Process Identification: Some Thoughts to the Structure of the Problem

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Outline

Starting point

- Been tickled by Steinar Kolås' promotion presentation
- Parameter identification - still a problem
- Little discussion on structure of the problem

Gas reactor – a toy example

- Fixed volume
- Gas - ideal
- No thermal effects
- Ideal valve – i.e. pulse feed – known
- Total pressure measured

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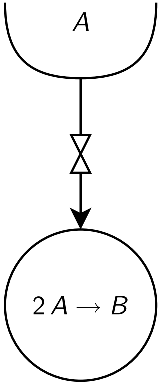

Figure: *Abstraction*

Model: balances, hydraulics and transposition

The component mass balance:

$$\underline{\dot{\mathbf{n}}} \quad := \quad \underline{\mathbf{s}}^T \, \tilde{n} + \underline{\hat{\mathbf{n}}} \tag{1}$$

The production rate

$$\tilde{n} \quad := \quad V \, \tilde{r} \tag{2}$$

The specific production rate

$$\tilde{r} \quad := \quad \frac{k}{|\nu_A|} \, p_A^2 \tag{3}$$

The partial pressures from the equation of state, here the ideal gas law:

$$\underline{\mathbf{p}} \quad := \quad \underline{\mathbf{n}} \, \frac{R\,T}{V} \tag{4}$$

Finally the total pressure:

$$p \quad := \quad \underline{\mathbf{e}}^T \, \underline{\mathbf{p}} \tag{5}$$

Expand production rate

Substitution of the pressure into the specific production rate, which in turn is substituted into the production rate gives:

$$\tilde{n} \quad := \quad \frac{k\,V}{|\nu_A|} \left(\frac{R\,T}{V} \right)^2 n_A^2 \quad := a(k)\, n_A^2 \tag{6}$$

Definitions for systems notation

Re-cast the model into systems notation by defining:

$$\underline{\mathbf{x}} := \underline{\mathbf{n}} \tag{7}$$

$$r := \tilde{n} \tag{8}$$

$$u := \hat{n}_A \tag{9}$$

$$y := p \tag{10}$$

$$\underline{\mathbf{f}} := [1, 0]^T \tag{11}$$

$$\alpha := \frac{V}{|\nu_A|} \tag{12}$$

$$\beta := \frac{R\,T}{V} \tag{13}$$

$$a(k) := k\,\alpha\,(\beta)^2 \tag{14}$$

Compressed model

We get the concise representation:

$$\dot{\underline{\mathbf{x}}} := \underline{\mathbf{s}}\, r + \underline{\mathbf{f}}\, u \tag{15}$$

$$r := a(k)\, x_1^2 \tag{16}$$

$$y := \beta\,(x_1 + x_2) \tag{17}$$

Ideal point observer/estimator

- Don't worry about noise - worry about the structure!
- Line of development: Kalman's observability for continuous systems
- Turns it into an algebraic problem !

Derivation

$$y := b\,\underline{\mathbf{e}}^T\,\underline{\mathbf{x}} \tag{18}$$

$$\dot{y} := b\,\underline{\mathbf{e}}^T\,\underline{\dot{\mathbf{x}}} \tag{19}$$

$$:= b\,\underline{\mathbf{e}}^T\,(r\,\underline{\mathbf{s}} + \underline{\mathbf{f}}\,u) \tag{20}$$

Isolate what can be "measured":

$$w := \dot{y} - b\,\underline{\mathbf{e}}^T\,\underline{\mathbf{f}}\,u \quad := \quad b\,\underline{\mathbf{e}}^T\,\underline{\mathbf{s}}\,r \tag{21}$$

$$\dot{w} := \ddot{y} - b\,\underline{\mathbf{e}}^T\,\underline{\mathbf{f}}\,\dot{u} \quad := \quad b\,\underline{\mathbf{e}}^T\,\underline{\mathbf{s}}\,\dot{r} \tag{22}$$

Manipulate:

$$\frac{w}{\dot{w}} := \frac{r}{\dot{r}} \tag{23}$$

$$:= \frac{ak\,x_1^2}{ak\,2\,x_1\,\dot{x}_1} \tag{24}$$

$$:= \frac{x_1}{\dot{x}_1} \tag{25}$$

Get state, then reaction, then reaction const

Solve for r and x_1:

$$r := \frac{w}{b\,\underline{\mathbf{e}}^T\,\underline{\mathbf{s}}} \tag{26}$$

$$x_1 := 2\,\frac{w}{\dot{w}}\,(s_1\,r + f_1\,u) \tag{27}$$

Only now nonlinearity hits: get reaction const

$$r := a(k)\,x_1^2 \tag{28}$$

$$\therefore \quad a(k) := r\,x_1^{-2} \tag{29}$$

$$\therefore \quad k := \frac{a(k)}{\alpha\,b^2} \tag{30}$$

Sequential approach

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  $\longrightarrow$ linear in flows and reaction

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- My PhD on observing composition in batch reactors from hydraulics and temp measurements

Case: State measurable

$$\underline{\dot{\mathbf{x}}} := \underline{\underline{\mathbf{F}}}\,\underline{\hat{\mathbf{x}}} + \underline{\underline{\mathbf{S}}}\,\underline{\mathbf{r}} \tag{31}$$

$$\underline{\hat{\mathbf{x}}} :: \text{measured} \tag{32}$$

$$\underline{\mathbf{r}} := V\,\underline{\underline{\mathbf{K}}}\,\underline{\mathbf{g}}(\underline{\mathbf{x}}) \tag{33}$$

Isolate reaction part:

$$\underline{\underline{\mathbf{S}}}\,\underline{\mathbf{r}} := \underline{\dot{\mathbf{x}}} - \underline{\underline{\mathbf{F}}}\,\underline{\hat{\mathbf{x}}} \tag{34}$$

Assume for simplicity square, invertible $\underline{\underline{\mathbf{S}}}$

$$\underline{\mathbf{r}} := \underline{\underline{\mathbf{S}}}^{-1}\left(\underline{\dot{\mathbf{x}}} - \underline{\underline{\mathbf{F}}}\,\underline{\hat{\mathbf{x}}}\right) \tag{35}$$

- Regularise and use for estimation of reaction constant(s).
- If necessary differentiate
- ..etc..

Case: Observation linear in state

$$\dot{\underline{\mathbf{x}}} := \underline{\underline{\mathbf{F}}}\,\hat{\underline{\mathbf{x}}} + \underline{\underline{\mathbf{S}}}\,\underline{\mathbf{r}} \tag{36}$$

$$\hat{\underline{\mathbf{x}}} :: \text{measured} \tag{37}$$

$$\underline{\mathbf{r}} := V\,\underline{\underline{\mathbf{K}}}\,\underline{\mathbf{g}}(\underline{\mathbf{x}}) \tag{38}$$

$$\underline{\mathbf{y}} := \underline{\underline{\mathbf{C}}}\,\underline{\mathbf{x}} \tag{39}$$

State reconstruction and estimation of reaction part is a linear problem.

Issues

- Modelling errors (dynamics) in hydraulics hurt
- Observation errors hurt
- Stochastic components can be filtered out
- Amplification of hydraulic and kinetic often very large.

Getting derivatives

- Use linear filter methods (example Schaufelberger, Maletinsky)
- Maletinsky's - Preisig: Multi-wavelets.
- Kalman filter, extended version also does estimation job. Bad control over estimation properties as variance-covariance becomes tuning parameters
- Fixed-gain observer with jacket etc.

Spline-type modulating functions: background

Given the SISO model in transfer function form

$$\sum_{i}^{n} a_i \, D^i \, y \quad := \quad \sum_{i}^{n} b_i \, D^i \, u \,, \tag{40}$$

elimination of the unknown initial conditions of the n integrators, except the last one which is directly measured by the output, transforms the model into

$$\sum_{i}^{n} a_i \, < \varphi_{n,i}, y > \quad := \quad \sum_{i}^{n} b_i \, < \varphi_{n,i}, u > \; . \tag{41}$$

The functions $\varphi_{n,0}$ are the modulating functions, B-splines of the order n, the first index, and 0-times differentiated, the second index.

properties

Some of the important characteristics of the B-spline functions are:

Compact base $\varphi_{a,\alpha}(t) = 0 \quad \text{for} \notin [0, nT]\,;$

Derivative | Integral $\varphi_{a,\alpha-1}(t) = \int_0^{nT} \varphi_{a,\alpha}(t)\, dt\,;$

Stem function order n $\varphi_{n,n}(t) = T^{-n} \sum_{i:=0}^{n} (-1)^i \binom{n}{i} \delta(t - i\,T)\,.$

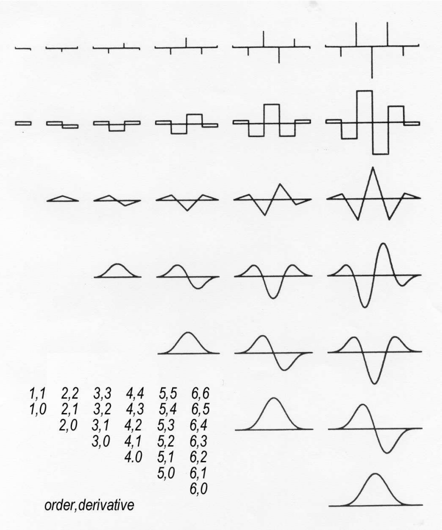
The upper triangle of functions is generated stepwise.

The first row are the Cholesky factors ± Pascal triangle entries.

Generator: consecutive convolution:

$\varphi_{a,a} \star \varphi_{b,b} = \varphi_{a+b,a+b}$

Example: convoluting $\varphi_{1,1}$ n-times with itself $((\varphi_{1,1})^{\star n})$ generates the first row.



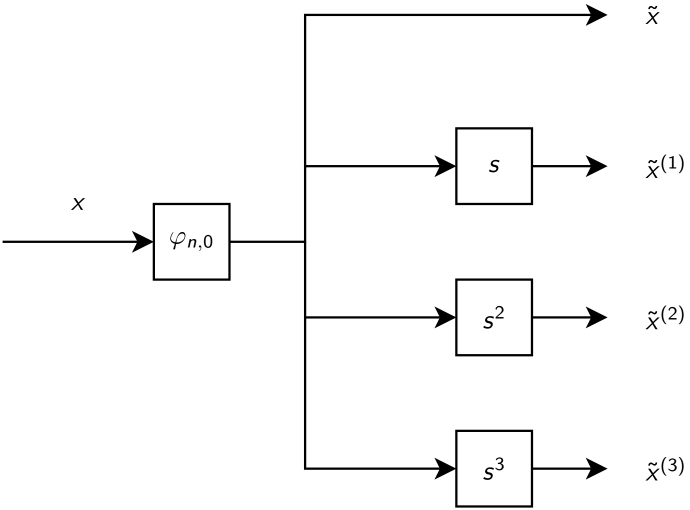
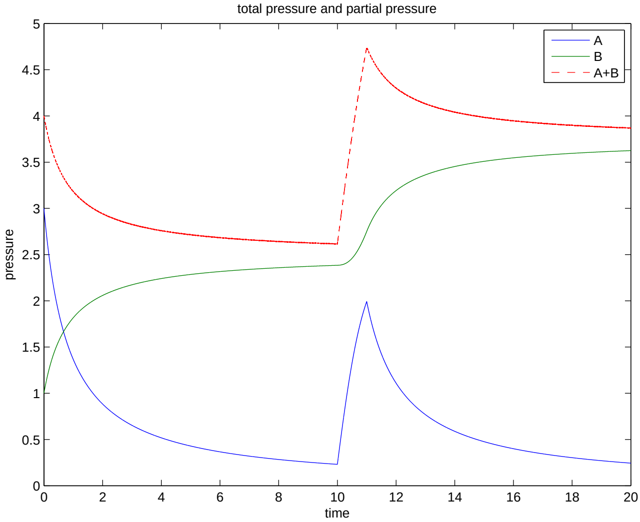
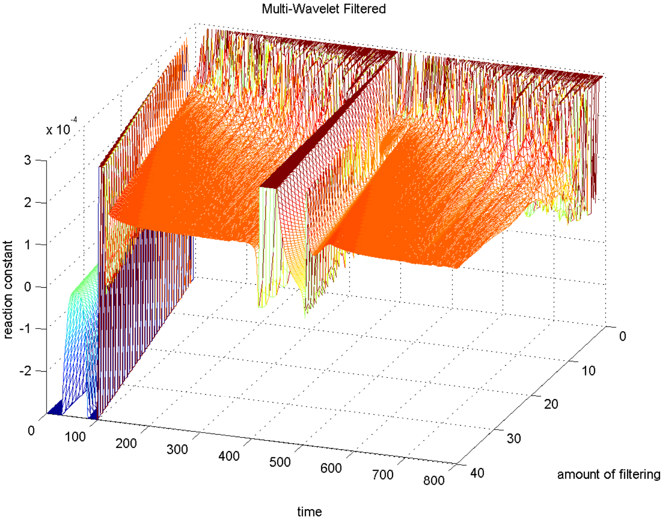


Figure: *filter*

Experiment


total pressure and partial pressure
A
B
A+B
pressure
time
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
2
4
6
8
10
12
14
16
18
20

Results


Multi-Wavelet Filtered
x 10^-4
3
2
1
0
-1
-2
reaction constant
0
100
200
300
400
500
600
700
800
time
0
10
20
30
40
amount of filtering

Structure

- Structure of the observer/estimation problem is important
- Linearity of the conservation principles can be used for estimating reaction first; next regularize and then estimate parameter.
- Linearity of the state observer problem – very handy

Methods

- Linear filter methods to get derivatives
- High-gain Kalman filter – about the same
- Extended Kalman filter – do things simultaneously...may not be a good idea (modelling errors, amplification)
- Multi-wavelets – very handy as state-variable filters (also no bias problem in estimator)
- Tuning: characteristic time $\approx$ time constant to be observed
- Multi-resolution: choose parallel filters with different characteristics

Do not use methods blindly

Less sophistication in the method usually provides more insight.