Neural Network Interest Group

Título/*Title*:

Process modeling strategy combining analytical and data based techniques

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Process modeling strategy combining analytical and data based techniques

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I. NN identification of reaction rates with known kinetics coefficients

II. NN identification of reaction rates with partially unknown kinetics coefficients

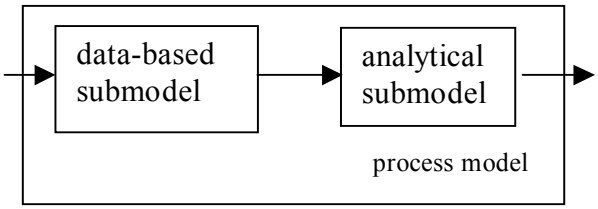


Fig. 1 hybrid (ANN + analytical) model

1. General dynamical macro model of biochemical reactors (matrix form)

$$\frac{dX}{dt} = K\varphi(X,T) + DX + F_{in} - F_{out}$$ **- mass balance** **(1)**

$$\frac{dT}{dt} = K_0\varphi(X,T) - D_0T + F_{in}$$ **- energy balance** **(2)**

$X = (x_1(t),.....x_n(t))^T$ — **concentrations of the *n* process variables at time *t*;**

T — **temperature of the reactor;**

$K = [k_1,.....k_m] \in R^{n\times m}$ — **stoichiometric matrix-kinetics coefficients**

$K_0 \in R^m_{\geq 0}$ — **coefficients of exothermicity;**

$\varphi = (\varphi_1,.....\varphi_m)^T$ — **reaction rate vector, where**

$\varphi_j(\cdot,\cdot) : R^{n+1}_{\geq 0} \rightarrow R_{\geq 0}$ — **are nonnegative continuous functions, j=1,…m;**

$F_{in}(\cdot) : R_{\geq 0} \rightarrow R^n_{\geq 0}$

$F_{in} = \left(F^{in}_1(t),.....F^{in}_n(t)\right)^T$ — **piecewise continuous and bounded function of *n* feed concentrations at time *t*.**

$F_{out}(\cdot): R_{\geq 0} \rightarrow R_{\geq 0}^{p}$ **piecewise continuous and bounded function of *n* effluent concentrations at time *t*;**

$F_{out} = \left(F_{1}^{out}(t), \ldots\ldots F_{p}^{out}(t)\right)^{T}$

D_x / D_0 **Dilution rate/heat transfer rate**

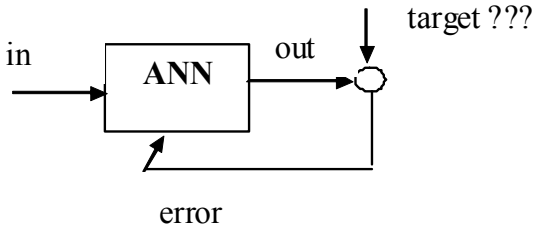
An augmented state vector is defined

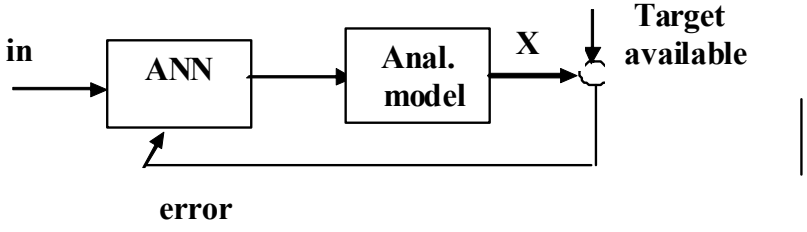
$$X_{aug} = \begin{bmatrix} X \\ T \end{bmatrix}, \; K_{aug} = \begin{bmatrix} K \\ K_0 \end{bmatrix} \; \dim(K_{aug}) = (n+1)xm, \quad rank(K_{aug}) = p$$

General dynamical macro model $\frac{dX_{aug}}{dt} = K_{aug}\varphi\left(X_{aug}\right) - DX_{aug} + F_{in} - F_{out}$ **(3)**

<u>Main challenges</u>

1. **Not all states are available (measurable) -** X_{aug}
2. **Not all kinetics coefficients are known -** K_{aug}
3. **Usually the reaction rates are not measurable -** $\varphi\left(X_{aug}\right)$





2. NN based identification of reaction rates when all kinetics coefficients are known and not all state variables are measured

Step 1: Model transformation

State partition 1 is defined: $X_{aug} = \begin{bmatrix} X_a & X_b \end{bmatrix}^T$ **- the partition is not unique**

$$\frac{dX_a}{dt} = K_a \varphi(X_a, X_b) - DX_a + F_{in\_a} - F_{out\_a} \quad \textbf{(4)}$$

$$\frac{dX_b}{dt} = K_b \varphi(X_a, X_b) - DX_b + F_{in\_b} - F_{out\_b} \quad \textbf{(5)}$$

A new vector Z is defined as the following linear combination of the states

$$Z = A_0 X_a + X_b \quad \textbf{(6)}$$

Where A_0 **is the unique solution of the equation**

$A_0 K_a + K_b = 0$ **,** K_a **is a *pxm* full rank arbitrary submatrix of** K_{aug} **(7)**

$$\frac{dZ}{dt} = -DZ + A_0(K_a, K_b)(F_{in\_a} - F_{out\_a}) + (F_{in\_b} - F_{out\_b}) \quad \textbf{(8)}$$

The purpose of the model transformation (8) is to get a vector Z, which is a linear combination of the process states, and is independent of the reaction rates. Eq. (8) will be used to recover the unmeasured states. The procedure for the state recovery, termed as state observer in the control theory, is discussed below.

Step 2: State observer independently of the reaction rates

State partition 2: $Z = A_1(K_{aug})X_1 + A_2(K_{aug})X_2$ **(9)**

X_1 **- measured** X_2 **-unmeasured - the partition is unique**

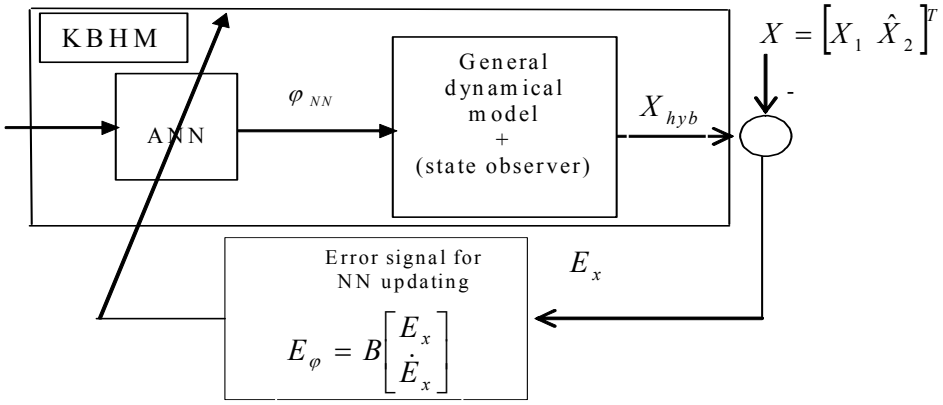
$$\frac{dX_1}{dt} = K_1 \varphi(X_1, X_2) - DX_1 + F_{in\_1} - F_{out\_1} \quad \textbf{(10.1)}$$

$$\frac{dX_2}{dt} = K_2 \varphi(X_1, X_2) - DX_2 + F_{in\_2} - F_{out\_2} \quad \textbf{(10.2)}$$

$$\frac{d\hat{Z}}{dt} = -D\hat{Z} + A_0(F_{in\_a} - F_{out\_a}) + (F_{in\_b} - F_{out\_b}) \quad \textbf{(11.1)}$$

$$\hat{X}_2 = A_2^{-1}(\hat{Z} - A_1 X_1) \quad \textbf{(11.2)}$$

Step 3: Error signal for NN updating



The true process behaviour: $\frac{dX}{dt} = K\varphi - DX + F_{in} - F_{out}$ **(12.1)**

The adaptive hybrid model (KBHM):

$$\frac{dX_{hyb}}{dt} = K\varphi_{NN} - DX_{hyb} + F_{in} - F_{out} + \Omega(X - X_{hyb}) \quad \textbf{(12.2)}$$

The model error dynamics:

$$\frac{d(X - X_{hyb})}{dt} = K(\varphi - \varphi_{NN}) - D(X - X_{hyb}) + \Omega(X - X_{hyb}) \quad \textbf{(13)}$$

The observation error is defined as: $E_x = (X - X_{hyb})$ **(14)**

The NN error signal is defined as: $E_\varphi = \varphi - \varphi_{NN}$ **(15)**

$$\frac{dE_x}{dt} = KE_\varphi - (\Omega + D)E_x \quad \textbf{(16.1)}$$

$$E_\varphi = K^{-1}[D + \Omega \quad 1]\begin{bmatrix} E_x \\ \dot{E}_x \end{bmatrix} = B\begin{bmatrix} E_x \\ \dot{E}_x \end{bmatrix} = \lambda_1 E_x + \lambda_2 \dot{E}_x \quad \textbf{(16.2)}$$

Ω is a design parameter, defines the influence of each of the terms in (16.2)

3. CASE STUDY A – ESTIMATION OF THE PRECIPITATION RATE OF CALCIUM PHOSPHATE

The calcium phosphate is recognized as an important product in the soil fertilizing and in the animal food engineering as the source of calcium supplement.
Depending on the temperature, the level of supersaturation, pH and initial concentration of reagents, the precipitation of calcium phosphate exhibits different dynamics and consequently different precipitation rates dynamics.

Analytical dynamical macro model:

$$\frac{dM_c}{dt} = -q_{m1}\varphi\left(M_c, M_B\right) \quad \textbf{(17)}$$

$$\frac{dM_{HAP}}{dt} = -K_{HAP}\left(M_{HAP}\right)^2 \quad \textbf{(18)}$$

$$\frac{dM_B}{dt} = \varphi\left(M_c, M_B\right) + 10q_{m2}K_{HAP}\left(M_{HAP}\right)^2 \quad \textbf{(19)}$$

M_c is the mass of calcium into solution, M_{HAP} is the mass of HAP and M_B is the mass of brushite; $\varphi(\cdot)$ is the precipitation rate, q_{m1}, q_{m2} are molar weight ratios.

State partition 1 and 2: $X_a = X_1 = M_c$, $X_b = X_2 = M_B$ **(20)**

$$K_a = -q_{m1},\ K_b = 1 \quad \textbf{(21)}$$

$$A_0 = A_1 = 1/q_{m1} \qquad A_2 = 1 \quad \textbf{(22)}$$

$$\frac{d\hat{M}_{HAP}}{dt} = -K_{HAP}\left(M_{HAP}\right)^2 \quad \textbf{(23.1)}$$

$$\frac{d\hat{Z}}{dt} = 10q_{m2}K_{HAP}\left(\hat{M}_{HAP}\right)^2 \quad \textbf{(23.2)}$$

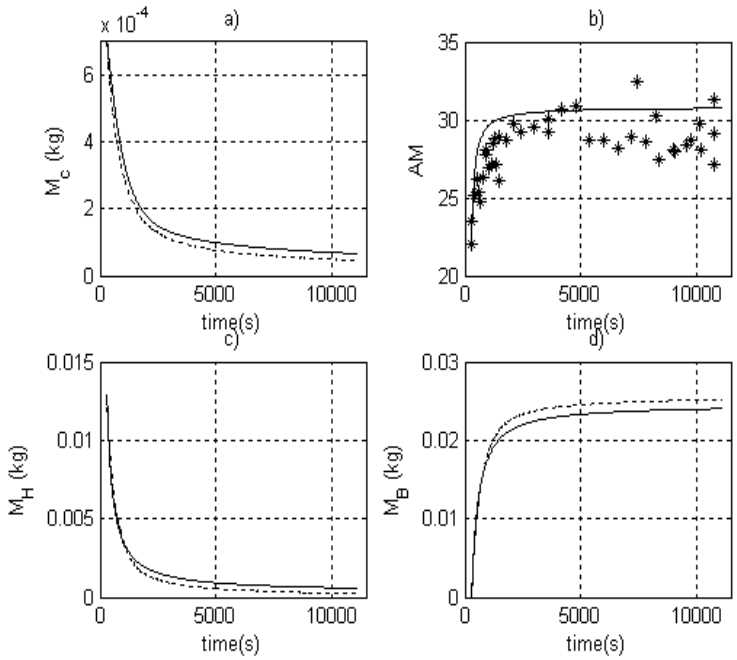
$$\hat{M}_B = \hat{Z} - \frac{1}{q_{m1}}M_c \quad \textbf{(23.3)}$$

The observation error $E_x = \begin{bmatrix} M_c - M_{chyb} \\ M_B - \hat{M}_{Bhyb} \end{bmatrix}$ **(24)**

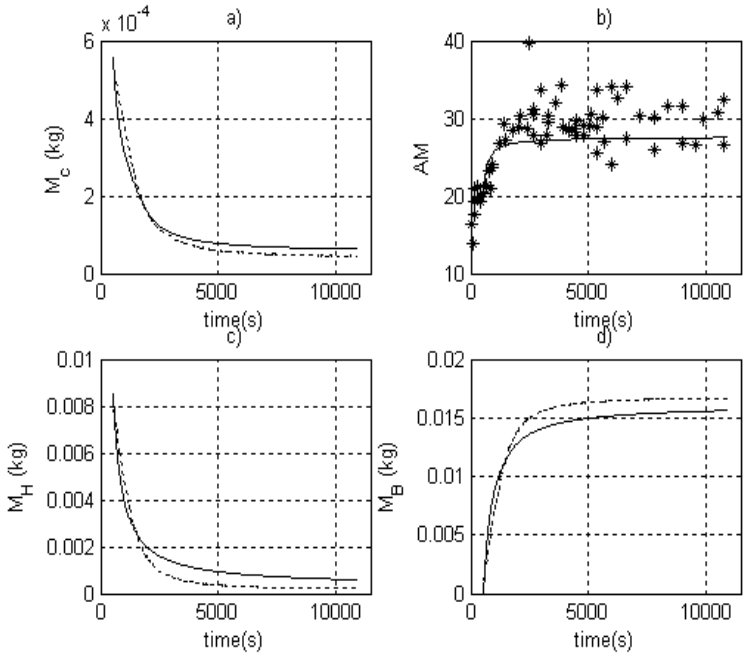
$$\Omega = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}, \quad D = 0 \quad \textbf{(25)}$$

$$E_\varphi = \frac{1}{q_{m1}}\begin{bmatrix} \left(\dot{M}_c - \dot{\hat{M}}_c\right) + 0.5\left(M_c - \hat{M}_c\right) \\ \left(\dot{M}_B - \dot{\hat{M}}_B\right) + 0.5\left(M_B - \hat{M}_B\right) \end{bmatrix} \quad \textbf{(26)}$$

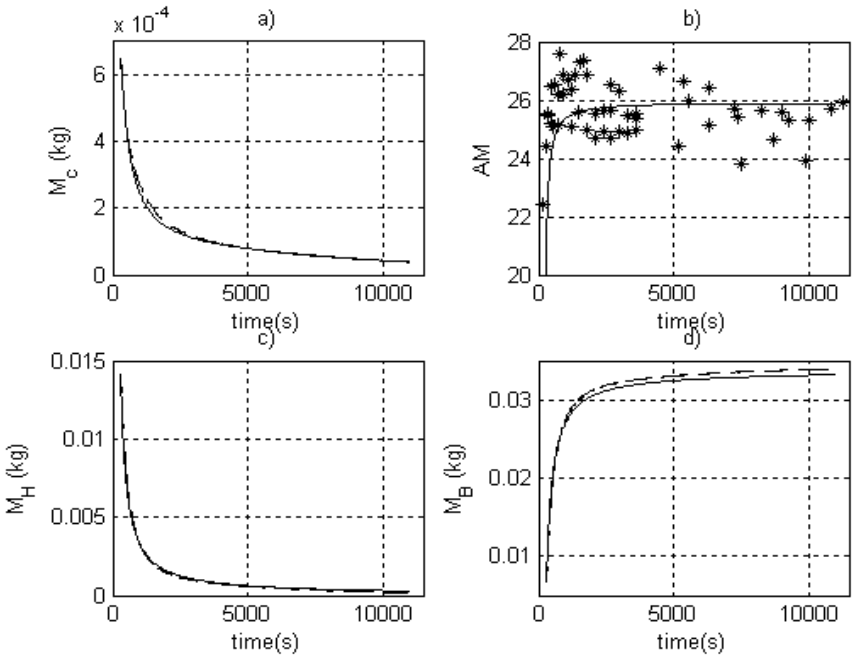
Numerical Results



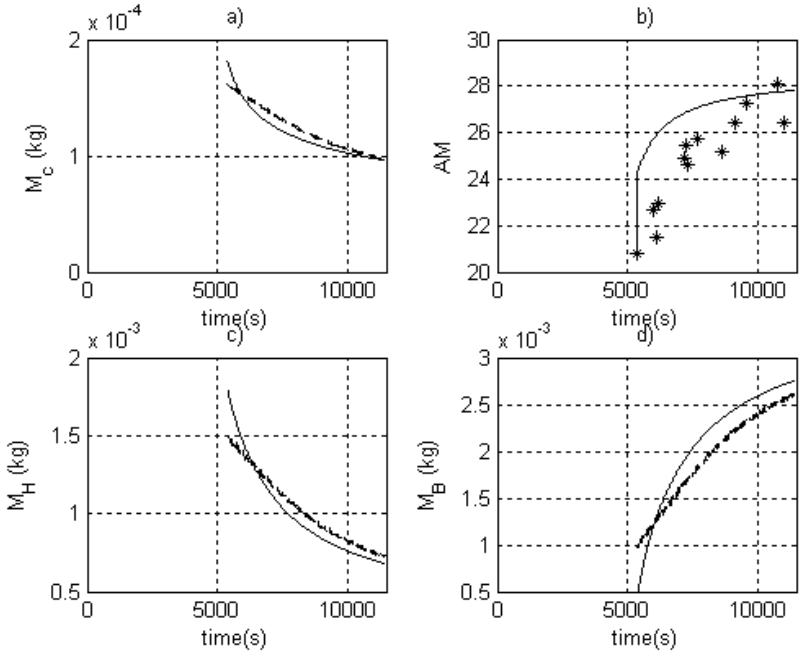
Training data - Initial concentration of reagents 0.3 M



Training data - Initial concentration of reagents 0.2 M
Numerical Results



Validation data - Initial concentration of reagents 0.4 M



Validation data - Initial concentration of reagents 0.05 M

TABLE 1 ESTIMATION RESULTS FOR 3 ANALYTICAL MODELS AND THE KBHM

Calcium phosphate precipitation rate models	**NDEI* for model validation data Mc – 0.4M**
Monod type model (Lubenova et al., 2003) $\varphi = \frac{\lambda_{B1} M_B}{\beta_{B1} + M_B} + \frac{\lambda_{c1} M_c}{\beta_{c1} + M_c}$	**0.404**

$\lambda_{B1}, \lambda_{c1}, \beta_{B1}, \beta_{c1}$ **- tuning parameters**	
Contois type model (Oliveira et al, 2002) $\varphi = \frac{\lambda_{B2} M_B}{\beta_{HAP2} M_{HAP} + M_B} + \frac{\lambda_{c2} M_c}{\beta_{c2} M_B + M_c}$ $\lambda_{B2}, \lambda_{c2}, \beta_{HAP2}, \beta_{c2}$ **- tuning parameters**	**0.096**
"Logistic" type model (Bastin and Dochain, 1990) $\varphi = \exp(-\lambda_3 M_B)$, λ_3 **- tuning parameter**	**0.062**
KBHM (this work) **A feedforward NN with 2 inputs (M_c, M_B), 1 output (φ_{NN}), one hidden layer with 7 sigmoid nodes**	**0.023**

***NDEI - nondimensional error index**
the root mean square error (RMSE) divided by the standard deviation of the target series

4. NN based identification of reaction rates when not all the states are measured and the kinetics coefficients related with the measured states are unknown

Step 1: Model transformation (the same as in the previous case) :

State partition 1: $Z = A_0 X_a + X_b$ **(27)**

Step 2: State observer

State partition 2:

$$Z = A_1(K_1, K_2) X_1 + A_2(K_1, K_2) X_2 \quad \textbf{(28)}$$

$$\frac{dX_1}{dt} = K_1 \varphi(X_1, X_2) - DX_1 + F_{in\_1} - F_{out\_1} \quad , \; X_1 \textbf{- measured, } K_1 \textbf{ is unknown} \quad \textbf{(29)}$$

$$\frac{dX_2}{dt} = K_2 \varphi(X_1, X_2) - DX_2 + F_{in\_2} - F_{out\_2} \; , \; X_2 \textbf{ -unmeasured, } K_2 \textbf{ is known} \quad \textbf{(30)}$$

$$\frac{d\hat{Z}}{dt} = -D\hat{Z} + A_0(\hat{K}_1, K_2)(F_{in\_a} - F_{out\_a}) + (F_{in\_b} - F_{out\_b}) \quad \textbf{(31)}$$

$$\hat{X}_2 = \left(A_2(\hat{K}_1, K_2)\right)^{-1} \left(\hat{Z} - A_1(\hat{K}_1, K_2) X_1\right) \quad \textbf{(32)}$$

Step 3: Observer based estimator

$$\frac{d\hat{Z}}{dt} = -D\hat{Z} + A_0(\hat{K}_1, K_2)(F_{in\_a} - F_{out\_a}) + (F_{in\_b} - F_{out\_b}) \quad \textbf{(31)}$$

$$\hat{X}_2 = \left(A_2(\hat{K}_1, K_2)\right)^{-1}\left(\hat{Z} - A_1(\hat{K}_1, K_2)X_1\right) \quad \textbf{(32)}$$

$$\frac{d\hat{X}_1}{dt} = \hat{K}_1\varphi_{NN} - D\hat{X}_1 + F_{in\_1} - F_{out\_1} + \Omega(X_1 - \hat{X}_1) \quad \textbf{(33)}$$

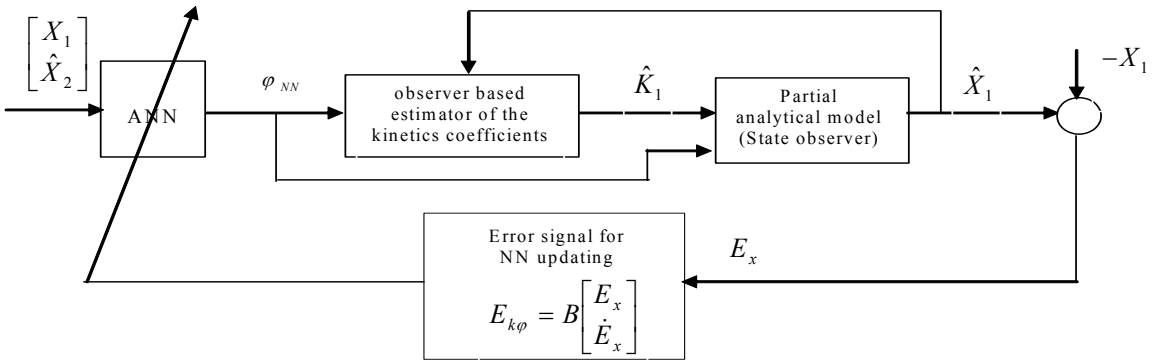
$$\frac{d\hat{K}_1}{dt} = \varphi_{NN}\Gamma(X_1 - \hat{X}_1) \quad \textbf{- adaptive estimator} \quad \textbf{(34)}$$

$$\Omega = diag\ \{\omega_i\},\ \Gamma = diag\ \{\gamma_i\},\ \ \gamma_i \in \Re^+,\ \omega_i \in \Re^+,\ \ i = 1..N \quad \textbf{(35)}$$

The actual value of K_1 is replaced by an estimate $\hat{K}_1$ which is updated by eq. (34)

Γ is a gain matrix such that the matrix $\Omega^T\Gamma + \Gamma\Omega$ is negative definite .
The updating law (34) is inspired by the theory of linear adaptive estimators, Narendra K.S. and Annaswamy A.M., 1989, Stable adaptive systems.

Step 3: Error signal for NN updating



Observation error $E_x = (X_1 - \hat{X}_1)$ **(36)**

$$\frac{dE_x}{dt} = K_1\varphi - \hat{K}_1\varphi_{NN} - (\Omega + D)E_x \quad \textbf{(37)}$$

Extended NN error signal $E_{K\varphi} = K_1\varphi - \hat{K}_1\varphi_{NN}$ **(38)**

$$E_{K\varphi} = \begin{bmatrix} D + \Omega & 1 \end{bmatrix}\begin{bmatrix} E_x \\ \dot{E}_x \end{bmatrix} = B\begin{bmatrix} E_x \\ \dot{E}_x \end{bmatrix} = \lambda_1 E_x + \lambda_2 \dot{E}_x \quad \textbf{(39)}$$

4. Case study B - estimation of the crystal growth rate (*G*) of sugar crystallization process

$$\frac{dM_s}{dt} = -k_1 G + F_f \rho_f B_f Pur_f$$

$$\frac{dM_c}{dt} = k_1 G$$

$$\frac{dm_0}{dt} = k_3 G$$

$$\frac{dT_m}{dt} = k_2 G + bF_f + cJ_{vap} + d$$

where M_s is the mass of dissolved sucrose, M_c is the mass of crystals, T_m is the temperature of the massecuite, m_0 is the number of crystals. Pur_f and ρ_f are the purity (mass fraction of sucrose in the dissolved solids) and the density of the incoming feed. F_f is the feed flowrate, J_{vap} is the evaporation rate and *b*, *c*, *d* are parameters incorporating the enthalpy terms and specific heat capacities derived as functions of physical and thermodynamic properties.

$$X_{aug} = \begin{bmatrix} M_s & M_c & m_0 & T_m \end{bmatrix}^T,\ K_{aug} = \begin{bmatrix} -k_1 & k_1 & k_3 & k_2 \end{bmatrix}^T \qquad \textbf{(40)}$$

k_1, k_2 – **unknown**

state partition 1 : $X_a = M_c$, $X_b = \begin{bmatrix} M_s & T_m & m_0 \end{bmatrix}^T$, $A_0 = \begin{bmatrix} 1 & -\frac{k_2}{k_1} & -\frac{k_3}{k_1} \end{bmatrix}^T$

state partition 2 : $X_1 = \begin{bmatrix} M_c & T_m \end{bmatrix}^T$, $X_2 = \begin{bmatrix} M_s & m_0 \end{bmatrix}^T$, $A_1 = \begin{bmatrix} 1 & -\frac{k_2}{k_1} & -\frac{k_3}{k_1} \\ 0 & 1 & 0 \end{bmatrix}^T$,

$$A_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}^T$$

Observer based estimator:

$$\hat{Z}_1 = M_c + \hat{M}_s$$

$$\hat{Z}_2 = -\frac{\hat{k}_2}{\hat{k}_1} M_c + T_m$$

$$\hat{Z}_3 = -\frac{k_3}{\hat{k}_1} M_c + \hat{m}_0$$

$$\begin{bmatrix} \frac{d\hat{M}_c}{dt} \\ \frac{d\hat{T}_m}{dt} \end{bmatrix} = \begin{bmatrix} \hat{k}_1 \\ \hat{k}_2 \end{bmatrix} G_{NN} + \begin{bmatrix} 0 \\ bF_f + cJ_{vap} + d \end{bmatrix} + \begin{bmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{bmatrix} \begin{bmatrix} M_c - \hat{M}_c \\ T_m - \hat{T}_m \end{bmatrix}, \quad D = 0$$

$$\begin{bmatrix} \hat{M}_s \\ \hat{m}_0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \left(\begin{bmatrix} \hat{Z}_1 \\ \hat{Z}_2 \\ \hat{Z}_3 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ -\frac{\hat{k}_2}{\hat{k}_1} & 1 \\ -\frac{k_3}{\hat{k}_1} & 0 \end{bmatrix} \begin{bmatrix} M_c \\ T_m \end{bmatrix} \right)$$

$$\begin{bmatrix} \frac{d\hat{k}_1}{dt} \\ \frac{d\hat{k}_2}{dt} \end{bmatrix} = G_{NN} \begin{bmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{bmatrix} \begin{bmatrix} M_c - \hat{M}_c \\ T_m - \hat{T}_m \end{bmatrix}$$

$$\omega_1 = \omega_2 = 0.5 \text{ , } \gamma_1 = \gamma_2 = 1$$

$$E_x = \begin{bmatrix} M_c - \hat{M}_c \\ T_m - \hat{T}_m \end{bmatrix}, \; E_{K\varphi} = \begin{bmatrix} \left(\dot{M}_c - \dot{\hat{M}}_c \right) + \omega_1 \left(M_c - \hat{M}_c \right) \\ \left(\dot{T}_m - \dot{\hat{T}}_m \right) + \omega_2 \left(T_m - \hat{T}_m \right) \end{bmatrix}$$

One step NN optimization

$$E_{\varphi(i)} = \frac{1}{q_{m1}} \left[\frac{M_{c(i)} - M_{c(i-1)}}{T} - \frac{\hat{M}_{c(i)} - \hat{M}_{c(i-1)}}{T} + \omega_1 \left(M_{c(i)} - \hat{M}_{c(i)} \right) \right] +$$

$$\left[\frac{T_{m(i)} - T_{m(i-1)}}{T} - \frac{\hat{T}_{m(i)} - \hat{T}_{m(i-1)}}{T} + \omega_2 \left(T_{m(i)} - \hat{T}_{m(i)} \right) \right]$$

Simulation Results

Table: Final average (in mass) crystal size (AM) and coefficient of variation (CV)

batch No.	experimental data		One step NN optimization		Batch NN optimization	
	MA [mm]	CV [%]	MA [mm]	CV [%]	MA [mm]	CV [%]
1	0.479	32.6	0.51	28.86	0.583	23.26
2	0.559	33.7	0.52	29.87	0.542	21.43
3	0.680	43.6	0.57	32.99	0.547	23.69
4	0.494	33.7	0.51	35.03	0.481	23.16
5	0.537	32.5	0.59	29.66	0.623	21.36
6	0.556	35.5	0.49	28.89	0.471	20.642
7	0.560	31.6	0.61	35.02	0.755	32.9
8	0.530	31.2	0.60	36.11	0.681	25.39
av. error			6.7%	12.6%	12.1%	27.3%

A feedforward NN with 3 inputs (M_c, T_m, M_s) , 1 output (G_{NN}), one hidden layer with 7 sigmoid nodes