Anaerobic Digestion as the core of the biomass exploitation. *The role of mathematical modeling*

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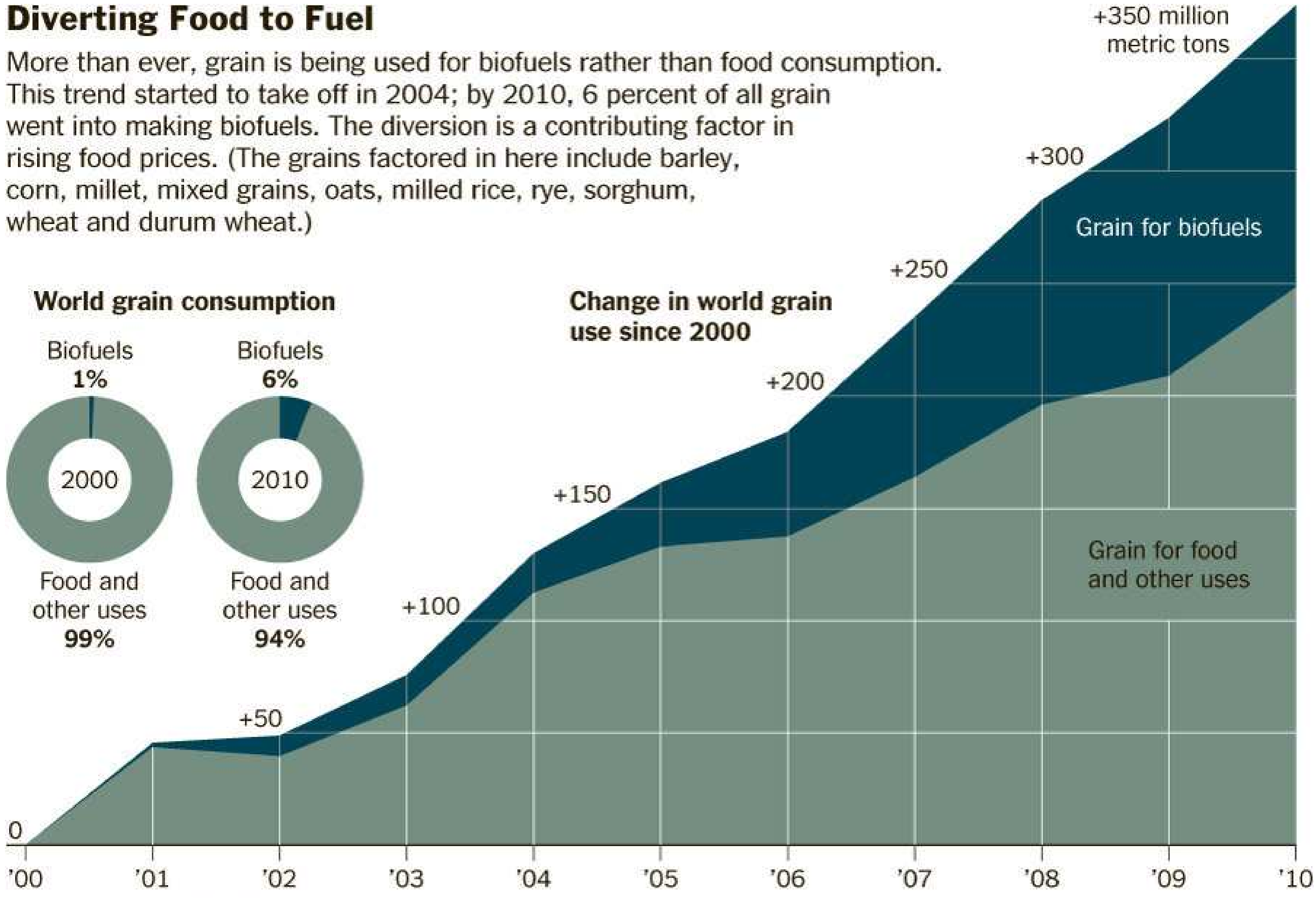
Diverting Food to Fuel

More than ever, grain is being used for biofuels rather than food consumption. This trend started to take off in 2004; by 2010, 6 percent of all grain went into making biofuels. The diversion is a contributing factor in rising food prices. (The grains factored in here include barley, corn, millet, mixed grains, oats, milled rice, rye, sorghum, wheat and durum wheat.)



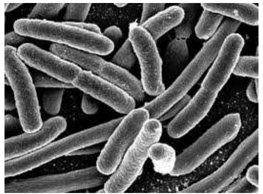
World grain consumption

Change in world grain use since 2000

Sources: United States Department of Agriculture; Food and Agricultural Policy Research Institute

Second generation biofuels are made from lignocellulosic biomass or woody crops, agricultural residues or waste

Anaerobic Digestion



Biomass

Anaerobic Microorganism

CH_4 (50-70%)

CO_2 (30-40%)

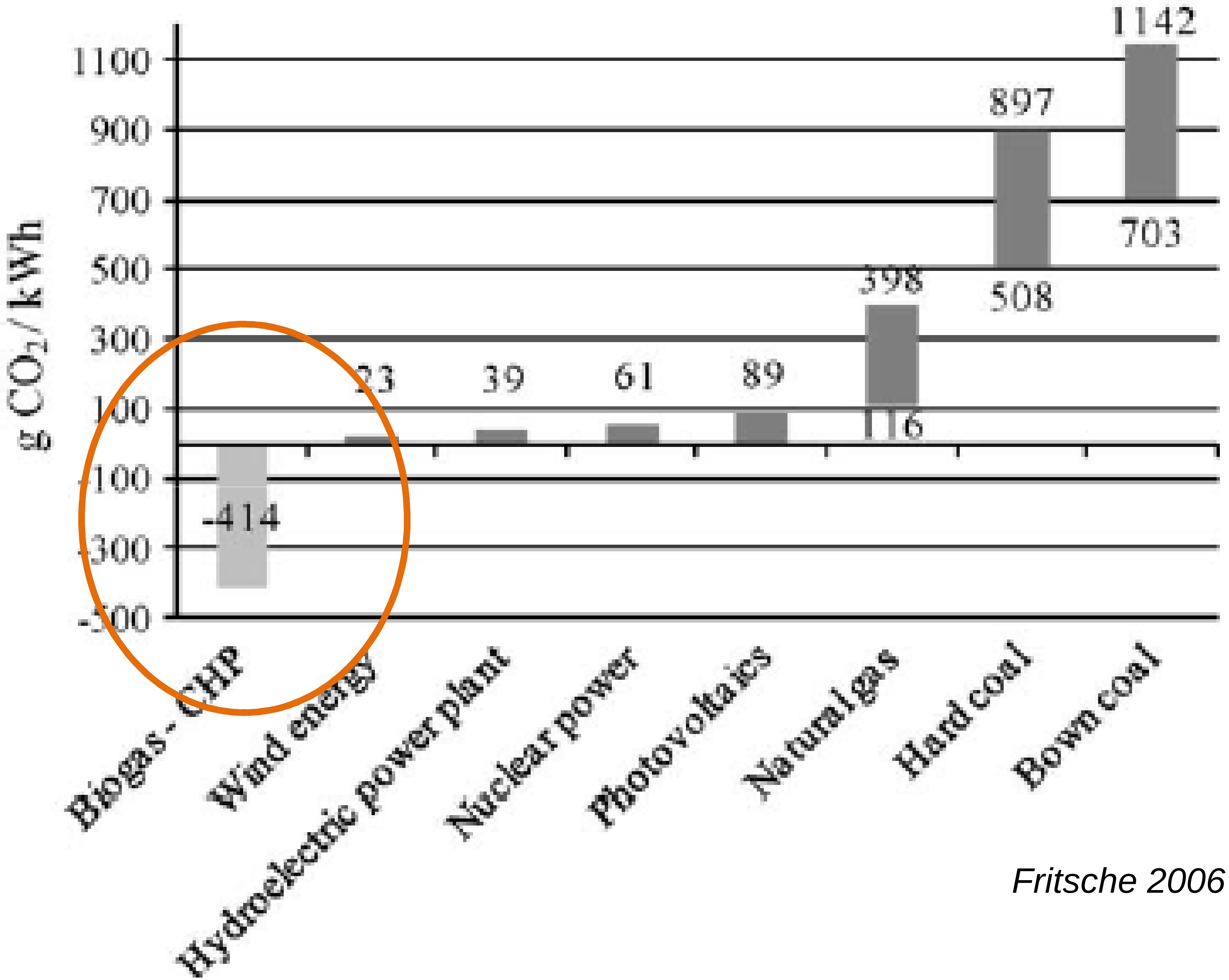
H_2S, H_2 (<1%)

Combined Heat Power (CHP)

Upgrade

CO_2

Biomethane CH_4 (>98%)



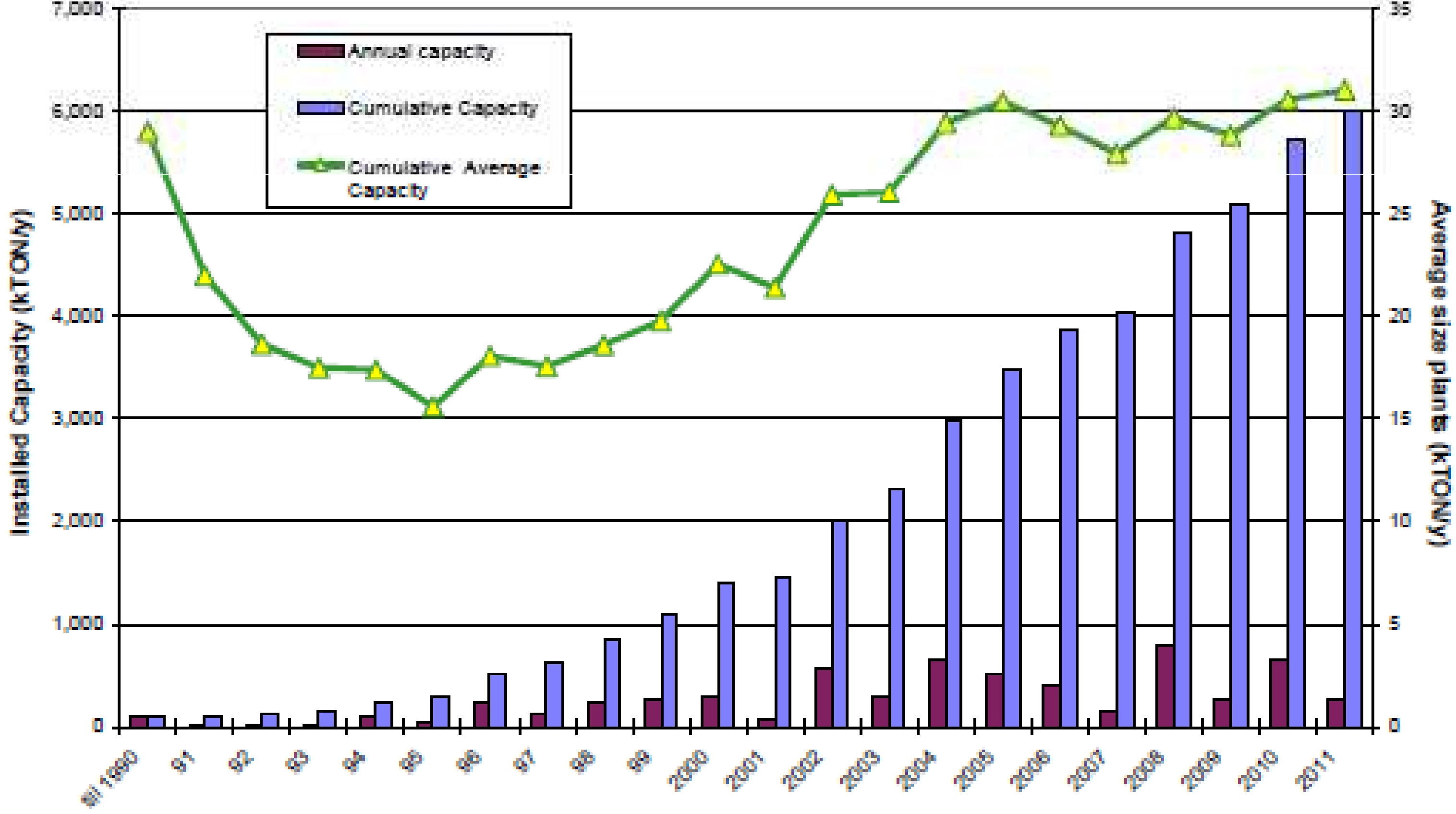
Fritsche 2006

Catching up….

Europe ➡

Organic fraction municipal solid waste (OFMSW)
Sewage sludge for WWTP
Manure livestock

de Baere et al (2010)



Germany

5,000 Biogas plants (CHP)

10 TWh electricty per year (2008) representing the 1.6% of the total demand (10,000 biogas-related jobs).

60 TWh electricity per year is the technical potential

Sweden

Biogas produced for heating, gas grid and injected in vehicules (24%)

12,000 vehicules, 70,000 projected by this year

City of Kristianstad (80,000 inhabs) relies completely on the biogas

United Kingdom

The UK's largest anaerobic digestion (AD) plant, Currently in a ramping up stage, 8 MW enough to power nearly 11,000 homes of electricity

Capacity to treat 165,000 tons of food waste per year (replacing landfill disposal)

China

by 2005, there were already 1,500 large-scale biogas plants at livestock farms and industrial waste sites

300 million rural residents will use biogas electricity by 2020 (10,000 large-scale plant)

Feeding time at the cow farm.

Nepal

Dalla’s approximately 550 residents use biogas for cooking in place of wood

India

public toilet complex serving visitors to the temple of the Indian guru Sai Baba generates enough biogas to provide back-up power for the temple complex

Chile

Largest biogas plant from sewage sludge in Latinamerica (La Farfana) connected to MEtroGas

At this stage…optimizing and improving the existing plants has become the new challenge in anaerobic digestion

Mathematical models….

Systems comprehension: microbial ecology or the different event occurring in the system

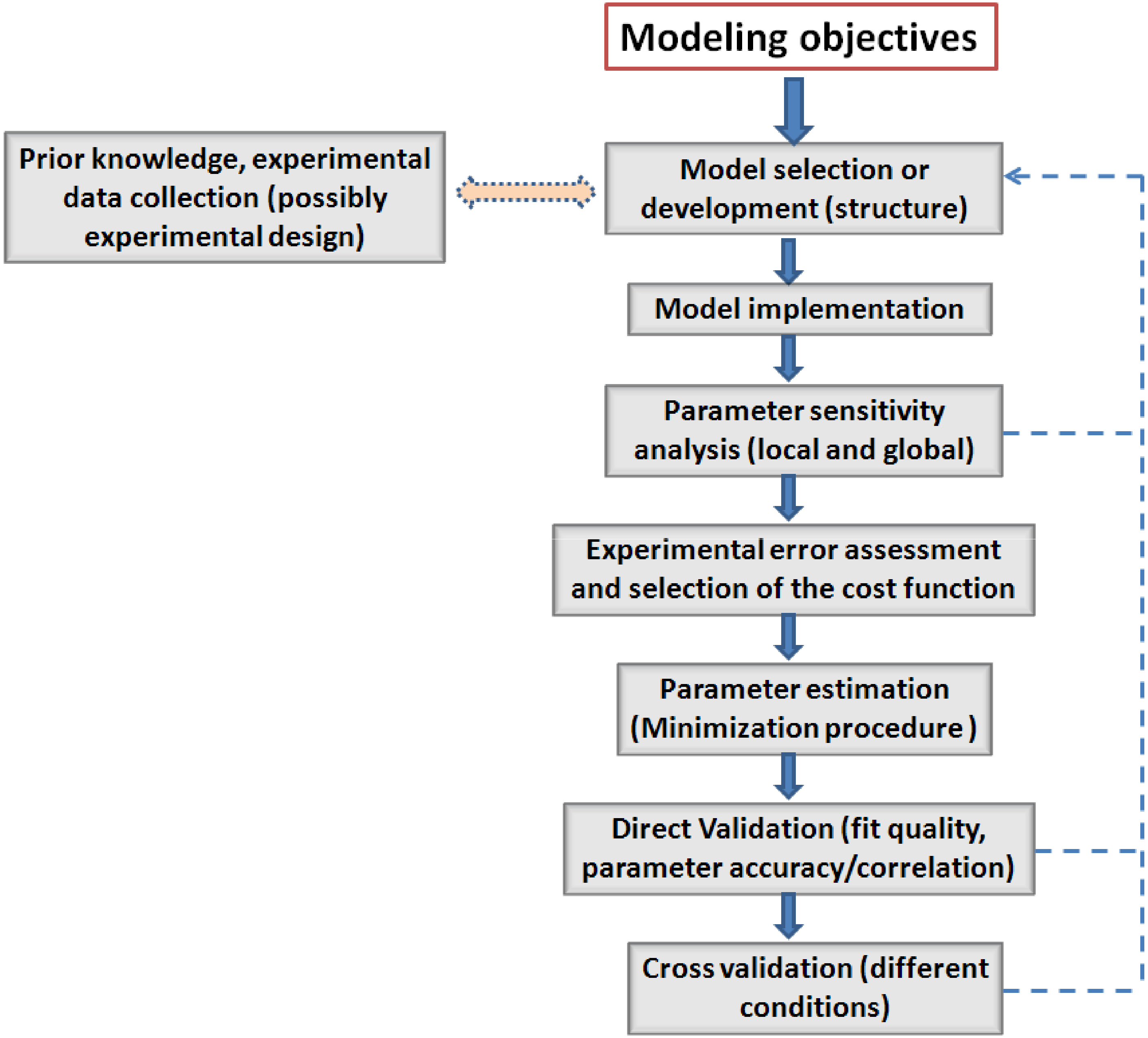
Formulation and evaluation of key hypothesis

Revealing information not apparent from pilot-scale studies

Identifying the most influential parameters of the system, giving guidance for the establishment of design criteria

Prediction of the system behavior at several conditions

$$\begin{aligned}
v_q &= -r_s i_q + \frac{\omega_r}{\omega_b}\Psi_d + \frac{p}{\omega_b}\Psi_q, & & \\
v_d &= -r_s i_d - \frac{\omega_r}{\omega_b}\Psi_q + \frac{p}{\omega_b}\Psi_d, & & \\
v_o &= -r_s i_o + \frac{p}{\omega_b}\Psi_o, & p\theta_r &= \omega_r, \\
0 &= r_{aq} i_{aq} + \frac{p}{\omega_b}\Psi_{aq}, & p\theta_e &= \omega_e, \\
v_f &= r_f i_f + \frac{p}{\omega_b}\Psi_f, & \delta &= \theta_r - \theta_e, \\
0 &= r_{ad} i_{ad} + \frac{p}{\omega_b}\Psi_{ad}, & \omega_m &= \frac{2}{p}\,\omega_r, \\
T_e &= \frac{3}{2}\,\frac{P}{2}\,\frac{1}{\omega_b}(\Psi_d i_q - \Psi_q i_d), & & \\
p\omega_r &= \frac{P}{2J}\,(T_a - T_e), & &
\end{aligned}$$



Modeling objectives

Prior knowledge, experimental data collection (possibly experimental design)

Model selection or development (structure)

Model implementation

Parameter sensitivity analysis (local and global)

Experimental error assessment and selection of the cost function

Parameter estimation (Minimization procedure)

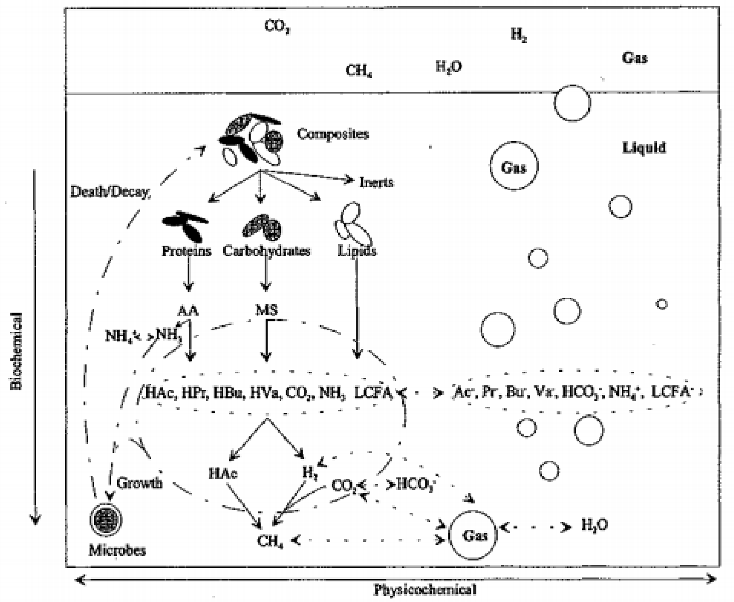
Direct Validation (fit quality, parameter accuracy/correlation)

Cross validation (different conditions)

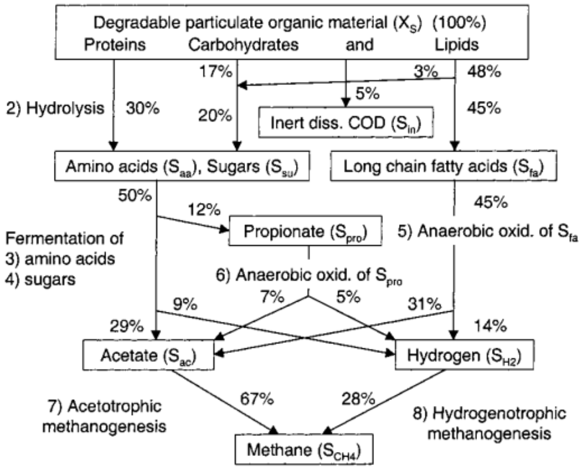
Anaerobic Digestion Model n°1 (ADM1)

The model describes the dynamics of 24 species and includes 19 bioconversion processes

43 differential equations !!!



Sewage sludge digestion model (Siegrist et al. 2002)



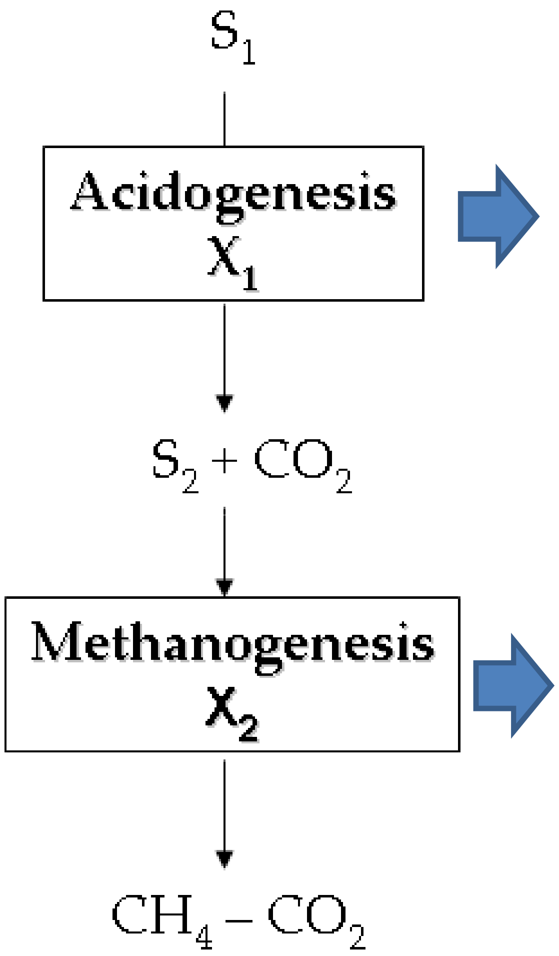
Two-reaction model (Bernard et al. 2001)

Three-reaction model (Haag et al. 2001)

Three-reaction model for microalgae (Mairet et al. 2012)

Among others…

Mathematical model 1 (AM2)



S_1

Acidogenesis
X_1

$S_2 + CO_2$

Methanogenesis
X_2

$CH_4 - CO_2$

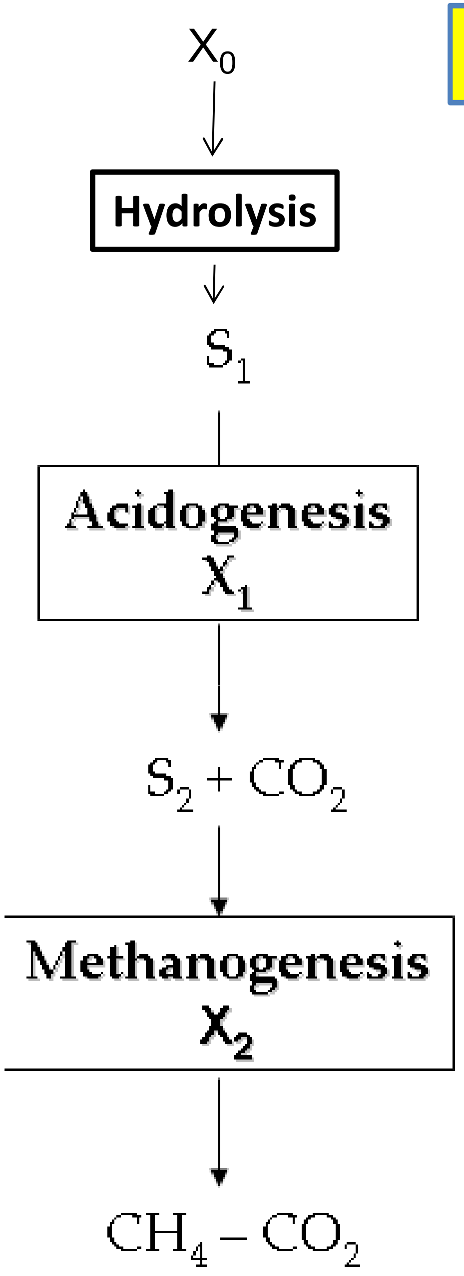
$$k_1 \cdot S_1 \xrightarrow{r_1} X_1 + k_2 \cdot S_2 + k_4 \cdot CO_2$$

$$r_1 = \mu_1 \cdot X_1 = \left(\mu_{1M} \cdot \frac{S_1}{K_{S1} + S_1} \right) \cdot X_1$$

$$k_3 \cdot S_2 \xrightarrow{r_2} X_2 + k_5 \cdot CO_2 + k_6 \cdot CH_4$$

$$r_2 = \mu_2 \cdot X_2 = \left(\mu_{2M} \cdot \frac{S_2}{K_{S2} + S_2 + \frac{S_2^2}{K_{12}}} \right) \cdot X_2$$

Mathematical model 2 (AM3)



Hydrolysis (X_1): $X_0 \xrightarrow{r_0} S_1$

Acidogenesis (X_1): $K_1 \cdot S_1 \xrightarrow{r_1} X_1 + K_2 \cdot S_2 + K_4 \cdot CO_2$

Methanogenesis (X_2): $K_3 \cdot S_2 \xrightarrow{r_2} X_2 + K_5 \cdot CO_2 + K_6 \cdot CH_4$

$$r_0 = k_0 \cdot X_0 \qquad r_1 = \mu_1 \cdot X_1 = \left(\mu_{1M} \cdot \frac{S_1}{K_{SA} + S_1} \right) \cdot X_1$$

$$r_2 = \mu_2 \cdot X_2 = \left(\mu_{2M} \cdot \frac{S_2}{K_{SM} + S_2 + \frac{S_2{}^2}{K_{IM}}} \right)$$

Mass balance

$$\frac{d\xi}{dt} = K \cdot r(\xi) + D(\xi_0 - \xi)$$

Gaseous stream and pH are expressed as functions of some state variables

$$q_C = k_L a\left(C + S_2 - Z - K_H \left(\frac{\phi - \sqrt{\phi^2 - 4K_H P_T (C + S_2 - Z)}}{2K_H} \right) \right)$$

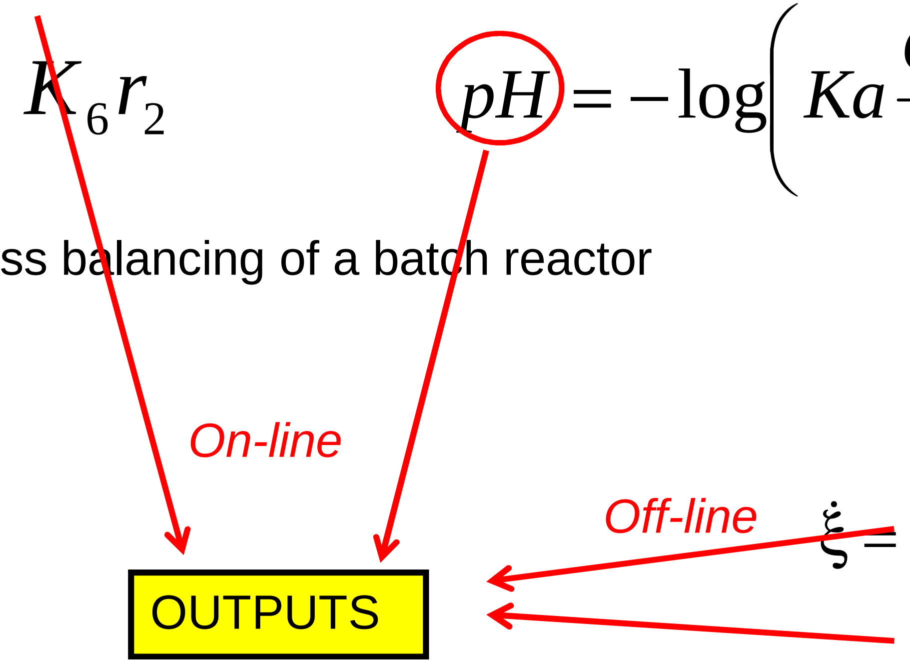
\+ *Biogas*

$$q_M = K_6 r_2$$

$$pH = -\log\left(Ka \frac{C + S_2 - Z}{Z - S_2} \right)$$

Mass balancing of a batch reactor

$$\dot{\xi} = \begin{bmatrix} \dot{X}_1 \\ \dot{X}_2 \\ \dot{S}_1 \\ \dot{S}_2 \\ IC \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -k_1 & 0 \\ k_2 & -k_3 \\ k_4 & k_5 \end{bmatrix} \begin{bmatrix} r_1(\xi) \\ r_2(\xi) \end{bmatrix}$$



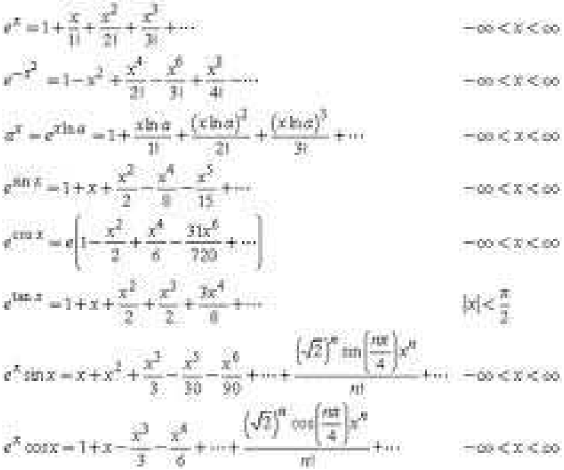
On-line

Off-line

OUTPUTS

Structural and parametric identifiability

Seldom addressed



$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \qquad -\infty < x < \infty$$

$$e^{-x^2} = 1 - x^2 + \frac{x^4}{2!} - \frac{x^6}{3!} + \frac{x^8}{4!} - \cdots \qquad -\infty < x < \infty$$

$$a^x = e^{x \ln a} = 1 + \frac{x \ln a}{1!} + \frac{(x \ln a)^2}{2!} + \frac{(x \ln a)^3}{3!} + \cdots \qquad -\infty < x < \infty$$

$$e^{\sin x} = 1 + x + \frac{x^2}{2} - \frac{x^4}{8} - \frac{x^5}{15} + \cdots \qquad -\infty < x < \infty$$

$$e^{\cos x} = e\left(1 - \frac{x^2}{2} + \frac{x^4}{6} - \frac{31x^6}{720} + \cdots\right) \qquad -\infty < x < \infty$$

$$e^{\tan x} = 1 + x + \frac{x^2}{2} + \frac{x^3}{2} + \frac{3x^4}{8} + \cdots \qquad |x| < \frac{\pi}{2}$$

$$e^x \sin x = x + x^2 + \frac{x^3}{3} - \frac{x^5}{30} - \frac{x^6}{90} + \cdots + \frac{\left(\sqrt{2}\right)^n \sin\left(\frac{n\pi}{4}\right) x^n}{n!} + \cdots \qquad -\infty < x < \infty$$

$$e^x \cos x = 1 + x - \frac{x^3}{3} - \frac{x^4}{6} + \cdots + \frac{\left(\sqrt{2}\right)^n \cos\left(\frac{n\pi}{4}\right) x^n}{n!} + \cdots \qquad -\infty < x < \infty$$

Taylor Series Expansion .
Calculating the successive derivatives of the output function with respect to the unknown model parameters, so as to obtain a system of independent equations in these parameters

Sensitivity analysis

One at a time techniques

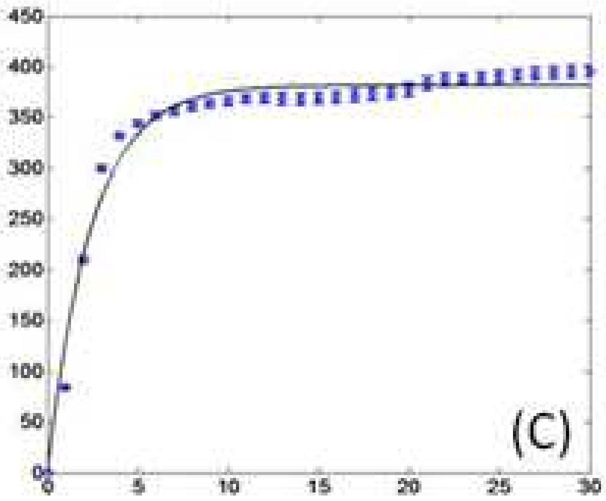
Global methods **(never used)**

$$\frac{\partial y_j}{\partial \theta_i} = \frac{y_j(\theta_i) - y_j(\theta_i + \Delta\theta_i)}{\Delta\theta_i}$$

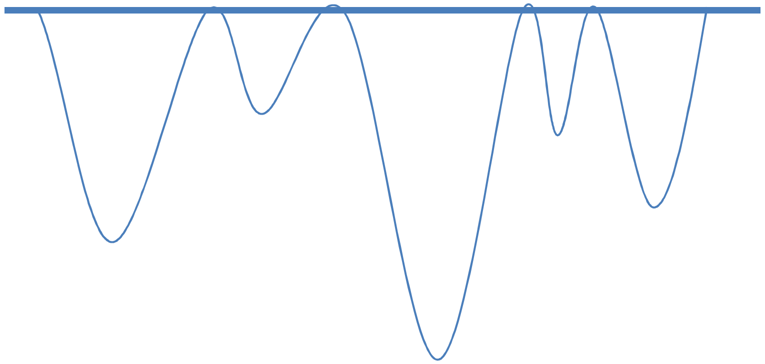
Parameters estimation

Measuring the deviation between the model and real system outputs

The selection of the objective function can play a crucial role in the results of the optimization



Optimization methodology



Local methods gradient-based

Multiple shooting

Direct-search methods: Levenberg-Marquardt method

Parameter uncertainty estimation

Error covariance matrix

$$\mathbf{F}(\theta) = \frac{1}{\hat{\sigma}^2} \sum_{t=1}^{N} \left[\frac{\partial \mathbf{y}(t,\theta)}{\partial \theta} \right]^T \left[\frac{\partial \mathbf{y}(t,\theta)}{\partial \theta} \right]$$

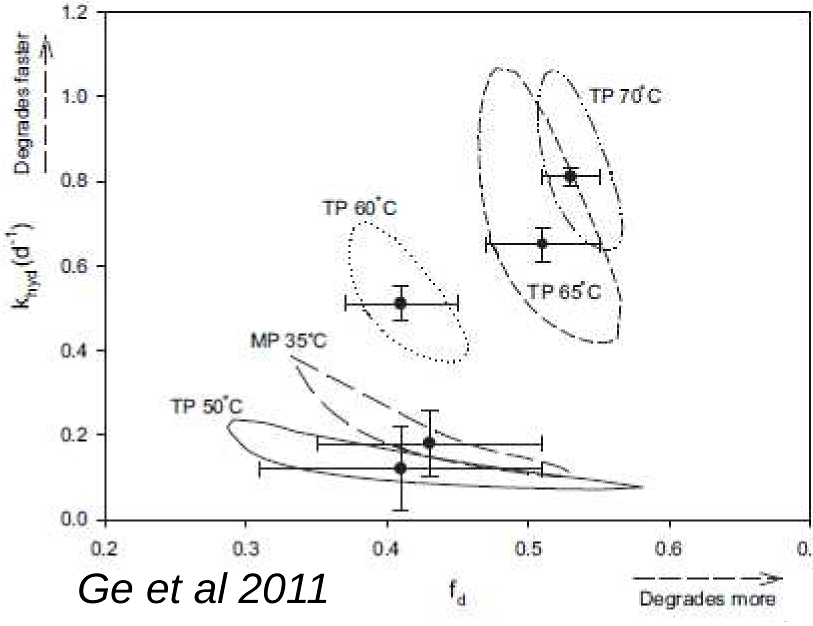
Inverse of the Fisher Information Matrix (FIM)

Optimistic estimate of the parameter error covariance matrix

Confidence intervals

$$J_{crit} = J_{opt} \cdot \left(1 + \frac{p}{N_{data} - p} F_{\alpha, p, N_{data-p}} \right)$$

More computationally demanding



Ge et al 2011

Final remarks and perspectives

Estudio en la identificación de dos modelos matemáticos

(1) Simulaciones preliminares para analizar la dinámica de los sistemas

(2) Identificación de parámetros bajo distintas circunstancias:

- Análisis matemático (Series de Taylor), Áreas de atracción, influencia del ruido en los experimentos, cantidad de variables medidas, diferentes condiciones iniciales, etc

Creación de un tutorial → **Creación de un tutorial (artículo, conferencia, capítulo de libro….**

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