A simplified approach for activity monitoring in complex wastewater treatment processes

Miguel Mauricio-Iglesias

Juan M. Garrido, Juan M. Lema

Environmental Biotechnology Group - BIOGROUP

Universidade de Santiago de Compostela

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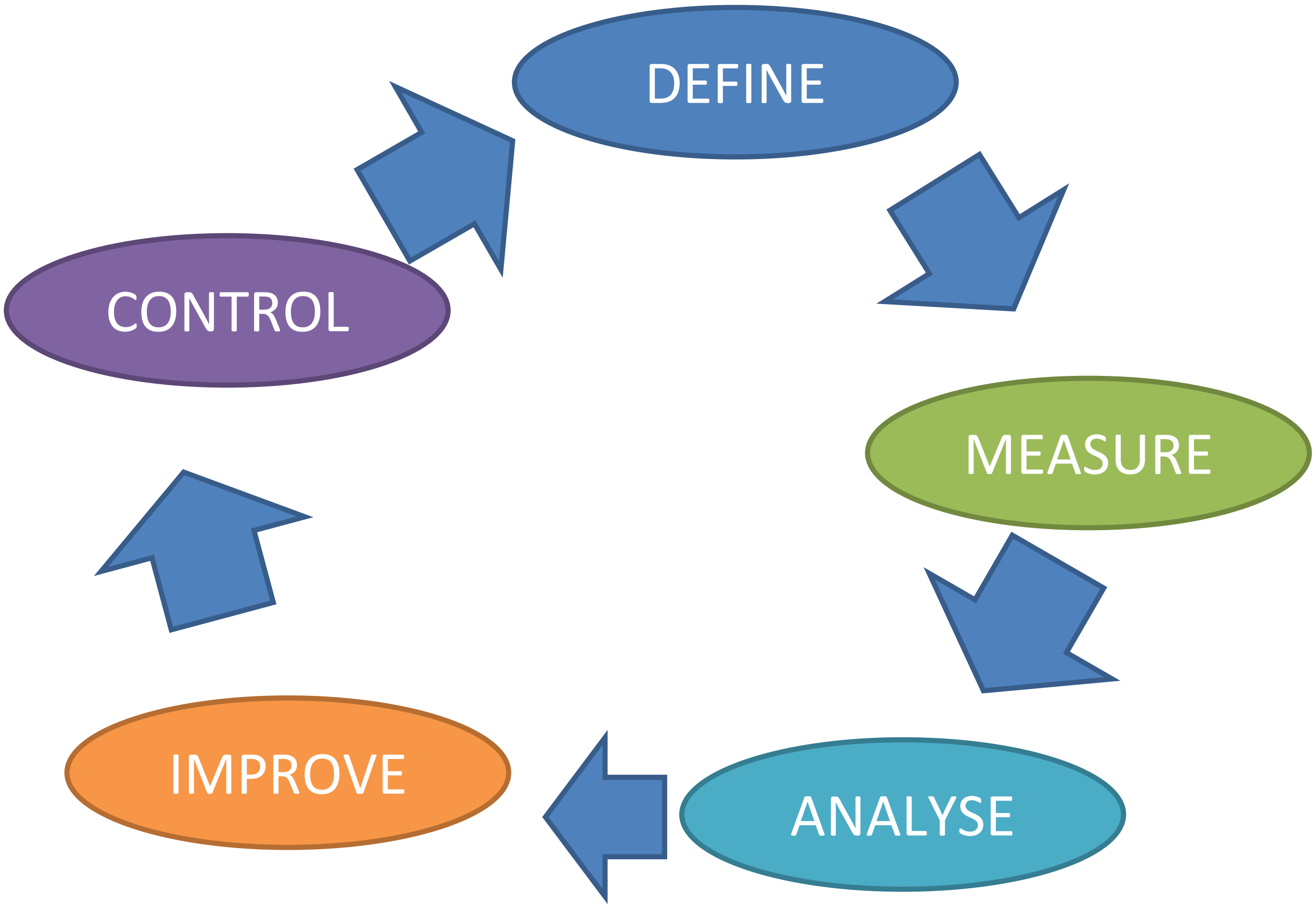
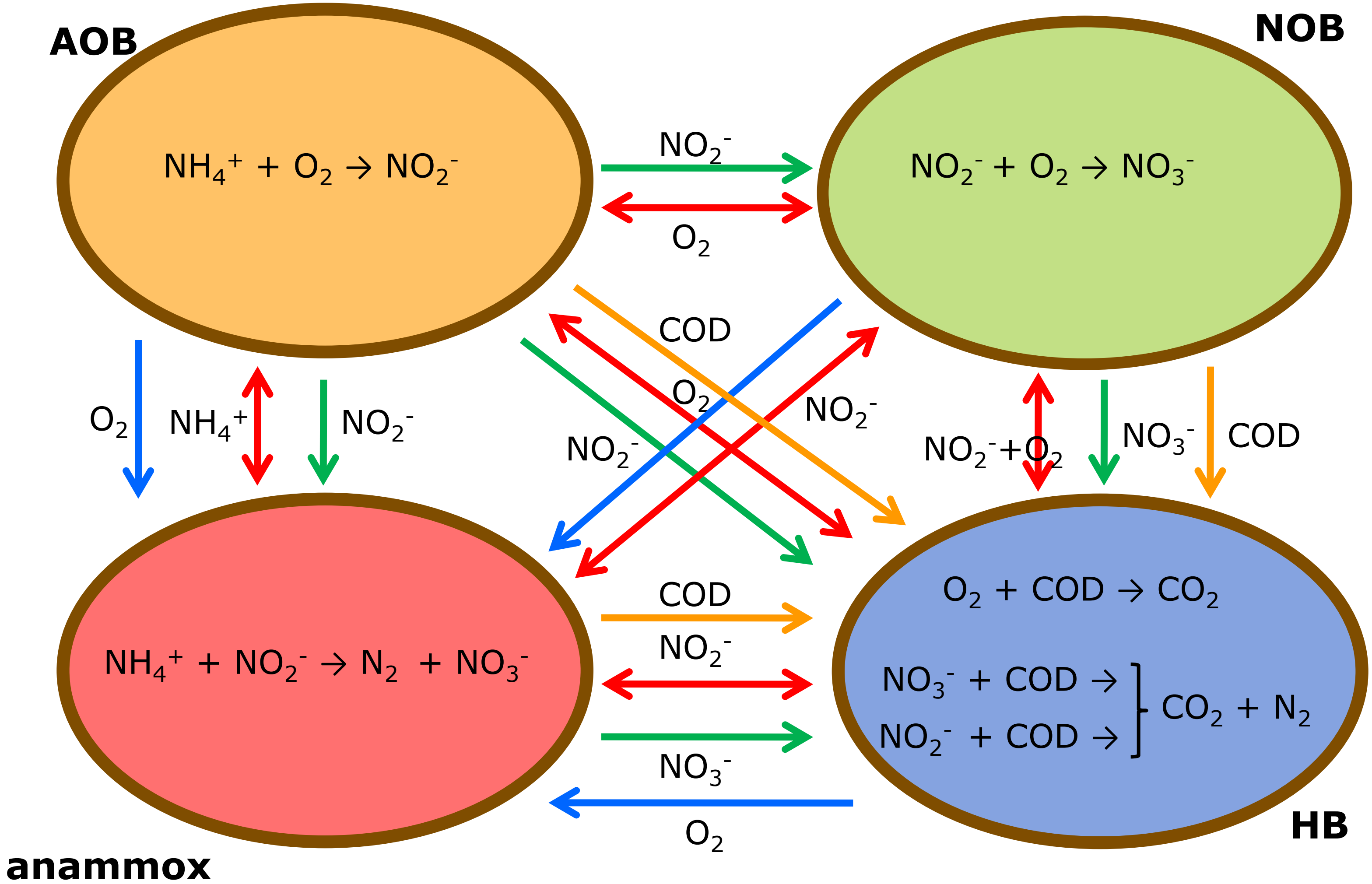
What you don't measure, you can't improve



Activity rate monitoring is useful in some processes



Vangsgaard, A.K.. (2014). PhD Thesis

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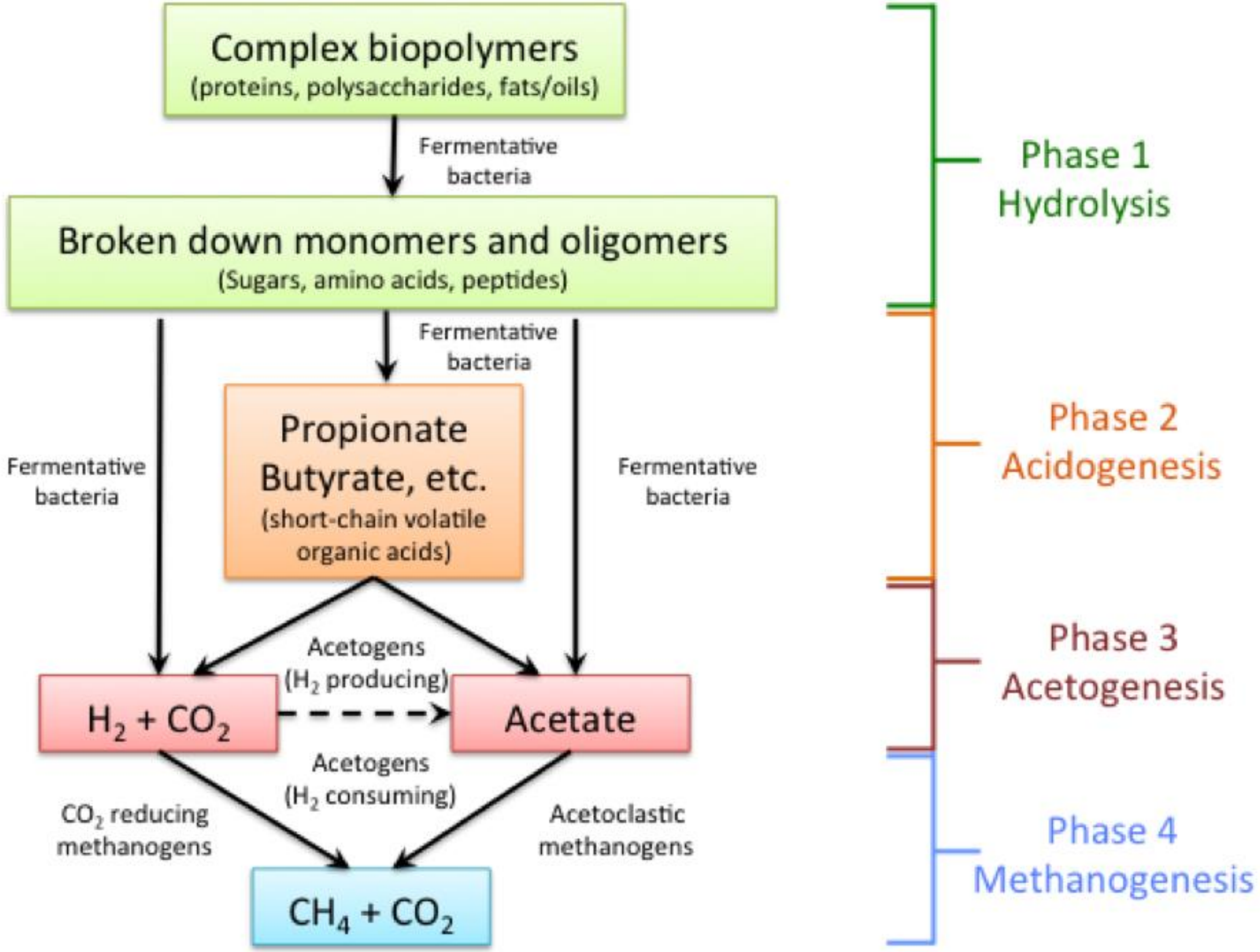
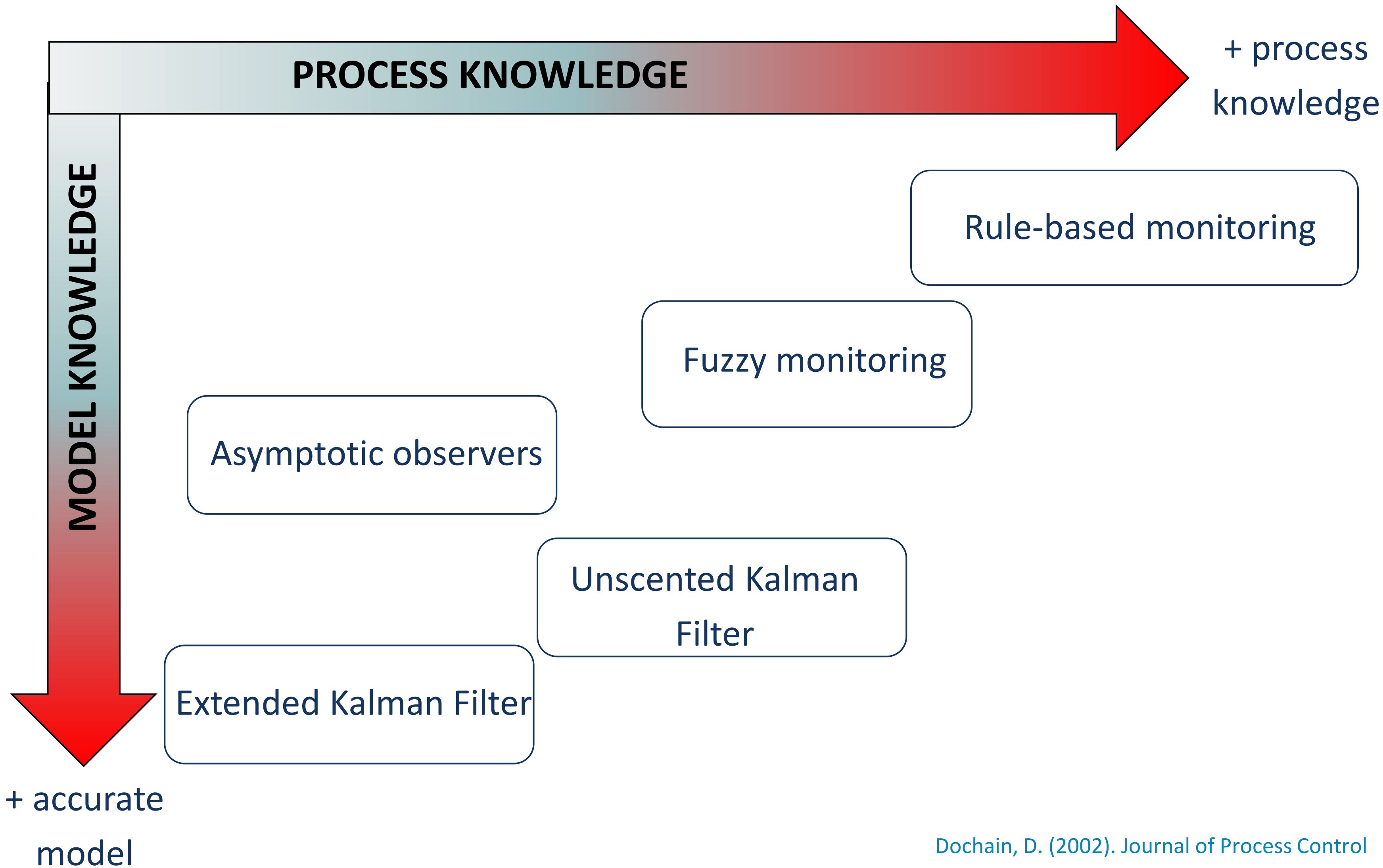


Figure Source: John A Datton e-education institute www.e-education.psu.edu

Most approaches rely on having a model or experience in running the process



Dochain, D. (2002). Journal of Process Control

The Continuous-Discrete Extended Kalman Filter is a very good tool if a model is available

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Plant model

$$x_{k+1} = x_k + \int_{t_k}^{t_{k+1}} f\left(x(\tau), u_k, d_k\right) d\tau + w_k$$

$$y_k = G(x_k) + v_k, \quad v_k \in \mathrm{N}_{iid}(0, R_v)$$

One step-ahead prediction

$$\hat{x}_{k+1|k} = \hat{x}_{k|k} + \int_{t_k}^{t_{k+1}} f\left(x(\tau), u_k, d_k\right) d\tau$$

$$\bar{A}_k = I + \int_{t_k}^{t_{k+1}} \frac{\partial f}{dx}\left(x(\tau), u_k, d_k\right) S_{\hat{x}_{k|k}} \, d\tau$$

$$P_{k+1|k} = \bar{A}_k P_{k|k} \bar{A}_k^T + R_w$$

Measurement update

Error $$e_k = y_k - C_k \hat{x}_{k|k-1}$$

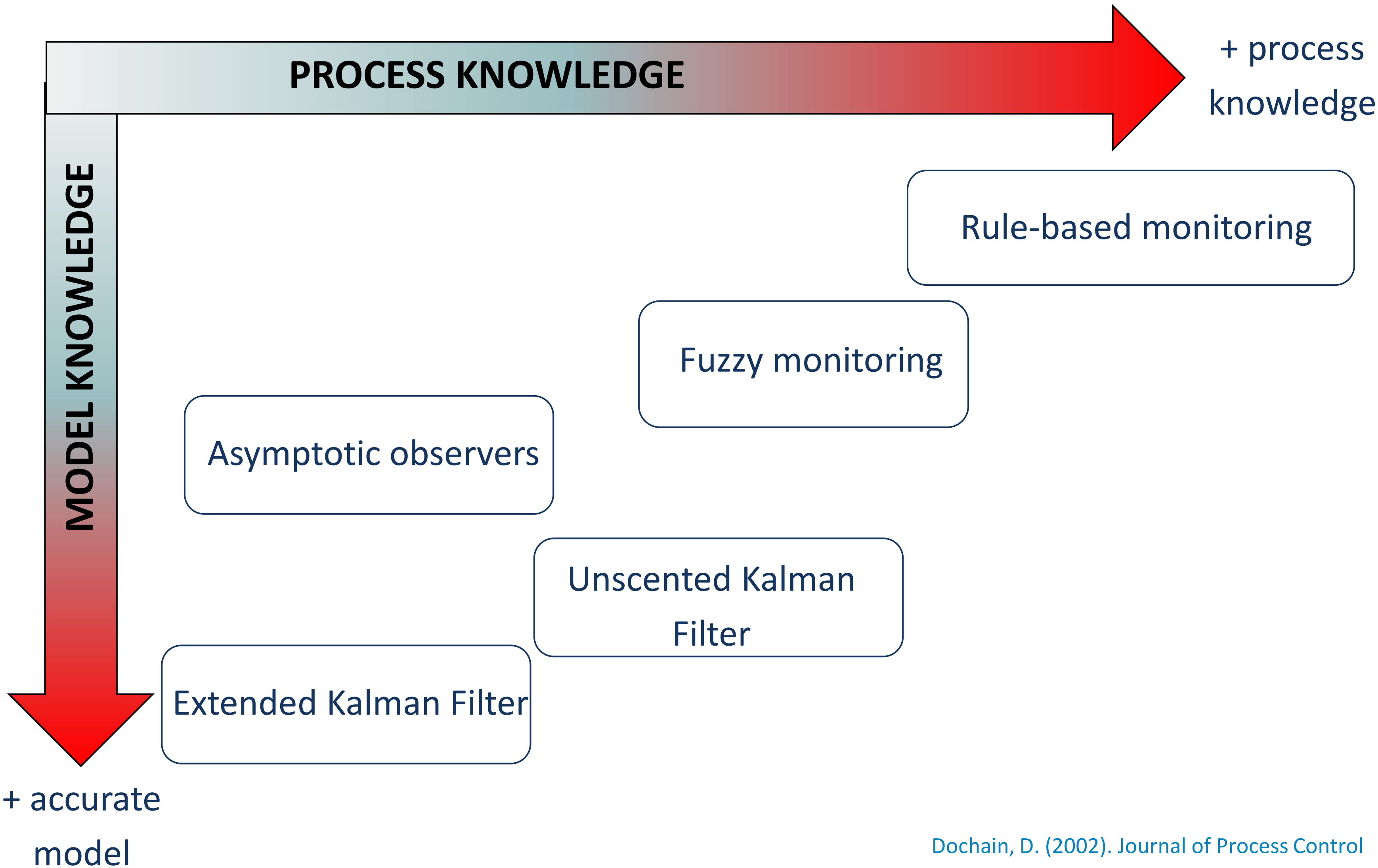
Gain $$K_{f,k} = P_{k|k-1} C_k^{\ T} \left[C_k P_{k|k-1} C_k^{\ T} + R_v\right]^{-1}$$

State estimate $$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_{f,k} e_k$$

Covariance $$P_{k|k} = P_{k|k-1} - K_{f,k} \left[C_k P_{k|k-1} C_k^{\ T} + R_v\right]^{-1} K_{f,k}^T$$

Mauricio-Iglesias et al. (2015). Computer Aided Chemical Engineering

What if we have little knowledge?



Dochain, D. (2002). Journal of Process Control

We propose stoichiometry-based monitoring as a very simple tool

$$r_S \approx \frac{s_t - s_{t-1}}{\Delta t} - F_{IN}\, s_{In} + F_{Out}\, s_t$$

Reaction = Accumulation – In + Out

This we know (partially)

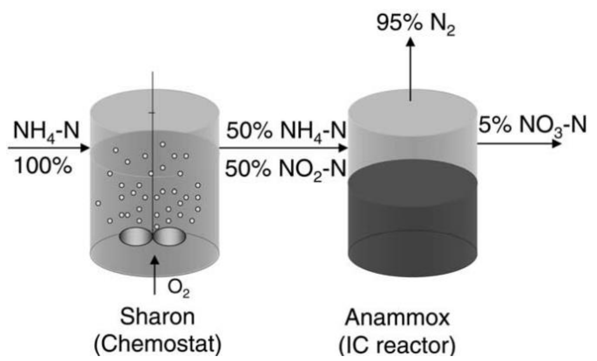
$$\boldsymbol{r_S} = \boldsymbol{S}\, \boldsymbol{\rho}$$

This we want to find out

$$\boldsymbol{r_S} = \boldsymbol{S}\, \boldsymbol{\rho}$$

- More r_s than ρ → The system is **overdetermined** → **Data reconciliation**
- As many r_s as ρ → The system is **determined** → **Unique solution**
- Fewer r_s than ρ → The system is **underdetermined** → **Infinite solutions**

A Sharon-Anammox process without HB gives place to a determined system of equations



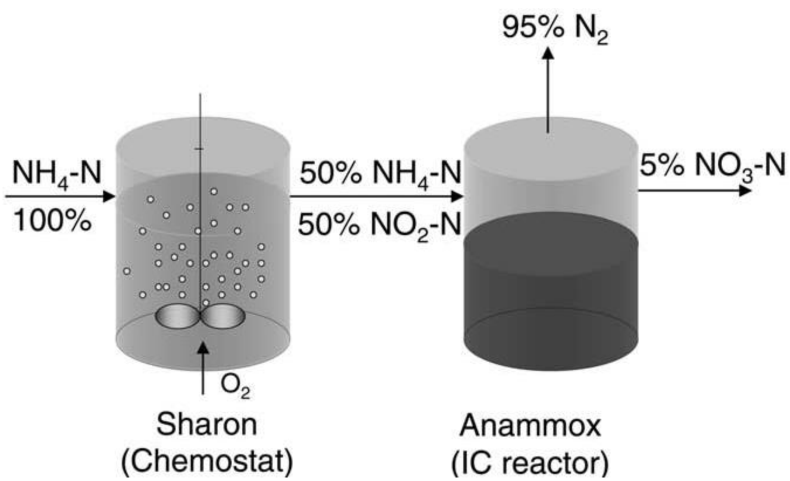
$$\begin{matrix} r_{NH} \\ r_{NO2} \\ r_{NO3} \end{matrix} = \begin{pmatrix} {}^{-1}/_{Y_{AOB}} & 0 & {}^{-1}/_{Y_{Amx/NH}} \\ {}^{1}/_{Y_{AOB}} & {}^{-1}/_{Y_{NOB}} & {}^{-1}/_{Y_{Amx/NO2}} \\ 0 & {}^{1}/_{Y_{NOB}} & 1.52 \end{pmatrix} \begin{pmatrix} \rho_{AOB} \\ \rho_{NOB} \\ \rho_{Amx} \end{pmatrix}$$

This we know (partially)

This we want to find out

Figure Source: Jetten et al (2002) Reviews in Environmental Science and Bio/Technology

Stoichiometry-based monitoring reproduces the reaction rates in an Sharon-Anammox process



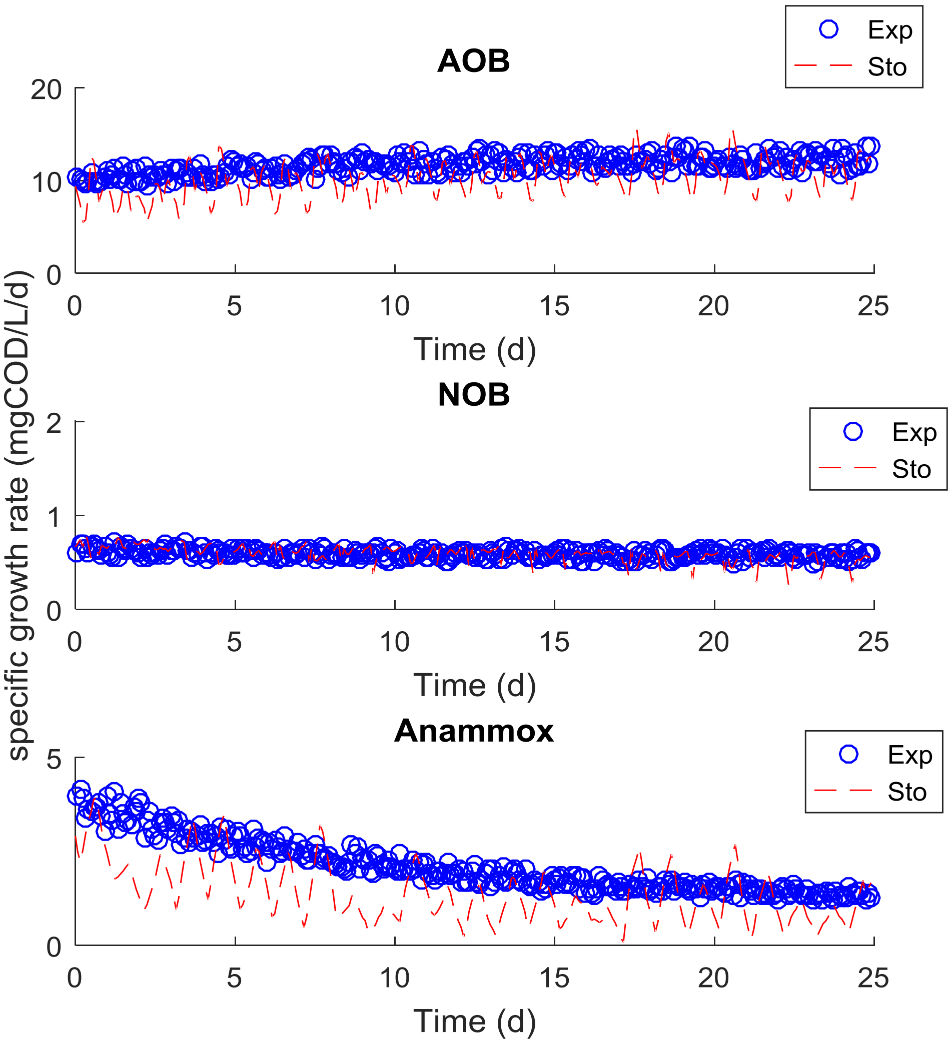


Figure Source: Jetten et al (2002) Reviews in Environmental Science and Bio/Technology

In many practical cases, the system is underdetermined…

$$\boldsymbol{r_S} = \boldsymbol{S}\,\boldsymbol{\rho}$$

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Activity rates cannot take any value. They are non-negative

$$\rho \in \mathbb{R}_{\geq 0}$$

We turn an underdetermined system of equations into a linear least squares program

$$\boldsymbol{r_S} = \boldsymbol{S}\,\boldsymbol{\rho} \quad \Rightarrow \quad \min_{\rho} \frac{1}{2} \|\boldsymbol{S\rho} - \boldsymbol{r_S}\|^2$$

And we enforce non-negativity by constraining the value of ρ

$$s.t.\ \ \boldsymbol{\rho_i} \geq \boldsymbol{0}\ and\ \boldsymbol{\rho_{inf}} \leq \boldsymbol{\rho_i} \leq \boldsymbol{\rho_{sup}}$$

Stoichiometry-based monitoring only requires substrate/product stoichiometry

Step 1

Determine the stoichiometry matrix (***S***), at least for substrate(s)/product(s) relationships

Step 2

Estimate the vector of observable rates (***r***) based on macroscopic measurements by mass balances

$$r_S \approx \frac{s_t - s_{t-1}}{\Delta t} - F_{IN}\, s_{In} + F_{Out}\, s_t$$

Step 3

Solve the constrained linear least-squares problem

$$\min_{\rho} \frac{1}{2} \|\boldsymbol{N\rho} - \boldsymbol{r}\|^2$$
$$s.t.\ \ \boldsymbol{\rho_i} \geq \boldsymbol{0}$$
$$and\ \boldsymbol{\rho_{inf}} \leq \boldsymbol{\rho_i} \leq \boldsymbol{\rho_{sup}}$$

Case study. Novel SIAM Process

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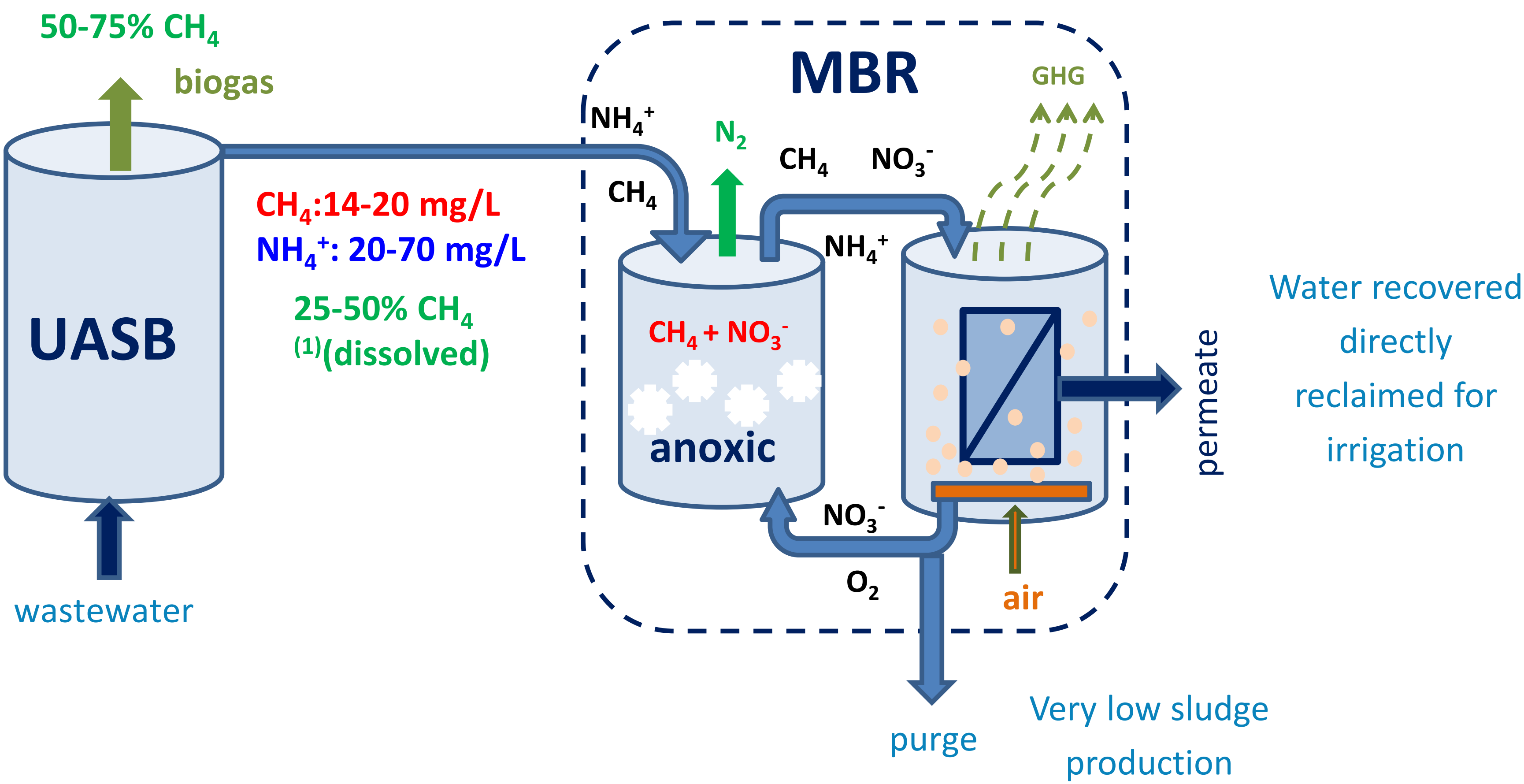
SIAM (*Sistema Integrado Anaerobio de Membrana*)

Membrane Integrated Anaerobic System. Buntner, D. et al(2011) Water Sci.Tech, 64(2), 397-402

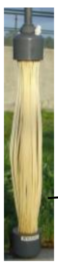


(1) Noyola, A. Morgan, J.M., Lopez, J.E. (2006). Reviews in Environmental Science and Bio-Technology 5, 93-114.

SIAM was patented at USC and demo plants are being built in Spain

Santiago de Compostela

Anaerobic reactor (UASB)



Aerobic membrane bioreactor

Outeiro de Rei (Lugo)
New plant in construction
in dairy company

Murcia

Many microbial groups play an important role in SIAM

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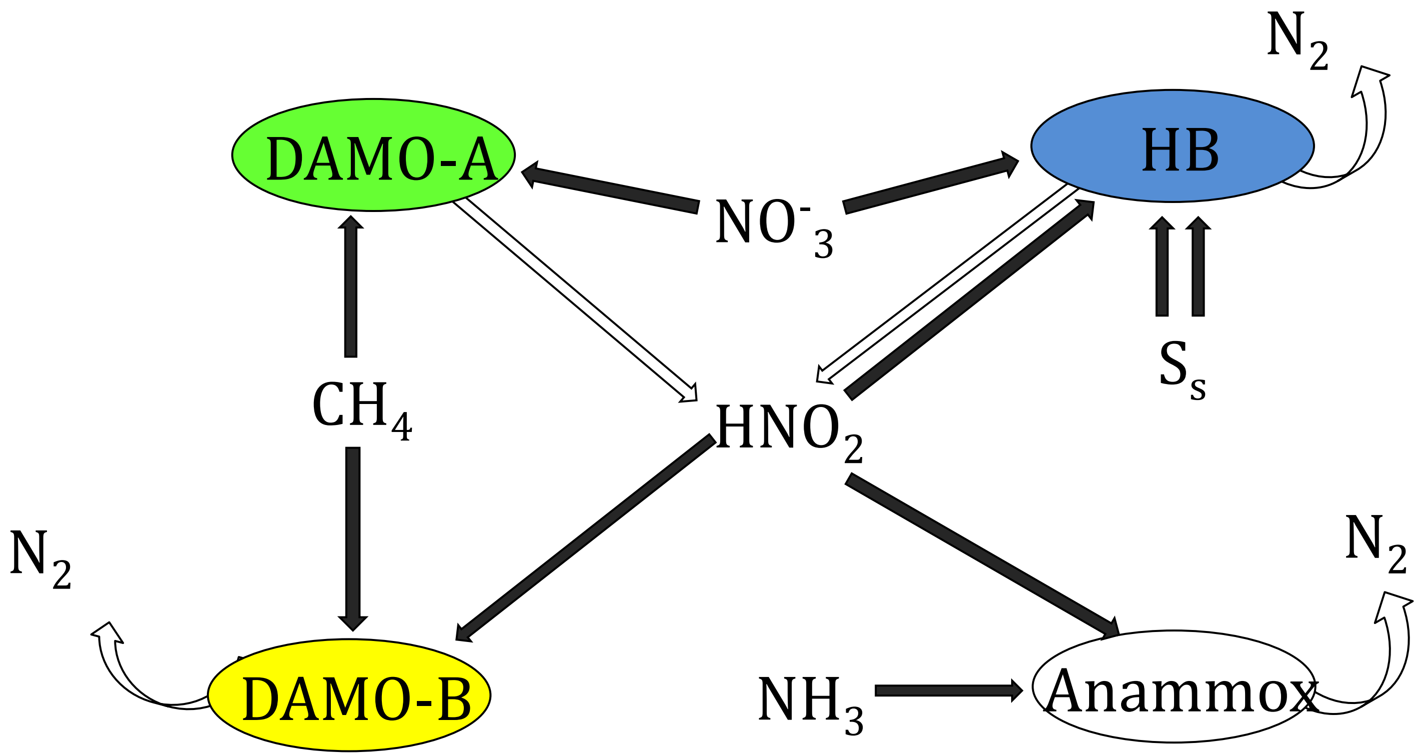
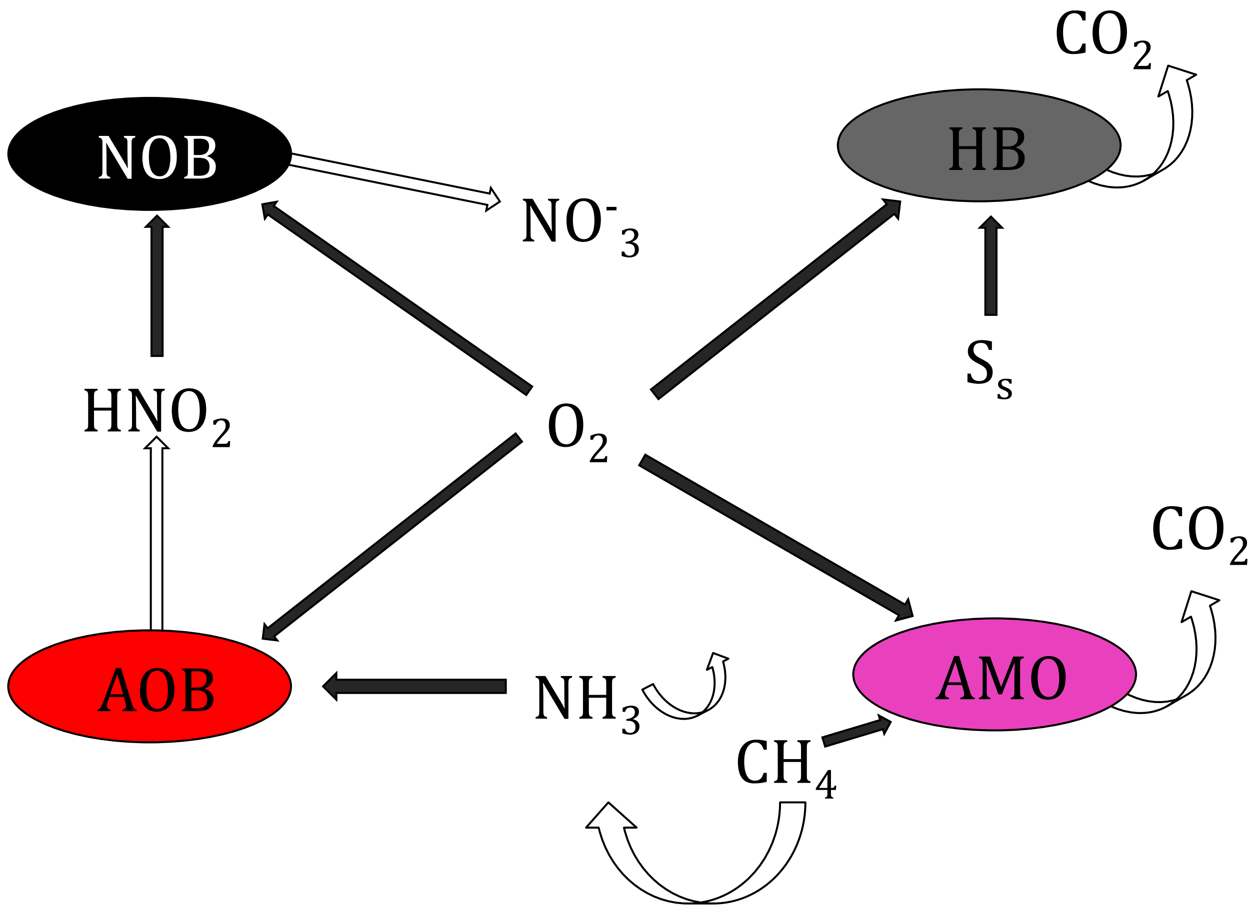


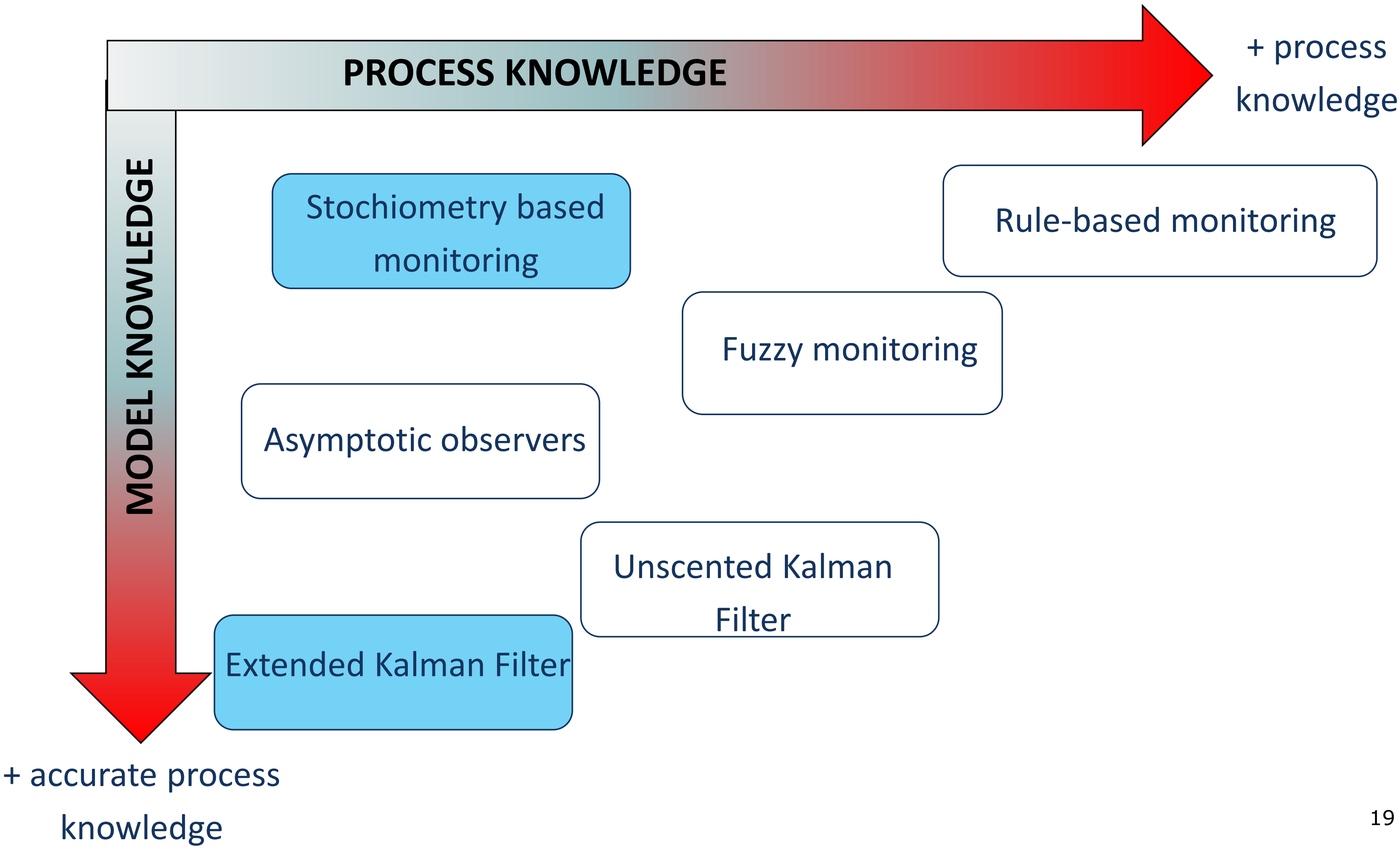
Main reactions in anoxic environment

Many microbial groups play an important role in SIAM

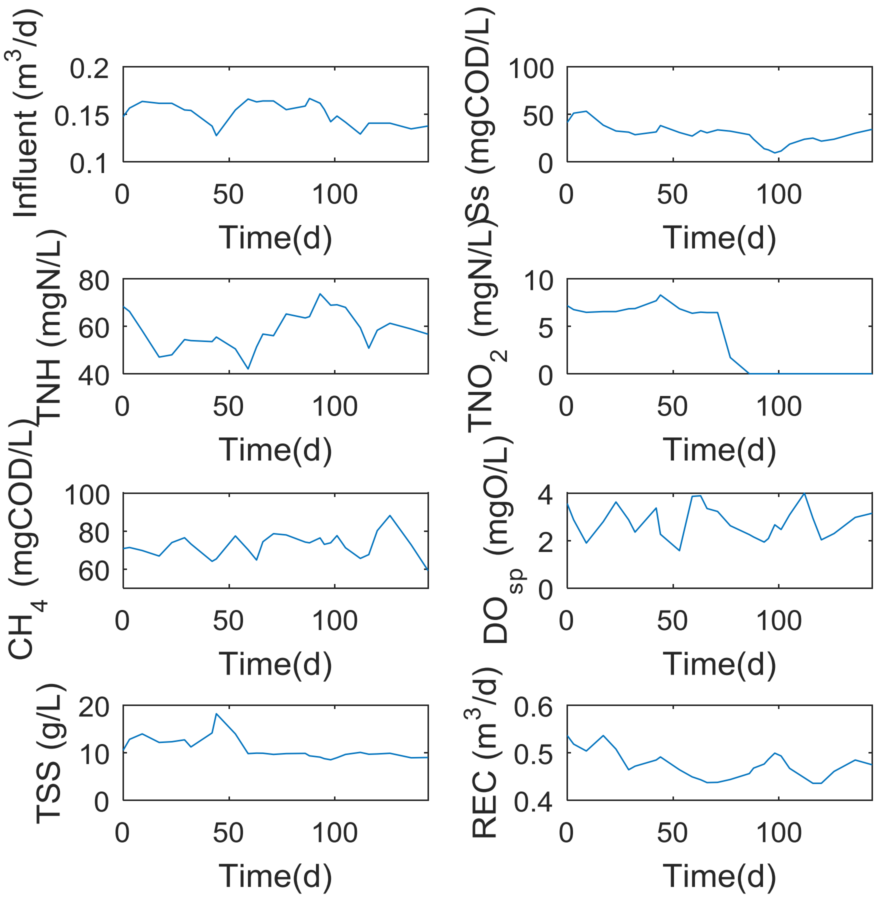


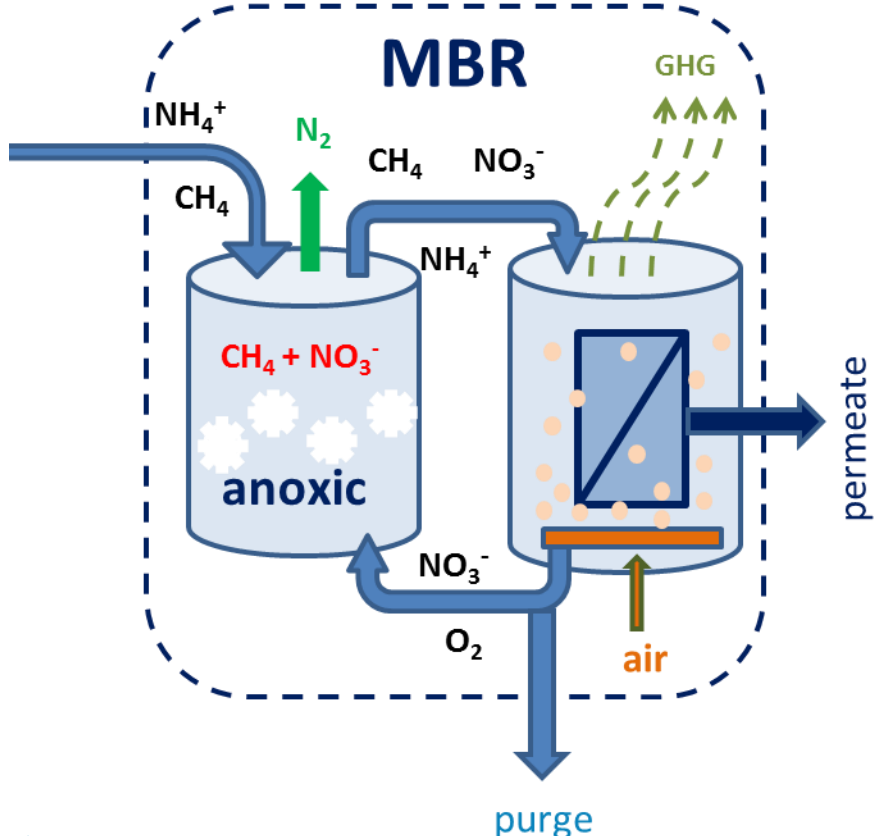
Main reactions in aerobic environment

Let’s benchmark the new method with the continuous-discrete Kalman filter



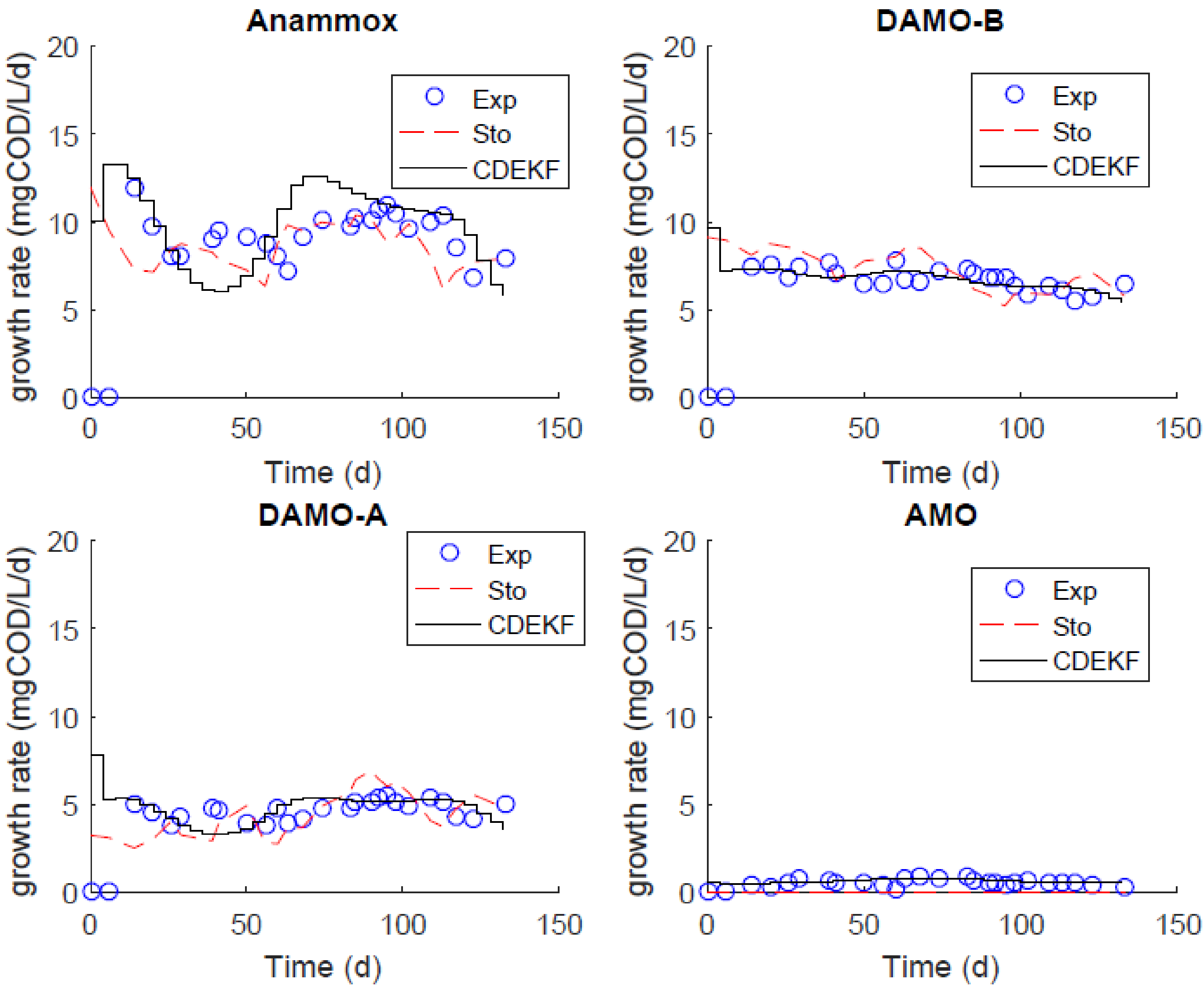
Using a realistic influent from our lab measurements



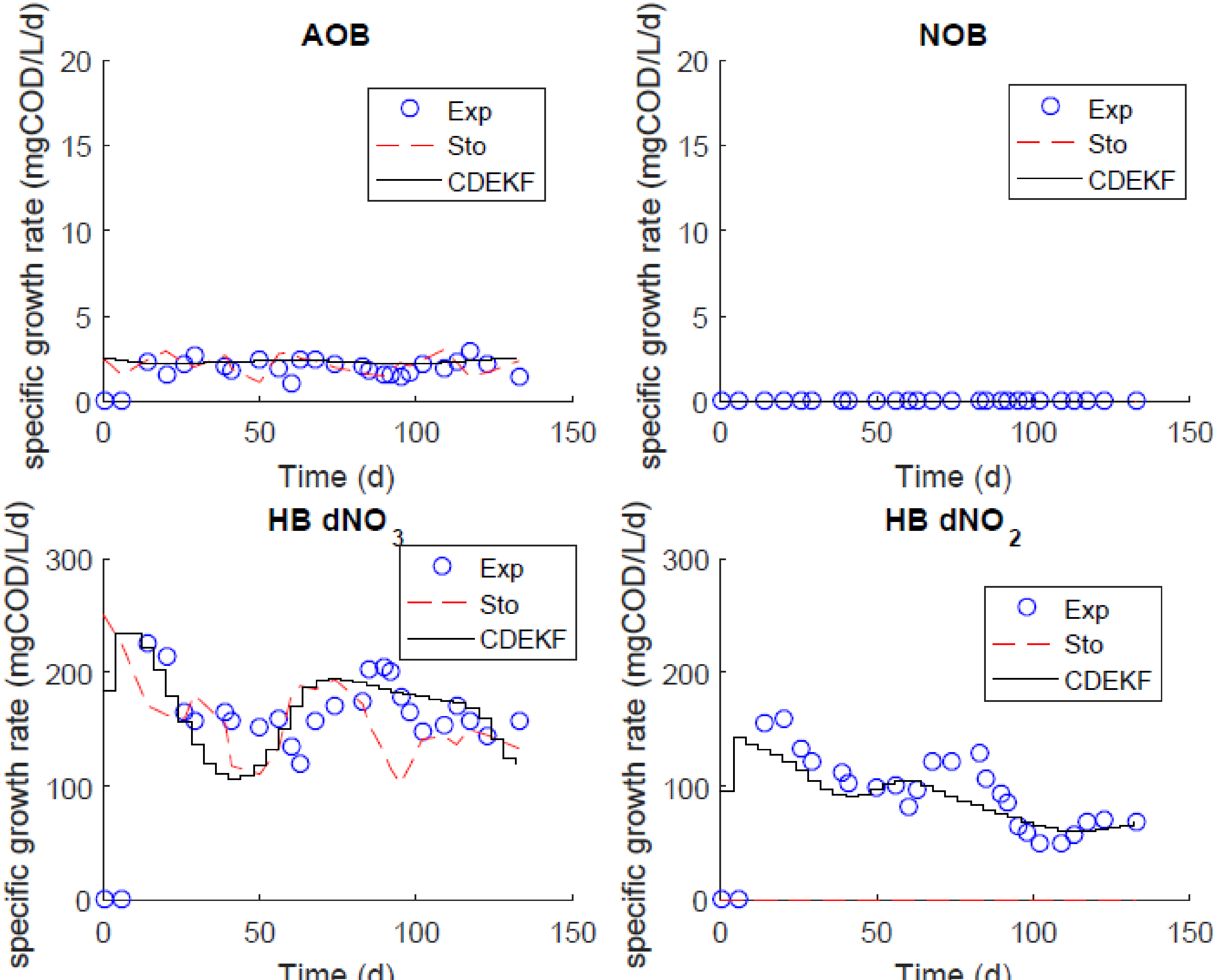


Measurements of ammonia, nitrite, nitrate, methane and oxygen in both chambers

The prediction of the rates is comparable for both methods …



… except for heterotrophic denitritation



A promising method and a lot of work to develop it further

Can it be extrapolated to other processes ?

Unicity ?

What is the minimum number of measurements ?

Appropriate sampling rate ?

✓ Simple

✓ Intuitive

✓ Limited amount of data

✓ Easy to program

✓ Surprisingly robust

Take home message

”There is no such a thing as simple methods;
there are methods adapted to a purpose” Gustaf Olsson (Academic’s Forum Sunday)

The stoichiometry-based monitoring is well adapted for the development of novel technologies

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www.life-siamec.eu/

Contact details

Miguel Mauricio-Iglesias miguel.mauricio@usc.es

Juan M. Garrido juanmanuel.garrido@usc.es

Juan M. Lema juan.lema@usc.es

BIOGROUP – Environmental Biotechnology Group www.usc.es/biogrup

Universidade de Santiago de Compostela (Spain)