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# EXPLORING MICROBIAL DYNAMICS BASED ON THE MICROBIAL TRANSITION STATE THERMOKINETIC THEORY

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## ABSTRACT

The Microbial Transition State (MTS) model, employing a thermokinetic approach rooted in statistical physics, establishes a link between growth kinetics and the energy balance of cell metabolism (Desmond-Le Quémener & Bouchez, 2014). This model has demonstrated success in simulating both microbial communities and pure cultures (Delattre et al., 2019).

Further development of the MTS theory is proposed to better grasp and represent the impact of environmental conditions (i.e. temperature, pH, salinity) on growth dynamics.

## MODEL FRAMEWORK

In the MTS theory, the specific growth rate ( $\mu$ ) is given by:

$$\mu = \mu_{\max} \prod_i \exp\left(\frac{v_{S_i}^{\text{met}}}{V_H * [S_i]}\right)$$

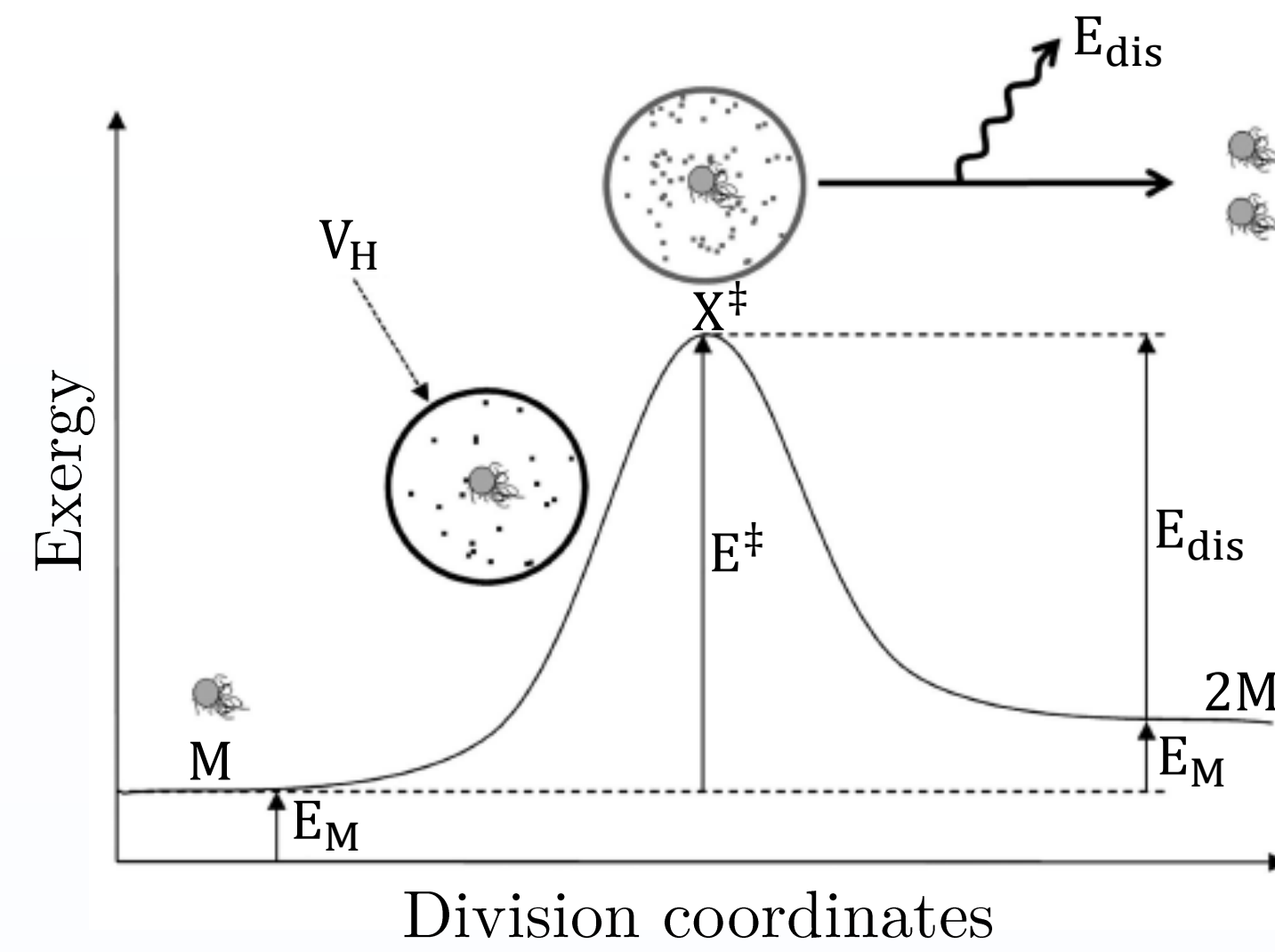


Fig. 1. Schematic representation of microbial energy levels along division coordinates. (Desmond-Le Quémener & Bouchez, 2014)

Where the model parameters are defined as follows:

$$v_{S_i}^{\text{met}} = v_{S_i}^{\text{an}} + \lambda * v_{S_i}^{\text{cat}}$$

- $\lambda$ : number of times the catabolic reactions is performed per mol of biomass produced (Kleerebezem, 2010).
- $v$ : stoichiometric coefficient of each chemical specie ( $S_i$ ).

▪ According to the Gibbs Energy Dissipation Method:

$$\lambda = -\frac{\Delta G_{\text{an}} + \Delta G_{\text{dis}}}{\Delta G_{\text{cat}}}$$

▪  $\Delta G_{\text{dis}}$  empirically defined by Heijnen (1992) as:

$$\Delta G_{\text{dis}} \approx 200 + 18(6 - NoC_{C_S})^{1,8} + \exp\left(\left((3,8 - \gamma_{C_S})^2\right)^{0,16} (3,6 + 0,4 NoC_{C_S})\right)$$

▪  $\Delta G_{\text{an}}$  and  $\Delta G_{\text{cat}}$  can be determined by thermodynamic calculations.

▪  $V_H$ : harvest volume.

## FOREGOING FINDINGS FROM OUR RESEARCH TEAM

Monod's growth rate:

$$\frac{\mu}{\mu_{\max}} = \frac{[S_i]}{K_S + [S_i]}$$

MTS growth rate:

$$\frac{\mu}{\mu_{\max}} = \exp\left(-\frac{\lambda}{V_H * [S_i]}\right)$$

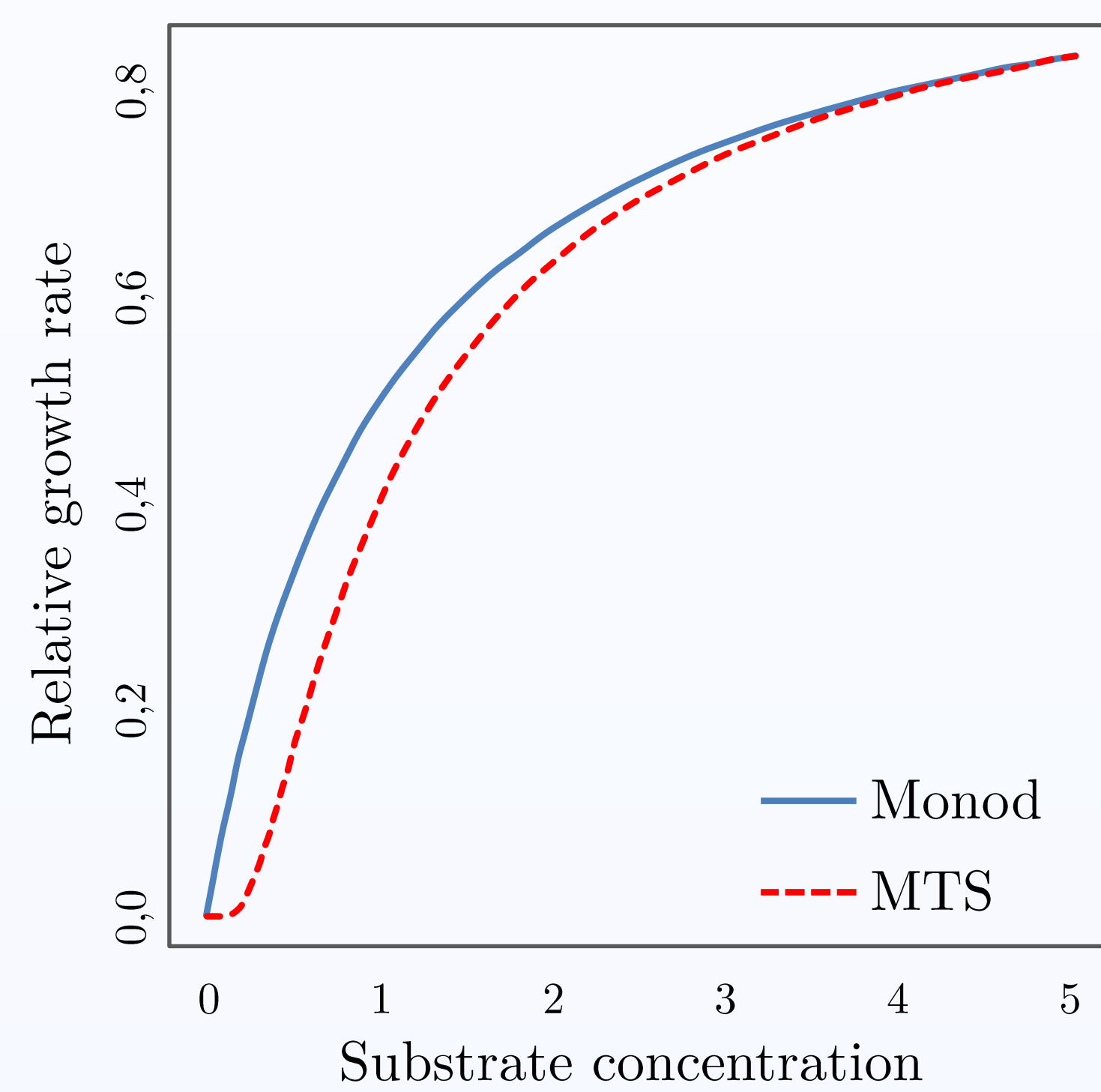


Fig. 2. Comparison between Monod's and MTS growth rate functions. (Ugalde-Salas et al., 2020)

Dependency on growth rate at low substrate concentrations.

Presence of an apparent threshold concentration for growth.

The growth of the most thermodynamically advantaged guild delays the growth of competing guilds.

With more incoming electron donor, molecules become available for a guild catalyzing a less exergonic reaction.

(Delattre PhD thesis; Delattre et al., 2019)

Case study: Wastewater treatment microbial assembly (Delattre et al., 2019).

$$|\Delta G_{\text{aerobic oxidation}}| > |\Delta G_{\text{denitrification}}| > |\Delta G_{\text{sulfate reduction}}| > |\Delta G_{\text{iron reduction}}|$$

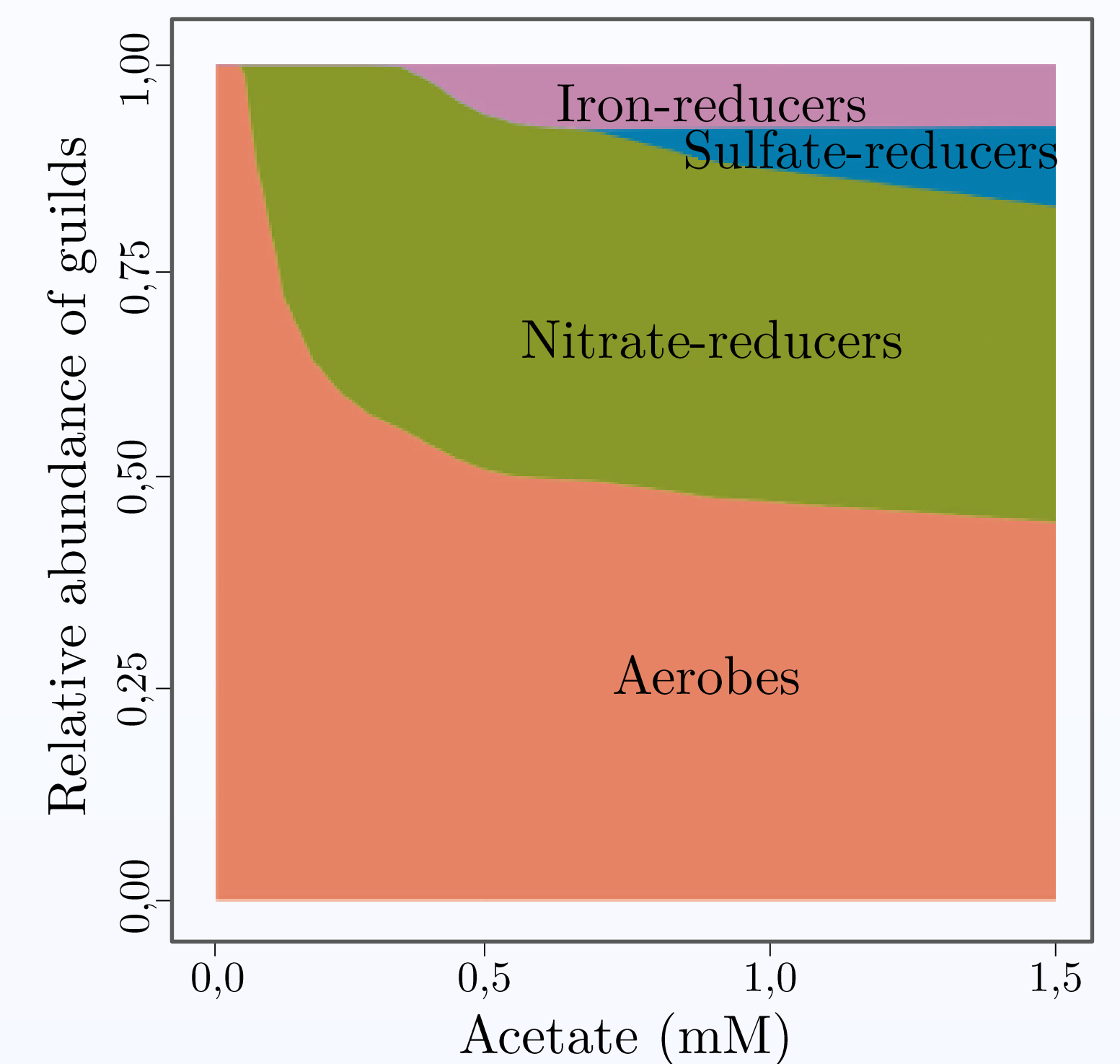
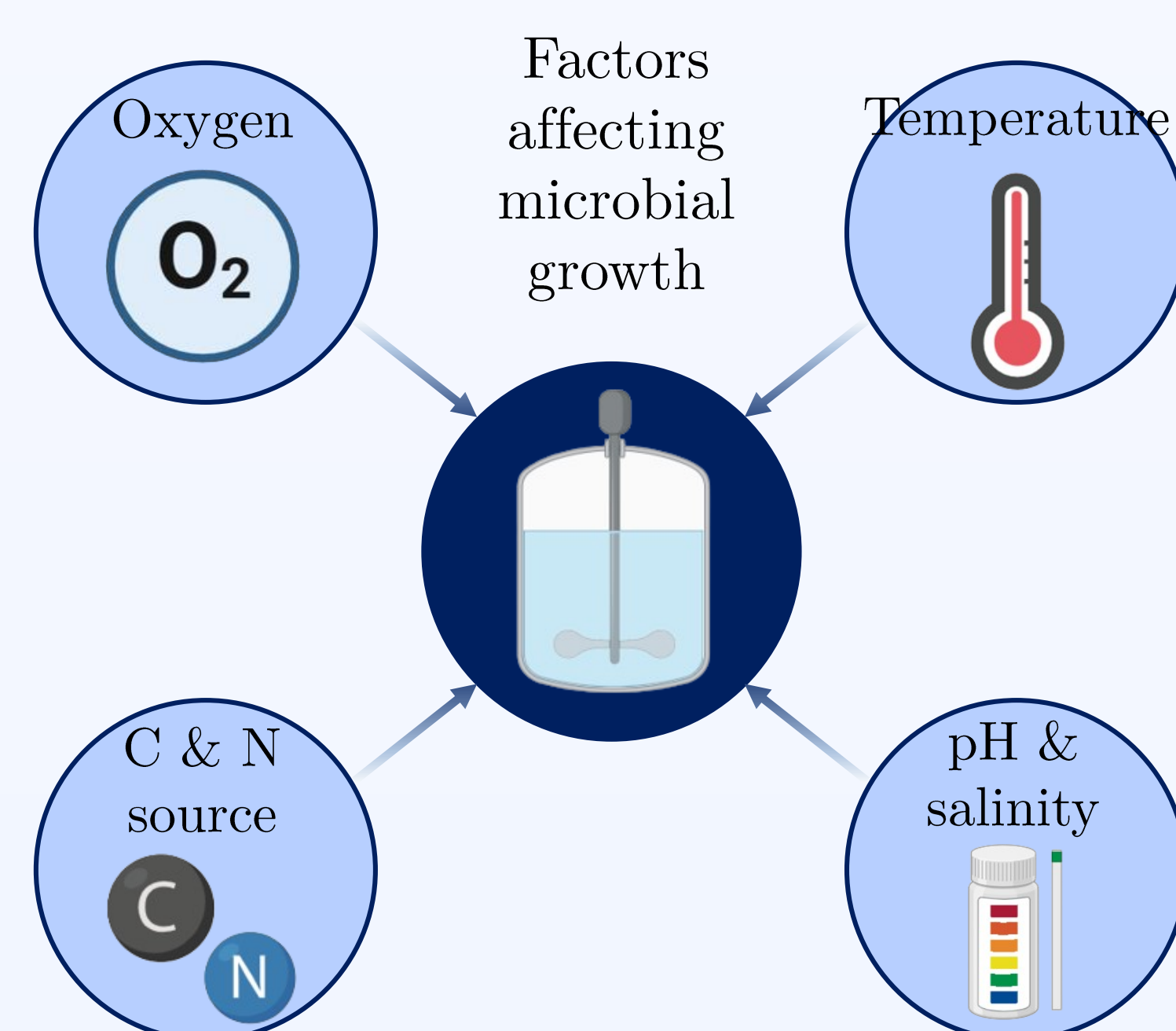
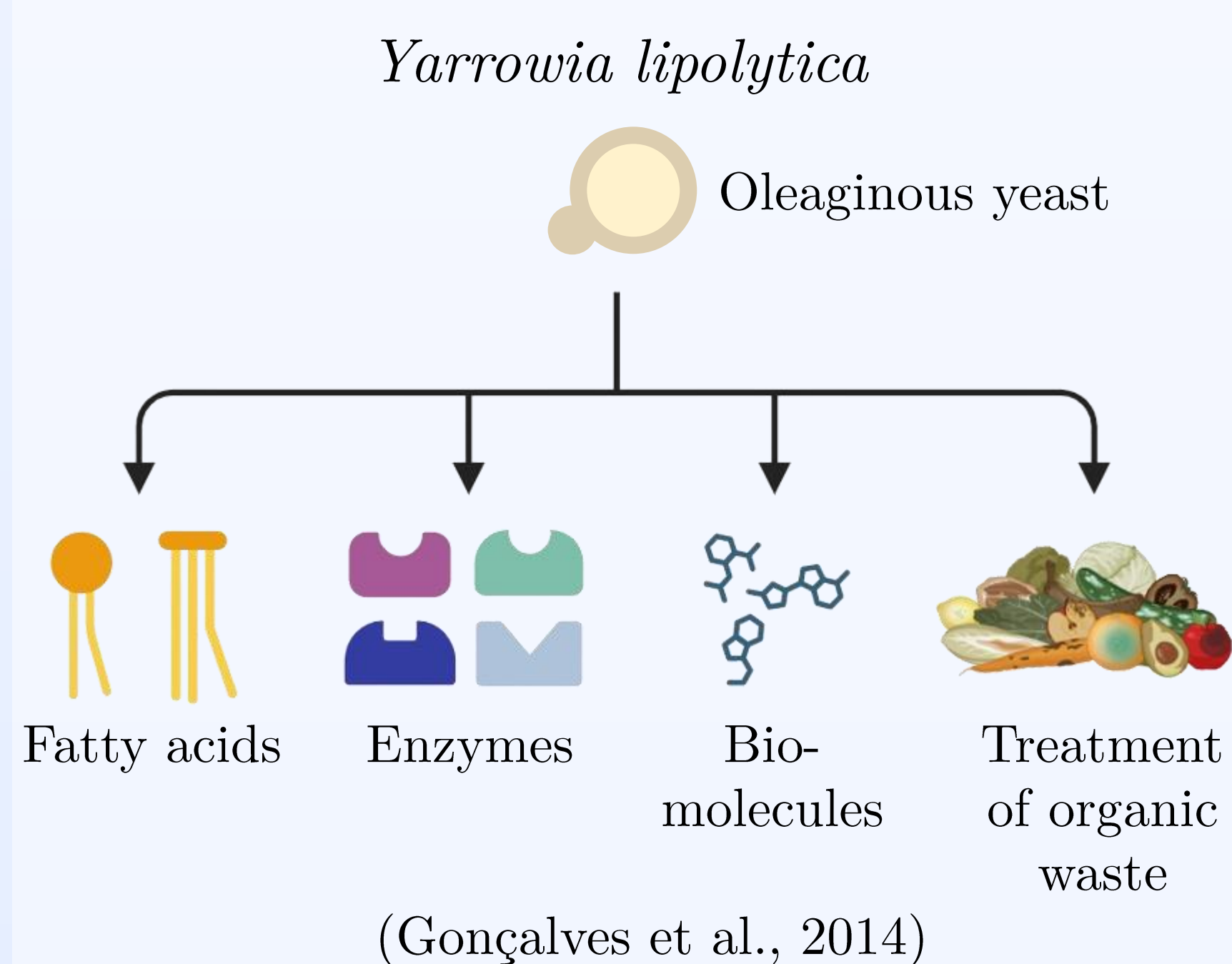


Fig. 3. Competition outcome in a chemostat in the presence of various electron acceptors as predicted by the MTS model. (Delattre et al., 2019)

## MY PHD THESIS



How is it possible to evaluate the effect of operating conditions on microbial growth dynamics from the fundamental principles of thermodynamics?

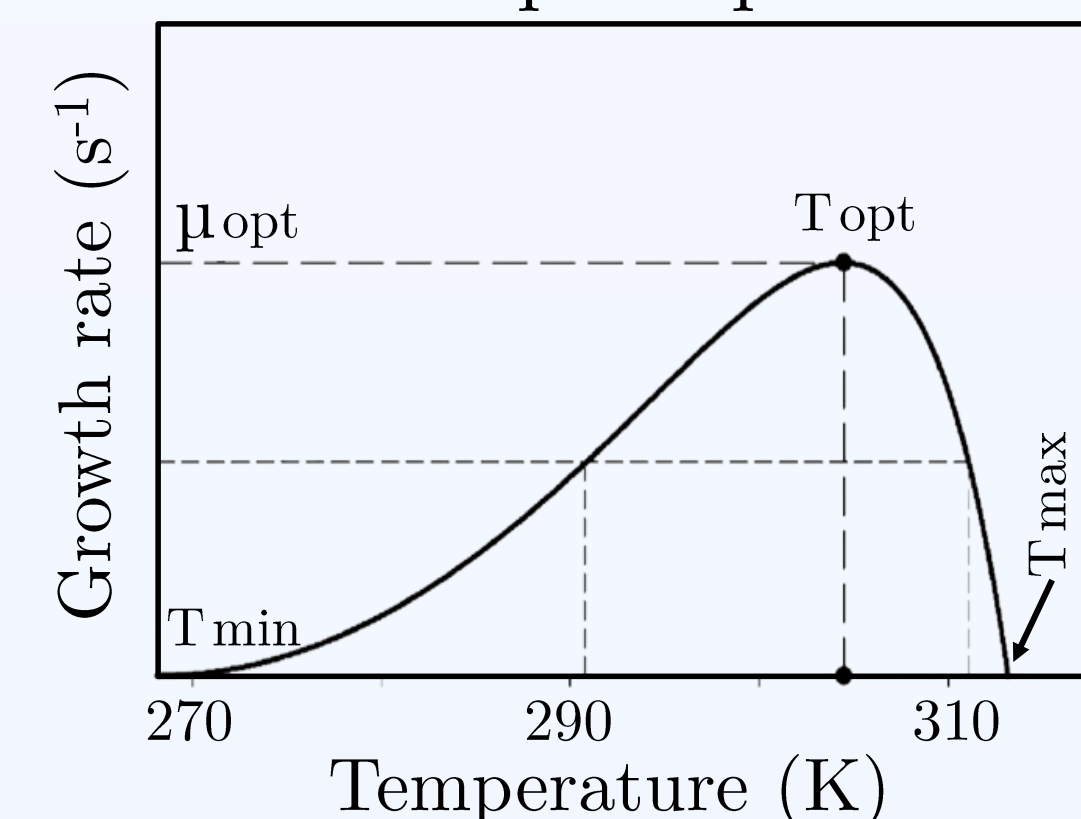


Fig. 4. Effect of temperature on microbial growth rate. (Noll et al., 2020)

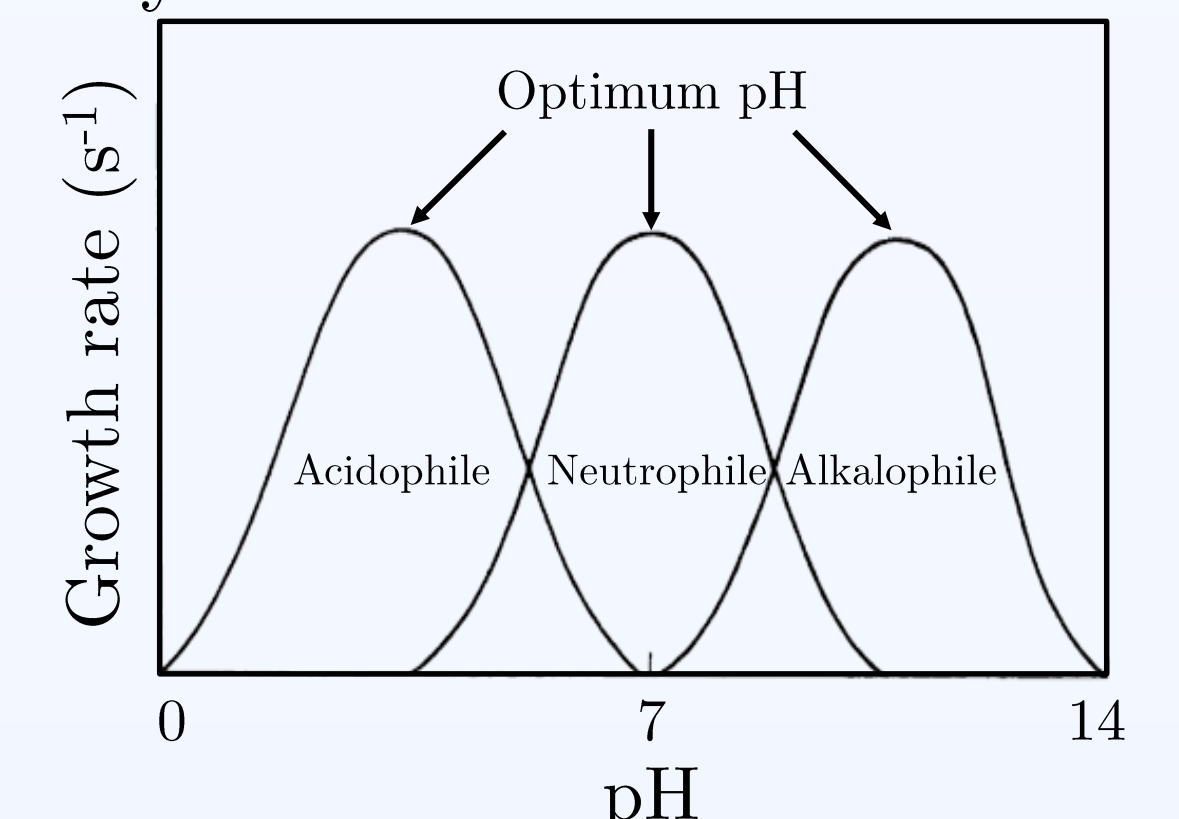


Fig. 5. Effect of pH on microbial growth rate. (Stuart Hogg, 2005)

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