Design of experiments for smoke depollution of diesel engine outputs

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ENBIS-EMSE 2009 Conference
1st July 2009

Ecole Nationale Supérieure des Mines SAINT-ETIENNE

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Talk Overview

1. **deNOx model: study case**
   1. **NOx trap: the way it works**
   2. **NOx trap: the mathematical formulation**
   3. **NOx trap: experimental and simulated results**
2. **Kriging with non linear trend (KNL)**
   1. **Presentation**
   2. **Kriging predictor**
   3. **Application on deNOx model and results**
3. **Conditioning by derivatives: improvement for KNL?**
   1. **Presentation**
   2. **Test model: presentation**
   3. **Application on test model and results**
   4. **First results on deNOx model**

Conclusions

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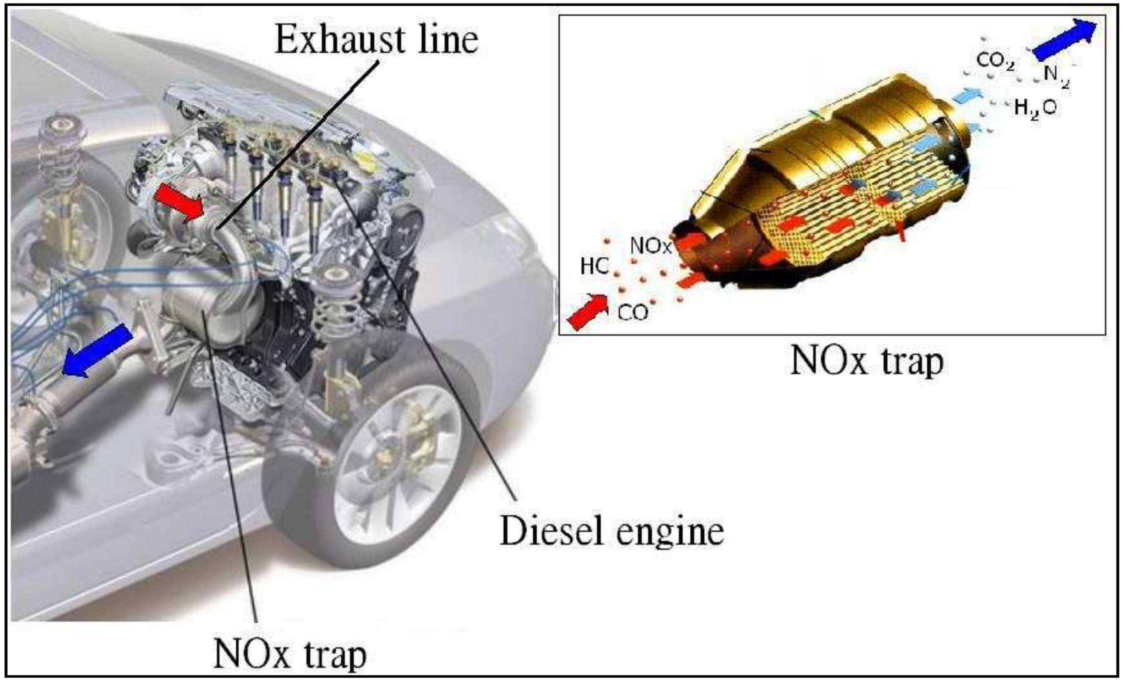
1. NOx trap: the way it works

Smoke post-treatment at the diesel engine output:

NOx trap



Reduce pollutants emissions at the diesel engine output

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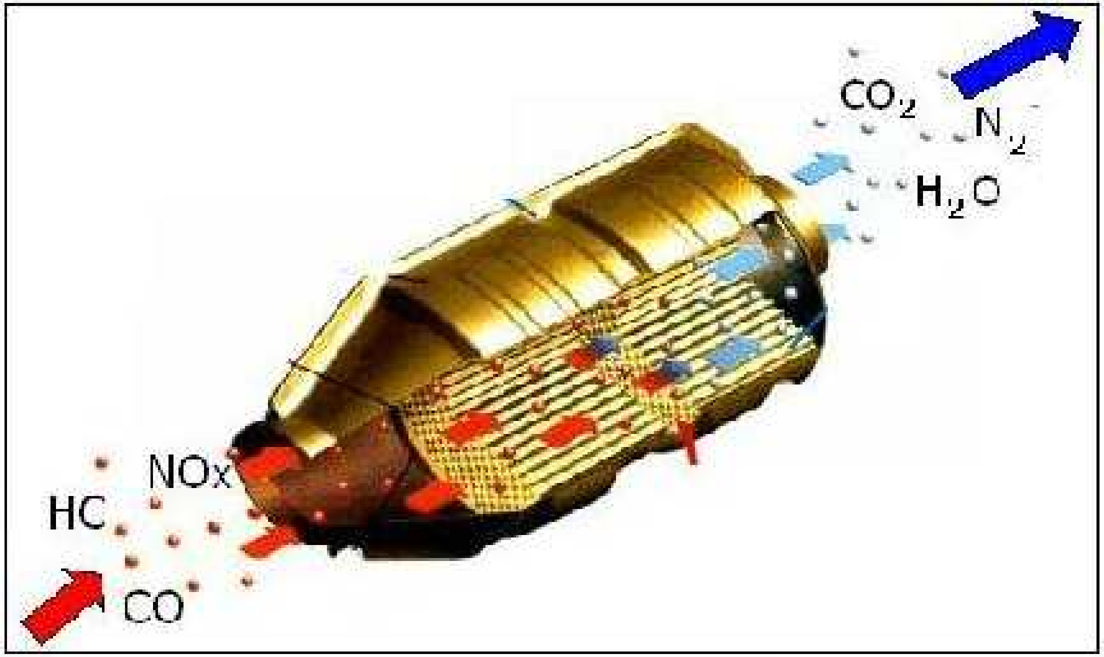

Reduce pollutants emissions at the diesel engine output

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1. NOx trap: the way it works

The NOx trap operates in two phases

1. NOx capture phase until saturation of active sites
2. NOx release phase after reducing the oxydated species

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Simplification of the problem

- Complex system: to reduce the complexity of the problem, at first, only capture phase is considered
- During this phase, the kinetic model have four dominant reactions: oxydation of CO, HC, NO et H_2

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Kinetic model

$$
\begin{aligned}
CO + 1/2 O_2 &\rightarrow CO_2 && (1)\\
1/a\ C_aH_b + (1 + b/4a)O_2 &\rightarrow CO_2 + b/2a\ H_2O && (2)\\
NO + 1/2\ O_2 &\Leftrightarrow NO_2 && (3)\\
H_2 + 1/2\ O_2 &\rightarrow H_2O && (4)
\end{aligned}
$$

Two kinetic parameters for each reaction

1. deNOx model: study case

2. NOx trap: the mathematical formulation

Mathematical model

The mathematical model of the NOx trap has the form,

$$Y = f(x, \beta)$$

where f results from a differential equation system (ODE)

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System inputs, denoted by *x*

On the experimental system, inputs are selected and controlled by the experimenter:

- Mass composition of five species present in the exhaust gas

$$c_1, c_2, c_3, c_4, c_5$$

- Mass flow of gas entering in the NOx trap, Q
- Entering gas temperature ⇒ increase linearly with the time

$$x = (c_1, c_2, c_3, c_4, c_5, Q, T)^t$$

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System outputs, denoted by Y

Mass composition of the three pollutants:

$$y_{HC}, y_{NOx}, y_{CO}$$

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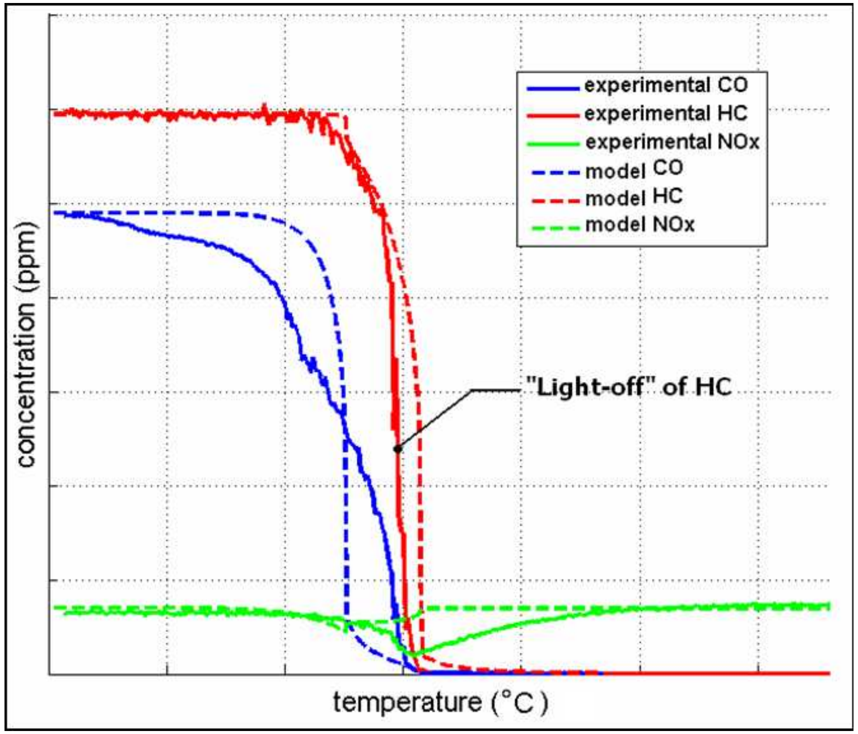
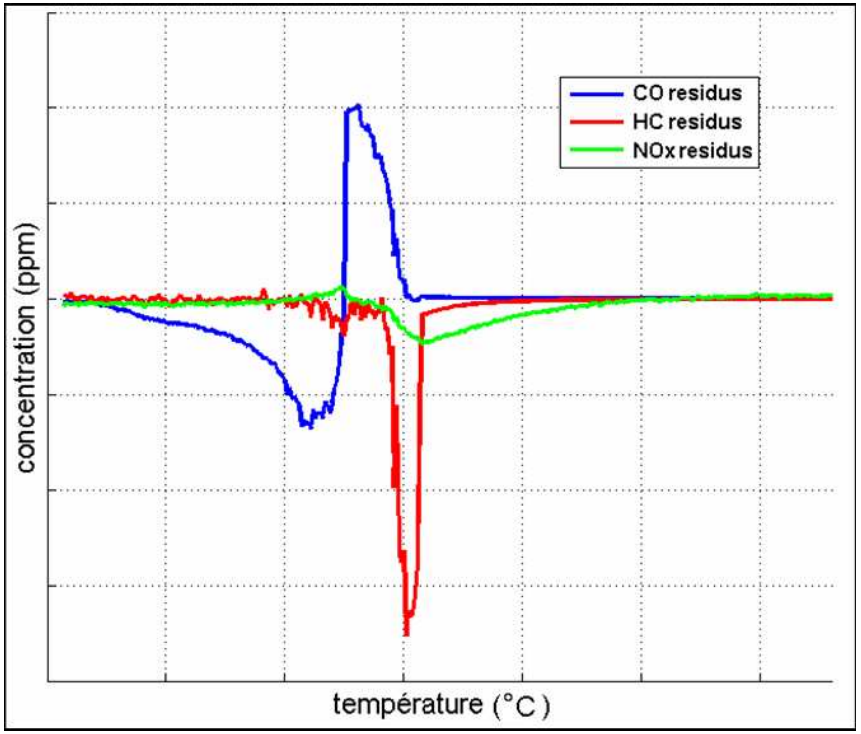
3. NOx trap: experimental and simulated results





Inadequacy of the computer model

Kinetic parameter estimation from a learning set of 20 experiments

Important differences between computer model and experiments

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2. Kriging with non linear trend (KNL)

1. Presentation

Why kriging?

1. To resolve the inadequacy of the mathematical model
2. To determine the new experimental points, through variance prediction

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1. Presentation

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Kriging with non linear trend

Differences between computer model and experiments = Gaussian process

$$y(x)=f\,(x,\beta\,) + z_{\sigma^2,\theta}\,(x)$$

where $z_{\sigma^2,\theta}(x)$ is a Gaussian process such as $E(z(x))=0$ et $cov(z(x),z(x+h))=\sigma^2 R_\theta(h)$

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Estimation of β, σ^2, θ

- Estimation by maximum likelihood
- The analytical formula for $\boldsymbol{\beta}$ is replaced by a minimization procedure

2. Kriging with non linear trend (KNL)

2. Kriging predictor

Kriging predictor

$$\hat{y}(x_0) = rR^{-1}Y - (F^T R^{-1} r - f)^T (F^T R^{-1} F)^{-1} F^T R^{-1} Y$$

Notation

- Let m be the number of design points
- $Y=(Y_1,\ldots,Y_m)^T$ output observed at location $S=(S_1,\ldots,S_m)^T$
- x_0 : point to be predicted
- R : correlation matrix between observations
- r : correlation vector between observations and the point to be predicted
- $F=f(S,\beta)$: value of computer model at design points
- $f=f(x_0,\beta)$: value of computer model at the prediction point

2. Kriging with non linear trend (KNL)

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$$\hat{y}(x_0) = rR^{-1}Y - (F^T R^{-1} r - f)^T (F^T R^{-1} F)^{-1} F^T R^{-1} Y$$

Prediction variance

$$\varphi(x_0) = \sigma^2 \left(1 + \left\| F^T R^{-1} r - f \right\|_{(F^T R^{-1} F)} + \left\| r \right\|_R \right)$$

where $\left\| u \right\|_A = u^T A^{-1} u$

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Parameters estimation

Parameters are obtained by solving recursively the simultaneous equations:

$$\begin{cases} \hat{\beta} = \min\limits_{\beta} (Y - F)^T R^{-1} (Y - F) \\ \hat{\sigma}^2 = (Y - F)^T R^{-1} (Y - F) / m \\ \hat{\theta} = \arg\min \left[\hat{\sigma}^2 \left| R^{-1} \right|^{1/m} \right] \end{cases}$$

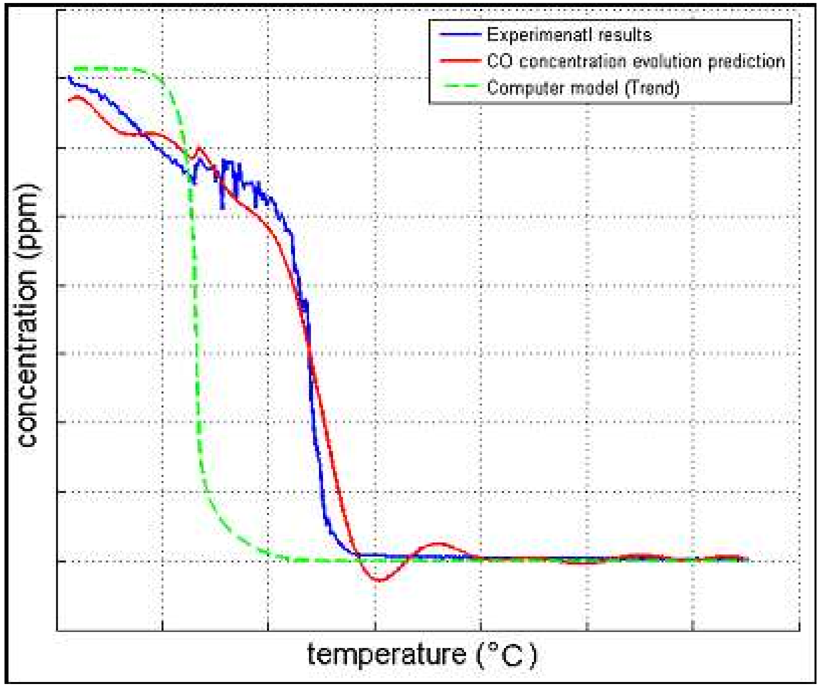
2. Kriging with non linear trend (KNL)

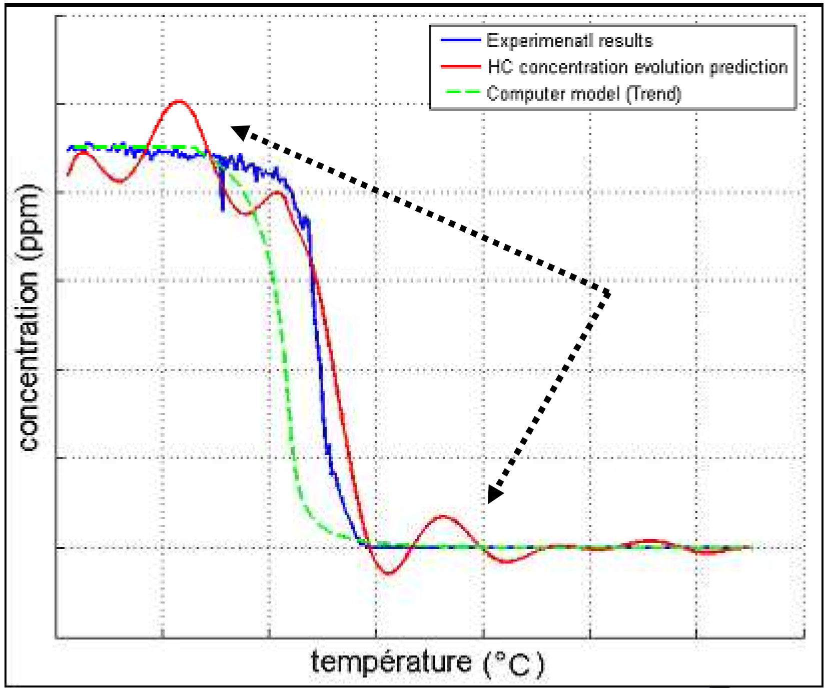
3. Application on deNOx model and results

Application

•12 experimental points are taken uniformly along the temperature for each of the 19 first experiments

•CO and HC prediction for the 20th experiment, outputs are treated independently





Oscillations appear on the initial and final stage

2. Kriging with non linear trend (KNL)

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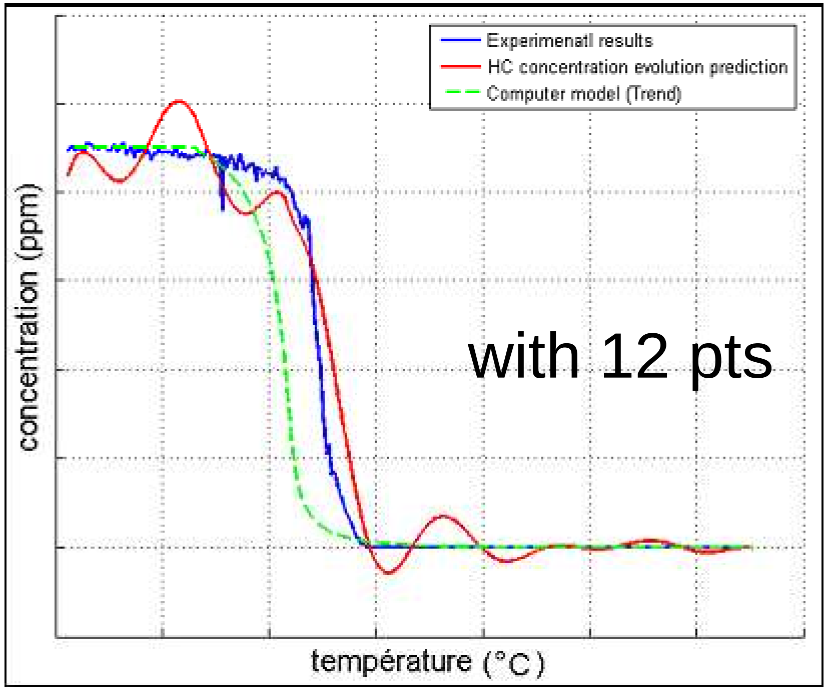
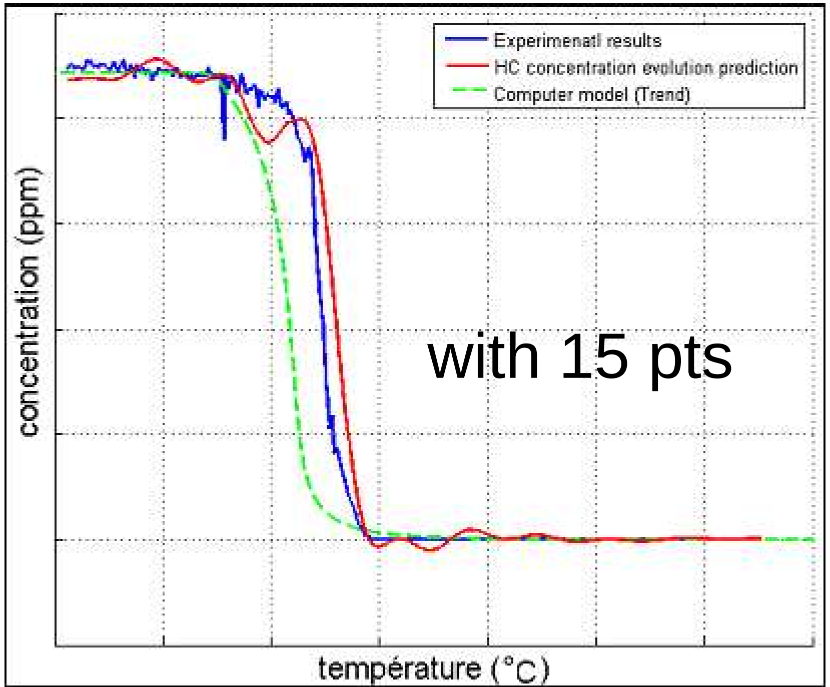
Influence of the number of design point

- HC concentration evolution prediction of the 20th experiment
- The approach is the same but 15 points are taken uniformly along the temperature instead of 12





Oscillations are still present

2. Kriging with non linear trend (KNL)

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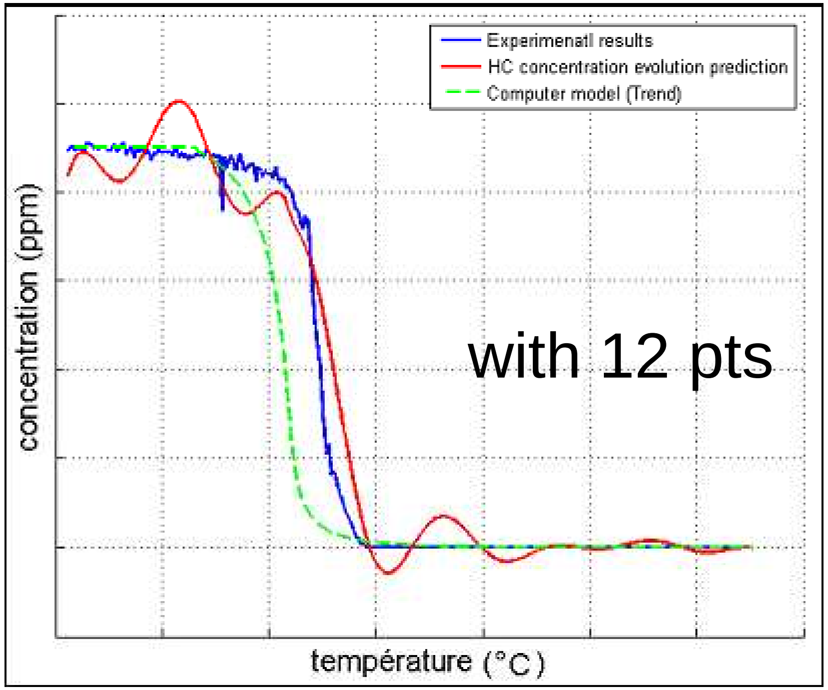

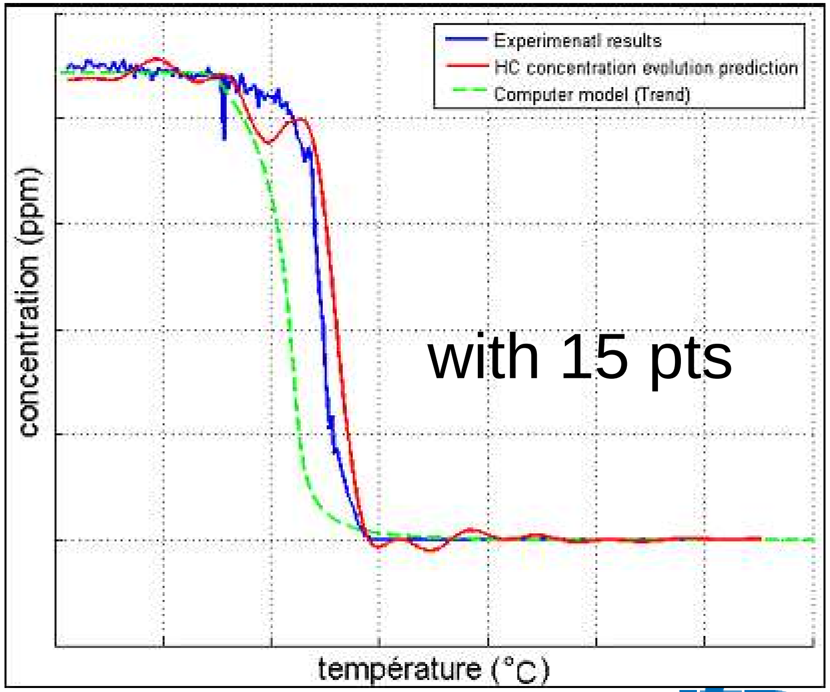

On both, initial and final stage, derivatives are constant

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3. Conditioning by derivatives: improvement for KNL?

1. Presentation

Notation

- Let $(s_1,\ldots,s_{m_1})$ the design points where function value is known
- Let $(v_1,\ldots,v_{m_2})$ the design points where partial derivative according to the first direction is known
- Exponent (1) denotes the output derivative along the first direction
- Let,

$Y=(Y_1,\ldots,Y_{m_1},Y_1^{(1)},\ldots,Y_{m_2}^{(1)})^T$ and $F=(f(s_1,\beta),\ldots,f(s_{m_1},\beta),f^{(1)}(v_1,\beta),\ldots,f^{(1)}(v_{m_2},\beta))^T$

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Covariance structure

Gaussian spatial correlation is used, defined by,

$$R(h) = \exp\left\{-\sum_{l=1}^{k}\theta_l h_l^2\right\}$$

The pairwise joint covariance of $Y(.)$ and $Y^{(1)}(.)$, is given by, (Santner, Williams and Notz, 2003)

$$Cov(Y(s_i),Y^{(1)}(v_j)) = \sigma^2 2\theta_1(s_i^1 - v_j^1)R(s_i - v_j)$$

$$Cov(Y^{(1)}(v_i),Y^{(1)}(v_j)) = \sigma^2(2\theta_1 - 4\theta_1^2(v_i^1 - v_j^1)^2)R(v_i - v_j)$$

1. Presentation

Covariance matrix C

Covariance matrix is defined by,

$$C = \begin{pmatrix} C_{00} & C_{01} \\ C_{01}^T & C_{11} \end{pmatrix}$$

where:

- C_{00} is the m_1xm_1 matrix of correlations between the elements of $Y_i, 1 \leq i \leq m_1$
- C_{01} is the m_1xm_2 matrix of correlations between Y_i and $Y_j^{(1)}, 1 \leq j \leq m_2$
- C_{11} is the m_2xm_2 matrix of correlations between the elements of $Y_j^{(1)}$

3. Conditioning by derivatives: improvement for KNL?

1. Presentation

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Kriging equations

Kriging equations are the same as for kriging with non linear trend

3. Conditioning by derivatives: improvement for KNL?

2. Test model: presentation

Application on two model

Kriging with non linear trend conditioning by derivatives (KNLD) is applied on:

- the test model: similar to study case but simpler and totally mastered
- the deNOx model

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Equations system: represents the experimental system

Langmuir-Hinshelwood formalization:

$$\begin{cases} \frac{d[A]}{dt} = & -\frac{k_0 \exp\{-\frac{E}{RT}\}[A]}{1 + b_0 \exp\{-\frac{\Delta H}{RT}\}[A]} \\ [A]_0 = & A_0 \end{cases}$$

Let ***g(x)*** be the model governed by this system

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Kinetic parameters choice

- ***g(x)*** depends on a hidden kinetic parameter vector, $\xi = \{k_o, E, b_o, \Delta H\}$,

- ξ *has* been chosen to conduct to very different concentration evolutions of A depending on the temperature

3. Conditioning by derivatives: improvement for KNL?

2. Test model: presentation

Second system: represents the mathematical model

Consider the following simple kinetic system:

$$\begin{cases} \dfrac{d[A]}{dt} = & -k'_0 \exp\{-\frac{E'}{RT}\}[A] \\ [A]_0 = & A_0 \end{cases}$$

Let ***f(x,β)*** be the model governed by this system, where ***β={ko',E'}***

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Consider the following simple kinetic system:

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Let $f(x,\beta)$ be the model governed by this system, where $\beta = \{ko', E'\}$

Objective

Determine parameters β, σ^2, θ such as:

$$g(x) = f(x, \beta) + z_{\sigma^2, \theta}$$

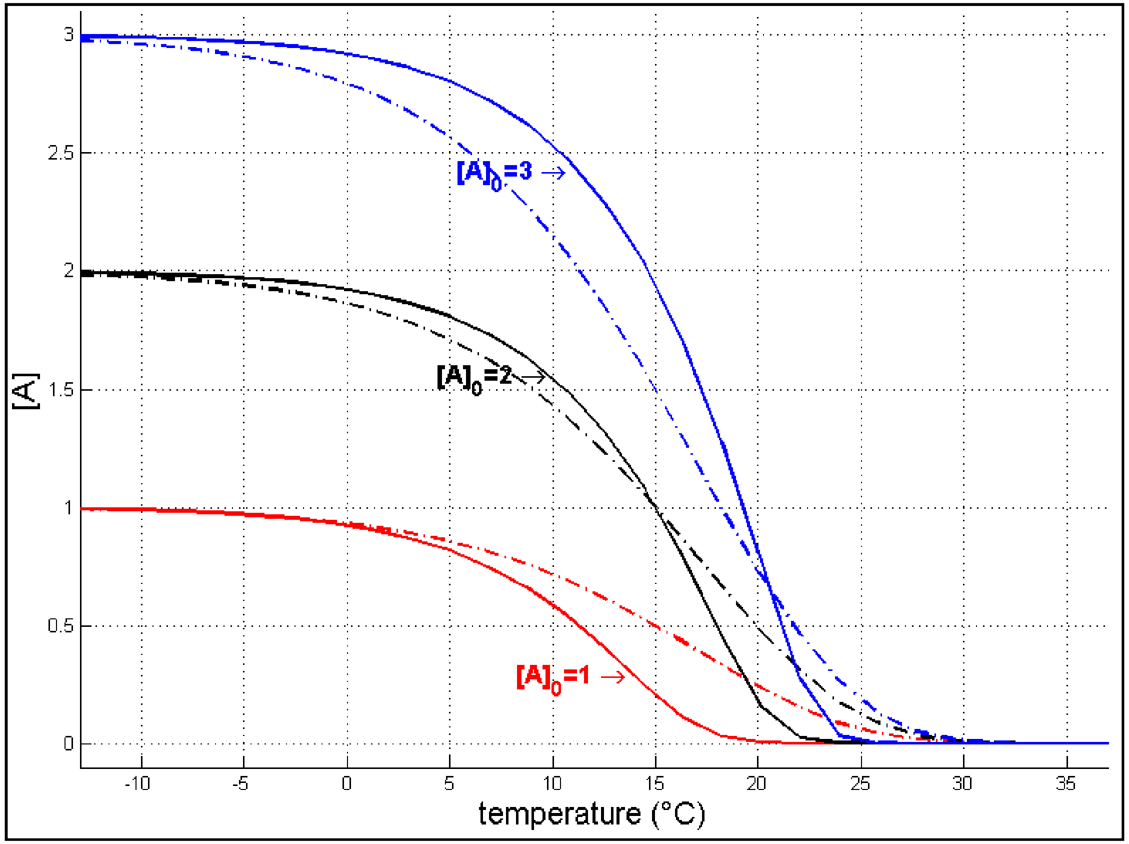
3. Conditioning by derivatives: improvement for KNL?

2. Test model: presentation

Simulations

Simulations for three different A_0 at a fixed time (80 seconds)

Solid line: ‘experimental results’ (function g), Dotted line: ‘estimated model’ (f)



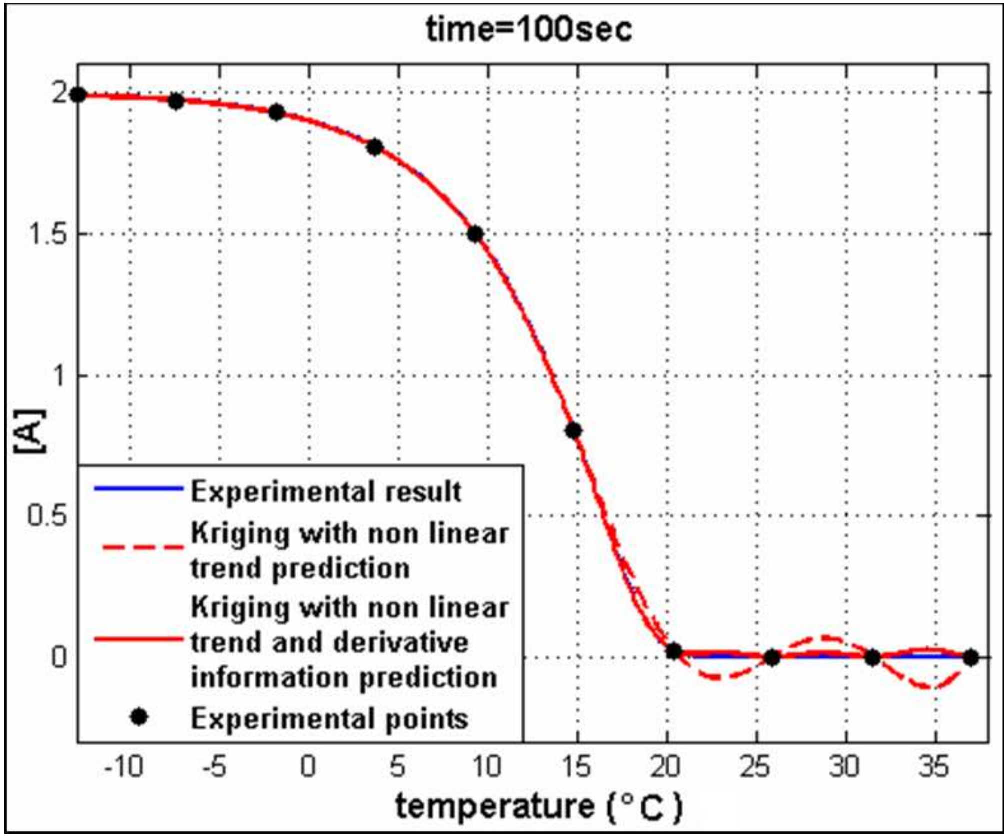
3. Conditioning by derivatives: improvement for KNL?

3. Application on test model and results

Application

Test model prediction by KNL (red dotted line) and kriging with non linear trend conditioning by derivatives (red solid line) compared to experimental results (blue line)

3 initial concentration, 8 fixed time and 10 temperatures on each simulation



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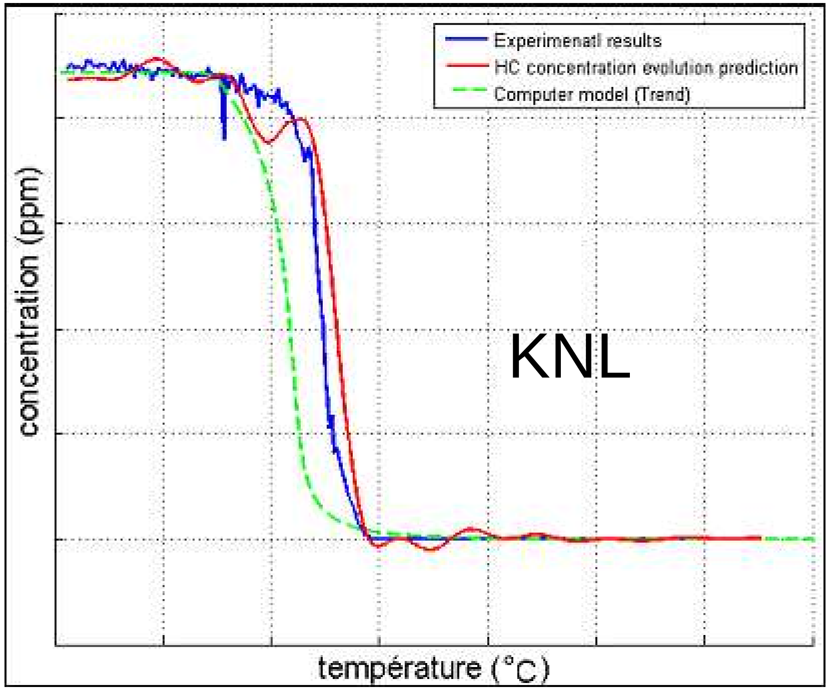
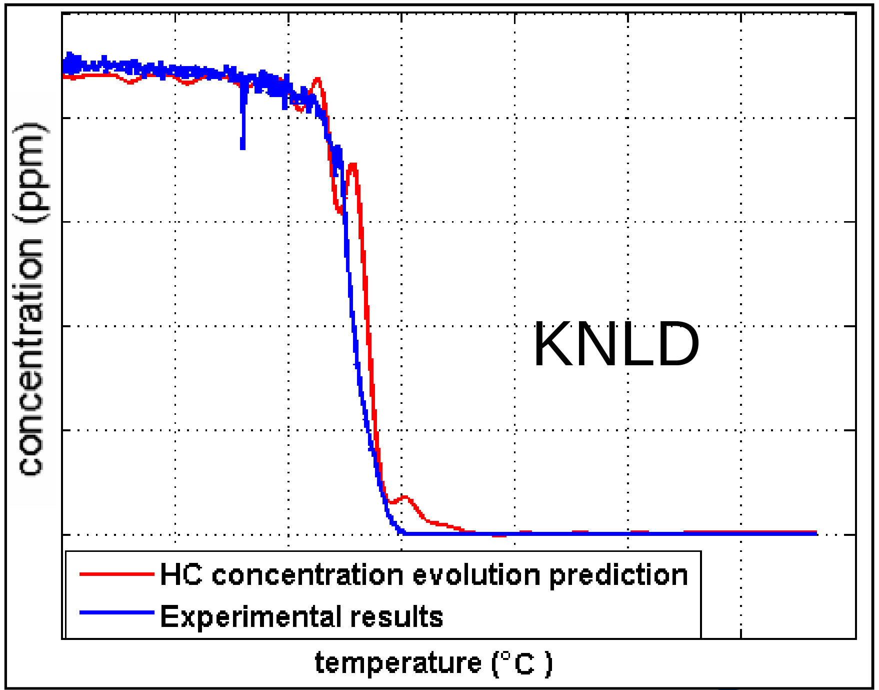
3. Conditioning by derivatives: improvement for KNL?

4. First results on deNOx model

Application

- **HC concentration evolution prediction of the 20th experiment by KNL and kriging with non linear trend conditioning by derivatives (KNLD)**
- **15 experimental points taken uniformly along the temperature on the 19 first experiments**
- **On each experimental point function and derivative values are supposed to be known**





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Points presented

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2. Kriging with non linear trend conditioning by derivatives (KNLD)

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2. Kriging with non linear trend conditioning by derivatives (KNLD)

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- Numerical problems when number of design sites increases
- Oscillations problems where response is less variable

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2. Kriging with non linear trend conditioning by derivatives (KNLD)

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2. KNLD: improvement for KNL

- Prediction is better, i.e. oscillations are less strong
- Model is too constrained

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Perspectives

1. Take into account derivative information only on both, initial and final stages for KNLD
2. Determine an experimental design through variance prediction
3. Compare this experimental design to classical ones

Thank you for your attention!

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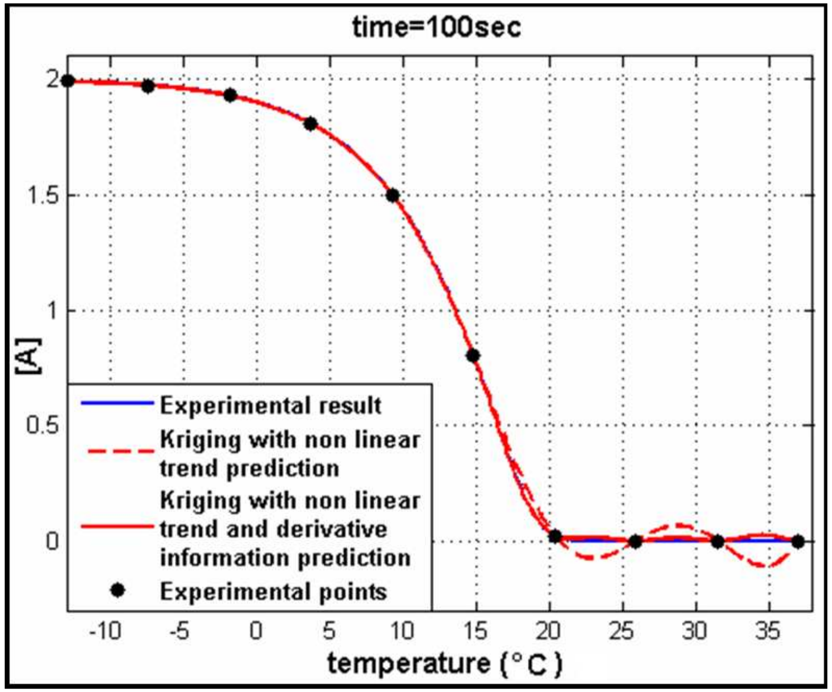

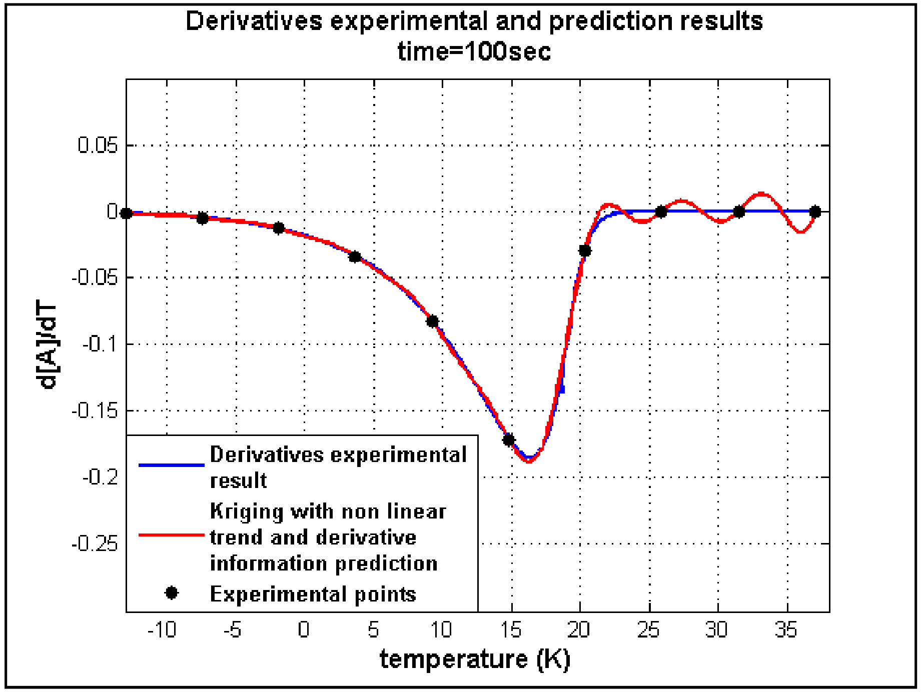

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