(h)m - m}{h} \text{ converges in } L^2(M) \text{ as } h \to +0\}. \quad (4)$$

From now on, let A_h be an operator defined by

$$A_h := \frac{G(h) - Id}{h} \quad (5)$$

with $A_h \in \mathfrak{L}(L^2(M)) \quad \forall h > 0$.

Semigroup Theory Notation III

Definition

Infinitesimal generator of a semigroup

An operator A defined as a linear mapping from $D(A)$ into $L^2(M)$, precisely as

$$\lim_{h \to +0} A_h m = Am$$

with $D(A)$ as in (4), is called the infinitesimal generator of the semigroup $\{G(t)\}_{t \geq 0}$.

Semigroup Theory Notation IV

Remark

Let A be the unbounded operator in $L^2(M)$ defined by

$$\begin{cases} (AW)(m) = -\mathbf{r} \cdot \operatorname{div}(W(m,t)) \\ D(A) = \{W \in L^2(M);\ AW \in L^2(M), W\big|_{\Theta} = 0\}. \end{cases}$$

Then, A is called advection operator. Problem $(\star)$ is equivalent to

$$\begin{cases} \dfrac{\partial W}{\partial t} = TW \\ W(0) = W_0 \end{cases}$$

with

$$T = A - \Sigma(m) + K$$

where K is an integral operator, defined by (2), which is bounded in $L^2(M)$ under certain assumptions which we have to make on the kernel f.

Idea of Proof I

- Existence and uniqueness of the solution shown based on semigroup theory (Idea of proof: Dautray and Lions,1993)
- Main steps:
  1. Show that the operator

$$\begin{cases} T = A - \Sigma(m) + K & (i) \\ D(T) = D(A) & (ii) \end{cases}$$

is infinitesimal generator of a semigroup of class $\mathcal{C}^0$ in $L^2(M)$ and the semigroup generated by T operates in cone of positive functions of $L^2(M)$

Idea of Proof II

2. Show that: Let $f(m, m')$ real positive function and measurable with respect to m or m' then there exist positive constants C_a and C_b, such that
$$\begin{cases} \int_M f(m, m')\, dm \leq C_a & \forall m' \in M \\ \int_M f(m, m')\, dm' \leq C_b & \forall m \in M \end{cases} \tag{6}$$
3. It follows that operator K defined by $(K\eta)(m) = \int_M f(m, m')\eta(m')dm' \quad \forall \eta \in L^2(M)$ is linear and continuous from $L^2(M)$ into $L^2(M)$.
4. Show $\Sigma \in L^\infty(M)$

Idea of Proof III

5. Show W weak solution of $(\star)$ if $y \in \mathcal{W}^2$ with

$$\mathcal{W}^2 = \{W \in L^2(M) : \mathbf{r} \cdot \operatorname{div} W \in L^2(M)\} \tag{7}$$

$W(0) = W_0$ and

$$\begin{aligned} &\int_M \left(\frac{d}{dt} v(m)\right) W(m,t)dm + \int_M (\mathbf{r} W(m,t)) \cdot \operatorname{div}(v(m))dm \\ &= -\int_M KW(m,t)v(m)dm + \int_M (\Sigma(m) + \tilde{\mathbf{r}}) W(m,t)v(m)dm \\ &\quad \forall v \in H^1(M), \end{aligned} \tag{8}$$

(follows from semigroup theory)

6. Show uniqueness via Gronwall's lemma

Nonlinear Case

- Quasilinear weakly hyperbolic partial integro-differential equations

$$\begin{cases} \dfrac{\partial W(m,t)}{\partial t} + r_\epsilon(m,N,S,O)\,\mathrm{div}(W(m,t)) \\ \qquad = -\Sigma(m)W(m,t) + KW(m,t) \\ \dfrac{\partial N}{\partial t} = -k_1 \int_M r_\epsilon(m,N,S,O)W(m,t)dm \\ \dfrac{\partial E}{\partial t} = \int_M q_E(m,S,E)W(m,t)dm \\ \dfrac{\partial S}{\partial t} = -\int_M q(m,N,E,S,O)W(m,t)dm \\ \dfrac{\partial O}{\partial t} = -k_4 \int_M r(m,N,S,O)W(m,t)dm \end{cases}$$

where K as before and Σ now represents positive function of m with

$$\Sigma(m) = \Gamma(m) + \Phi(E)m + k_d m + \tilde{r}_\epsilon$$

with $r_\epsilon(m,N,S,O) = m\tilde{r}_\epsilon(N,S,O)$.

Idea of Proof

1. Assumptions: Kinetic parameters and temperature all positive, initial conditions belong to $L^\infty(M, \mathbb{R}^5)$, are non-negative and temperature is bounded by predefined upper and lower bound, such that linear temp. dependent functions nonnegative
2. Show entries of the Jacobian $\mathcal{J}_{h_y}(m, t, y)$ (h(m,t,y) right hand side) are up to a constant bounded by Z^2 for y with values in $[0, Z]$, i.e. $0 \leq y_i \leq Z$ for $i = 1, \ldots, 5$
3. With mean value theorem, right hand side h is locally Lipschitz continuous for non-negative arguments, i.e. there exists a constant $L > 0$ not dependent on Z and

$$|h(m, t, y) - h(m, t, \tilde{y})|_{\mathbb{R}^5} \;\leq\; LZ^2\, |y - \tilde{y}|_{\mathbb{R}^5},$$

   holds, where $|\cdot|_{\mathbb{R}^5}$ denotes the componentwise absolute value in $\mathbb{R}^5$.
4. **<u>BUT</u>**: Limitations for approaches in literature

Approaches in Literature I

- Glimm method: Existence result via formulating and studying the Riemann problem for nonlinear strictly hyperbolic systems of equations which are smooth in some region with a sufficiently small total variation of the initial data (Glimm, 1965)
- Existence and uniqueness of entropy solutions for weakly coupled hyperbolic systems via its parabolic regularization and then letting viscosity vanish (artificial diffusion) (Natalini and Hanouzet, 1996; Rohde, 1998; Korsch and Kröner, 2017)
- Approaches via semigroup theory very useful for semilinear equations with nonlinear operator independent of solution y, e.g. Pazy (1992); Engel et al. (1999)
- Pazy (1992) even applies to quasilinear evolution equation but with linear operator that explicitly depends on solution

Approaches in Literature II

- Dreher (2003) shows local existence and uniqueness for systems of quasilinear weakly hyperbolic differential equations via pseudodifferential operators and a reformulation with a special right hand side that has to show asymptotic behavior
- Existence and uniqueness for systems of hyperbolic equations via sesquilinear forms requires linearity of the flux to fulfill properties for forming sesquilinear form (Wloka, 1982)
- Rozhdestvenskii et al. (1972) show existence for weakly nonlinear systems of quasilinear weakly hyperbolic equations where solution stays bounded, derivatives also stay bounded for all points in time apart from the initial one (even global existence of solutions to these kind of systems for all finite time values)

Approaches in Literature III

- **BUT**: All these approaches not applicable for our problem without modification $\rightarrow$ Ideas welcome!
- Main problem for strongly nonlinear systems of quasilinear weakly hyperbolic equations: Derivatives can become infinite for some finite point in time $\rightarrow$ For any point in time larger than latter one no solution exists

Discretization of PIDE “in Mass”

- Using finite-volume method (to ensure mass conservation) with first order upwind scheme for the flux approximation results in the following discrete scheme:

$$\dot{w}_i = \frac{1}{m_{i+1} - m_i}\Bigg[-\left(r_\epsilon(m_{i+1}, N, S, O)w_i(t) - r_\epsilon(m_i, N, S, O)w_{i-1}(t)\right)$$
$$+ 2\sum_{j=0}^{N_W}\left(w_j(t)\int_{\Omega_i}\int_{\Omega_j} p(m, m')\Gamma(m')dm'dm\right) - w_i(t)\int_{\Omega_i}\Gamma(m)\,dm$$
$$- \Phi(E)w_i(t)\int_{\Omega_i} m\,dm - k_d w_i(t)\int_{\Omega_i} m\,dm\Bigg], \quad i = 1, 2, \ldots, N_W - 1,$$

where N_W: #cells FVM

Whole Model Considered for Simulation

- Add the differential equations for our product and substrate concentration development to the system above
- Yields the following system of differential equations

$$\dot{y} = f(t, y(t))$$

where $\dot{y} = (\dot{w}_i, \dot{N}, \dot{E}, \dot{S}, \dot{O})^T$ with for example

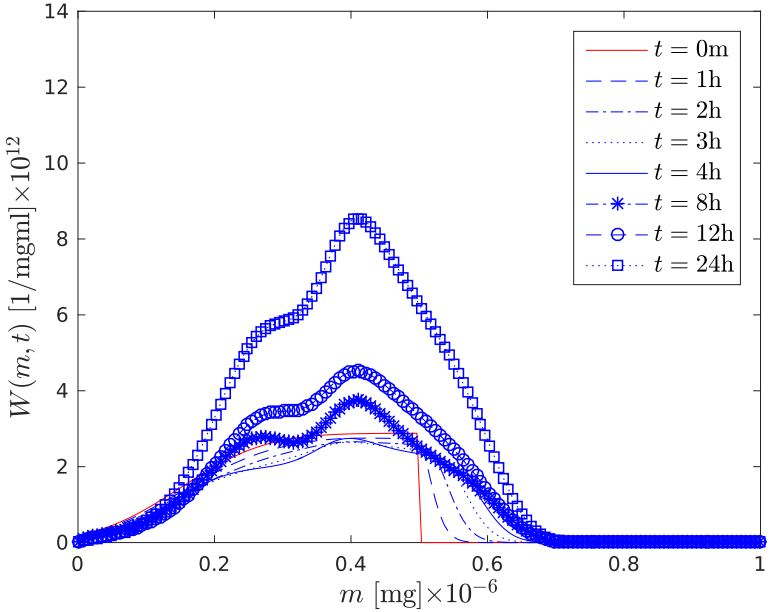
$$\dot{S} = -\sum_{i=1}^{N_W-1} \tilde{q}(N, S, E, O) \left(\frac{m_{i+1} + m_i}{2} \right) w_i (m_{i+1} - m_i),$$

where $q = \tilde{q}(N, S, E, O)m$

- Numerical integration of this system using backward differentiation formula (BDF) method or implicit trapezoidal rule
- Implementation in MATLAB
- In the following: time step of $1/192 \approx$=0.0052, 150 mass cells

Numerical Modeling Results: First 24 Hours

Small to medium cell initial distribution



Two normal peaks initial distribution

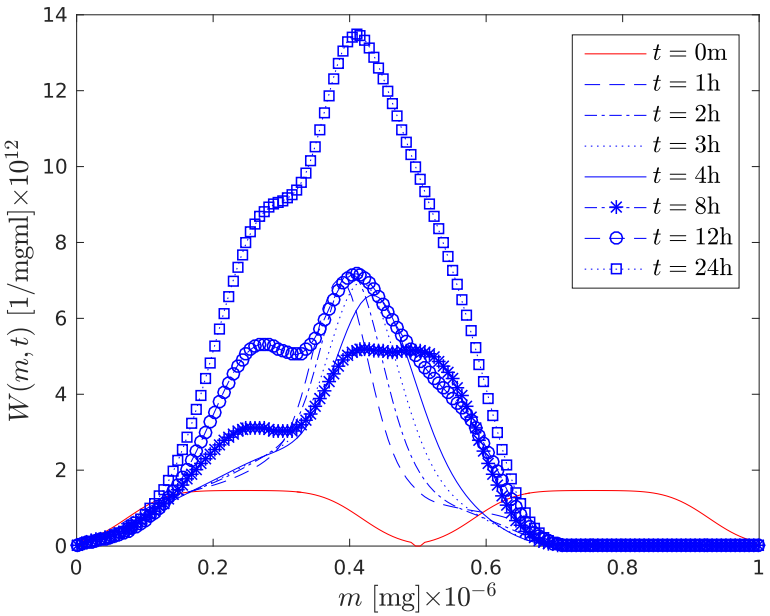


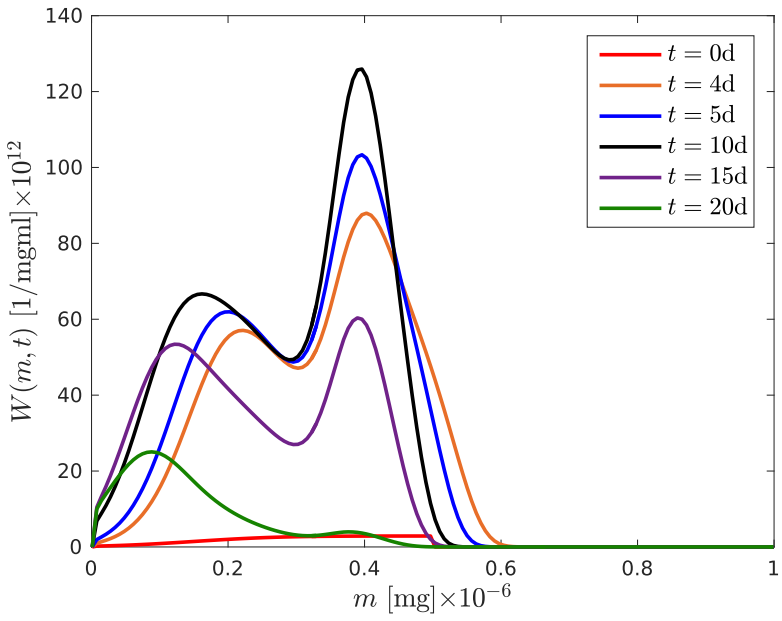
Figure: Cell number density for different cell masses for first 24 hours with implicit trapezoidal rule

- Lagged division

- Large cells disappear within first two hours
- Same trend but peaks much larger
- Similarity of two normal peaks to constant

Cell Number Density for Entire Time Horizon

Small to medium cell initial distribution



Two normal peaks initial distribution

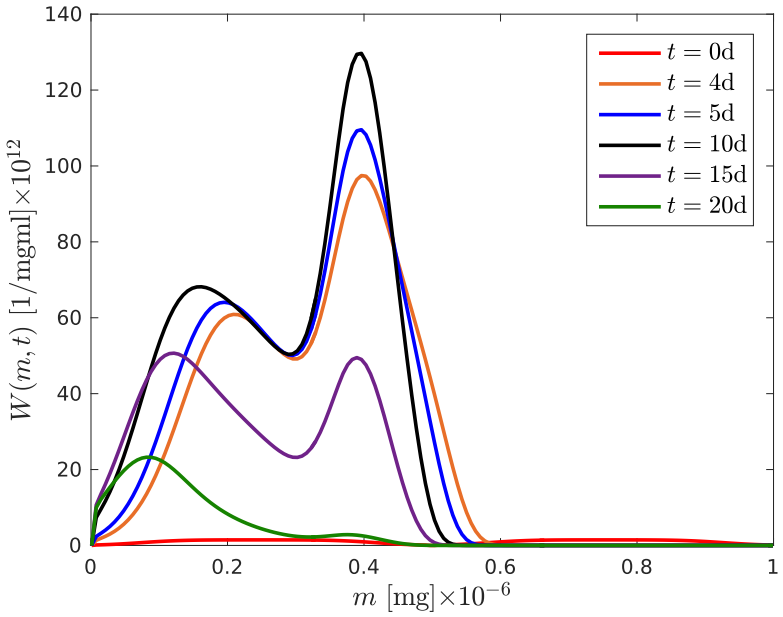
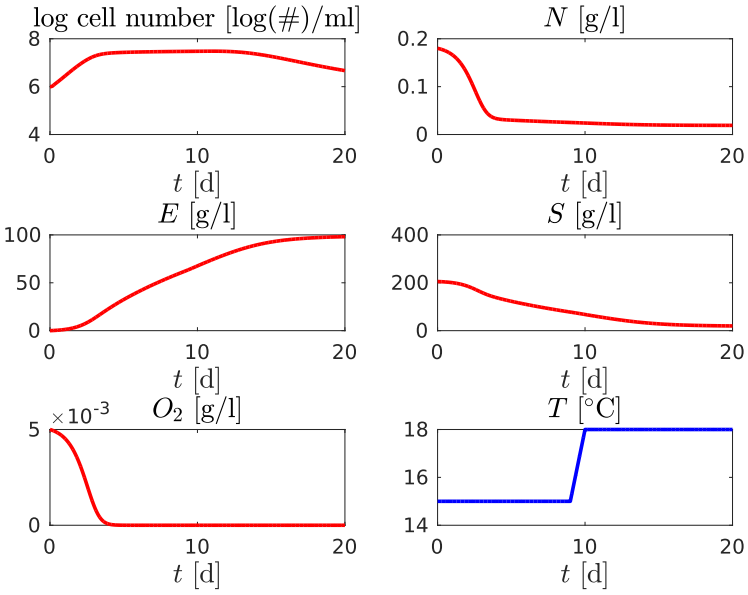


Figure: Cell number density for different cell masses for twenty days with implicit trapezoidal rule

- Similar but different

All the Trajectories

Small to medium cell initial distribution



Two normal peaks initial distribution

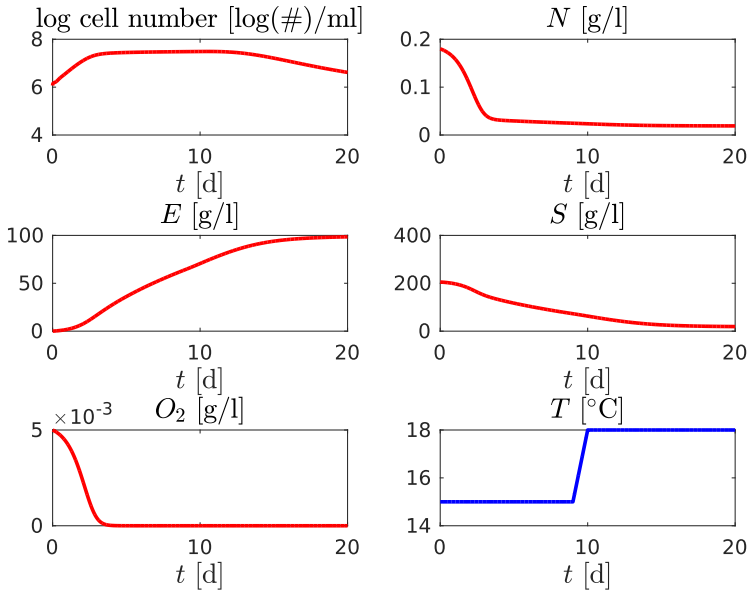


Figure: Log cell number and all other substrate/product concentration trajectories for entire time horizon with implicit trapezoidal rule

- 1 million cells / ml initially
- Yeast growth phases
- Sugar, nitrogen, oxygen consumption due to yeast growth
- Conversion into ethanol
- No visible difference

Challenges Facing with the IDE Model

- Problem of receiving data
- Computational cost of IDE model:
  - Accuracy of integral approximation
  - Accuracy of mass discretization
  - Accuracy of time discretization
  - with respect to Courant Friedrichs Levy condition (assurance of stability properties)

$\rightarrow$ ODE model for description $\leftarrow$ regarding optimization

Model Based on ODEs

$$
\begin{cases}
\dfrac{dX}{dt} = \mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\left(\dfrac{O}{K_O+O}+\epsilon\right)X \\
\qquad - k_d X - \Phi(E)X \\
\dfrac{dN}{dt} = -\,k_1\mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\left(\dfrac{O}{K_O+O}+\epsilon\right)X \\
\dfrac{dE}{dt} = \beta_{max}(T)\dfrac{S}{K_{S_2}+S}\dfrac{K_E(T)}{K_E(T)+E}X \\
\dfrac{dS}{dt} = -\,k_2\dfrac{dE}{dt} \\
\qquad -k_3\mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\left(\dfrac{O}{K_O+O}+\epsilon\right)X \\
\dfrac{dO}{dt} = -k_4\mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\dfrac{O}{K_O+O}X
\end{cases}
$$

with $\Phi(E) = \left(0.5 + \dfrac{1}{\pi}\arctan(k_{d_1}(E-tol))\right)k_{d_2}(E-tol)^2$

[Borzì et al. (2014); Schenk et al. (2017)]

IDE Model vs. ODE Model

IDE model (two normal peak initial distribution)

ODE model with approx. same initial yeast concentration

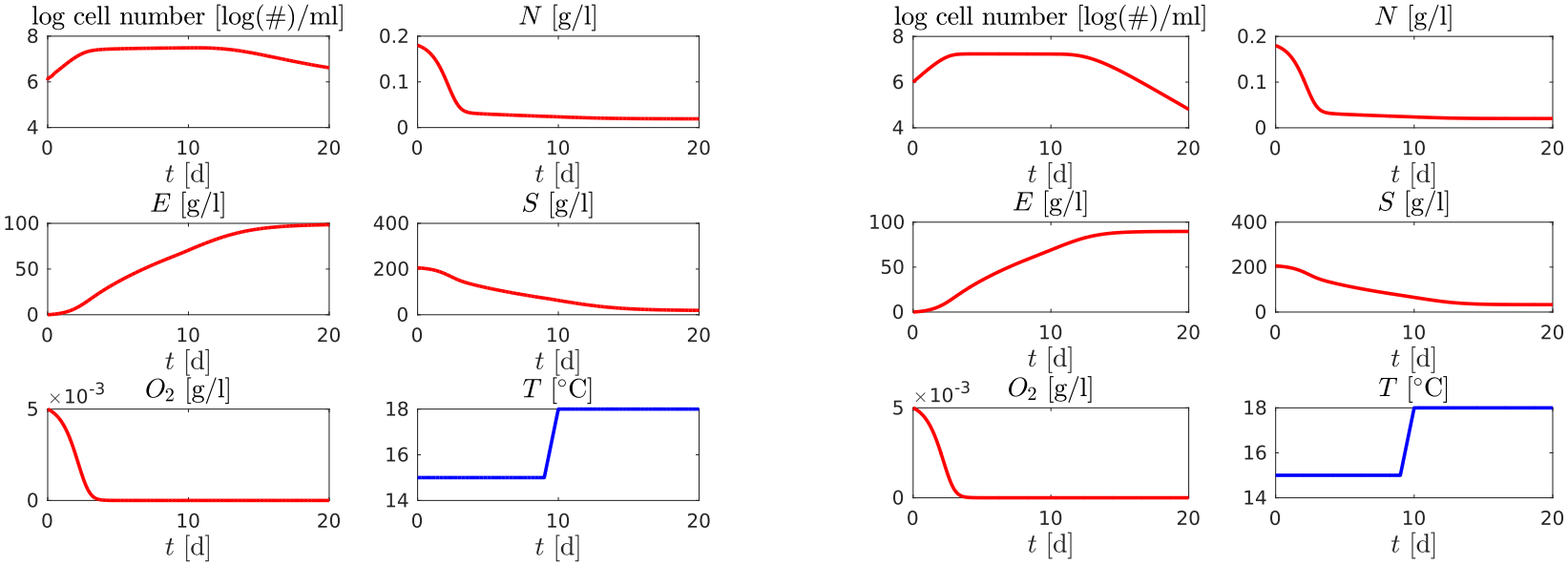


Figure: Log cell number and all other substrate/product concentration trajectories for entire time horizon

- Main differences for yeast growth, yeast death and accumulation of alcohol
- BUT: Challenges

Further Research

- ODE model for optimization
- Economic nonlinear model predictive control with parameter and state estimation and application in several experiments with industry partners
- Novel optimization problem formulation including temperature development equation
- Temperature control with objective of energy conservation and quality maintenance
- Reduction of cooling costs by approximately 52%
- Quality assured by performance of triangle test

Outcomes and Outlook

- Model derivation, existence and uniqueness studies, and numerical results
- Ideas of proof available in literature not applicable for existence and uniqueness proof for nonlinear IDE system without modification
- More data and computational efficient methods needed for IDE model $\rightarrow$ ODE model for optimization
- More information: Borzì et al. (2014); Schenk and Schulz (2015); Schenk et al. (2017); Schenk (2018); Bartsch et al. (2019)

[Source: ruter.de]

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Outlook

- Further investigations related to nonlinear system
- Stability and convergence analysis for IDE problem

References I

Bartsch, J., Borzì, A., Schenk, C., Schmidt, D., Müller, J., Schulz, V., and Velten, K. (2019). An extended model of wine fermentation including aromas and acids. *ArXiv-Preprint*, arXiv:1901.03659. http://arxiv.org/abs/1901.03659.

Borzì, A., Merger, J., Müller, J., Rosch, A., Schenk, C., Schmidt, S., Schulz, V., Velten, K., von Wallbrunn, C., and Zänglein, M. (2014). Novel Model for Wine Fermentation Including the Yeast Dying Phase. *ArXiv-Preprint*. http://arxiv.org/abs/1412.6068.

Daoutidis, P. and Henson, M. A. (2002). Dynamics and Control of Cell Populations in Continuous Bioreactors. *AIChE Symposium Series*, 326:274–289.

Dautray, R. and Lions, J.-L. (1993). *Mathematical Analysis and Numerical Methods for Science and Technology*, volume 6. Springer.

Dreher, M. (2003). *Local Solutions to Quasi-Linear Weakly Hyperbolic Differential Equations*, pages 157–205. Birkhäuser Basel, Basel.

Engel, K. J., Brendle, S., Nagel, R., Campiti, M., Hahn, T., Metafune, G., Nickel, G., Pallara, D., Perazzoli, C., Rhandi, A., et al. (1999). *One-Parameter Semigroups for Linear Evolution Equations*. Graduate Texts in Mathematics. Springer New York.

Galitzky, C., Worrell, E., Healy, P., and Zechiel, S. (2005). Benchmarking and self-assessment in the wine industry. *In Proceedings of the 2005 ACEEE Summer Study on Energy Efficiency in Industry*.

Glimm, J. (1965). Solutions in the Large for Nonlinear Hyperbolic Systems of Equations. *Communications on Pure and Applied Mathematics*, 18:697–715.

Henson, M. A. (2003). Dynamic Modeling and Control of Yeast Cell Populations in Continuous Biochemical Reactors. *Computers and Chemical Engineering*, 27:1185–1199.

Houska, B., Ferreau, H., Vukov, M., and Quirynen, R. (2009–2013). ACADO Toolkit User's Manual. http://www.acadotoolkit.org.

Korsch, A. and Kröner, D. (2017). On Existence and Uniqueness of Entropy Solutions of Weakly Coupled Hyperbolic Systems on Evolving Surfaces. *Computers & Fluids*.

Mantzaris, N., Srienc, F., and Daoutidis, P. (2002). Nonlinear Productivity Control Using a Multi-Staged Cell Population Balance Model. *Chemical Engineering Science*, 57:1–14.

Morgan, D. O. (2007). *The Cell Cycle: Principles of Control*. Primers in Biology. OUP/New Science Press.

Natalini, R. and Hanouzet, B. (1996). Weakly Coupled Systems of Quasilinear Hyperbolic Equations. *Differential Integral Equations*, 9:1279–1292.

Pazy, A. (1992). *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Applied Mathematical Sciences. Springer New York.

Rohde, C. (1998). Entropy Solutions for Weakly Coupled Hyperbolic Systems in Several Space Dimensions. *Zeitschrift für Angewandte Mathematik und Physik ZAMP*, 49(3):470–499.

References II

Rozhdestvenskii, B. L., Yanenko, N. N., Science, A. F., and Technology Center Charlottesville, V. (1972). *Systems of Quasilinear Equations and Their Applications to Gas Dynamics*. Defense Technical Information Center.

Schenk, C. (2018). *Modeling, Simulation and Optimization of Wine Fermentation*. PhD thesis, Trier University. https://ubt.opus.hbz-nrw.de/frontdoor/index/index/year/2018/docId/860.

Schenk, C. and Schulz, V. (2015). Energy-Optimal Control of Temperature for Wine Fermentation Based on a Novel Model Including the Yeast Dying Phase. *IFAC-PapersOnLine, 5th IFAC Conference on Nonlinear Model Predictive Control (NMPC'15), Seville, Spain*, 48(23):452–457. http://www.sciencedirect.com/science/article/pii/S240589631502604X.

Schenk, C., Schulz, V., Rosch, A., and von Wallbrunn, C. (2017). Less cooling energy in wine fermentation - a case study in mathematical modeling, simulation and optimization. *Food and Bioproducts Processing*, 103:131–138. http://www.sciencedirect.com/science/article/pii/S0960308517300421.

Smyth, M., Russell, J., and Milanowski, T. (2011). Solar energy in the winemaking industry. *Green Energy and Technology*. Springer.

Wikipedia (2017). Saccharomyces Cerevisiae — Wikipedia, The free Encyclopedia. [Online; accessed 17-October-2017].

Wloka, J. (1982). *Partielle Differentialgleichungen: Sobolevräume und Randwertaufgaben*. Mathematische Leitfäden. Teubner.

Zhang, Y., Zamamiri, A. M., Henson, M. A., and Hjortso, M. A. (2002). Cell Population Models for Bifurcation Analysis and Nonlinear Control of Continuous Yeast Bioreactors. *Journal of Process Control*, 12(6):721–734.

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