Optimal Experiment Design for the estimation of moisture material properties

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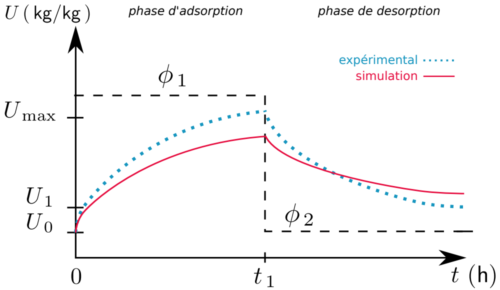
Context

Comparison numerical prediction *VS.* experimental observations

Some discrepancies observed [1] :

- for different materials,
- for different facilities,
- at different scales : material & wall.



Possible explanation :

$\Rightarrow$ estimation of material properties according to standards

$$\text{standards} = \begin{cases} \text{gravimetric method ISO 12571} \\ \text{cup method ISO 12572} \end{cases} = \text{steady state measurements}$$

Issues

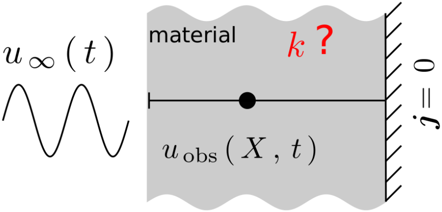
Objective : Estimating the material properties using transient measurements.

Methodology,

1. Define a configuration
2. Define a physical model :

$$c\,\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial u}{\partial x}\right),$$

$$\frac{\partial u}{\partial x} = \mathrm{Bi}\left(u - u_{\infty}(t)\right), \qquad x = 0$$



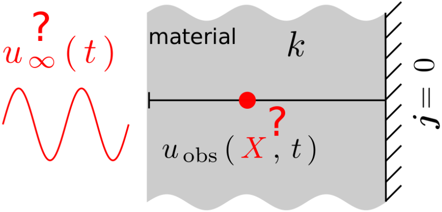
3. Obtain the experimental observations $u_{\mathrm{obs}}(t)$ with local sensor(s)
4. Solve the inverse problem : $k = \arg\min_{k} \left|\left| u(X, t, k) - u_{\mathrm{obs}}(X, t) \right|\right|_2$

Problem statement

Estimation of material properties

However,

- Where to place the sensors ?
- What variations for $u_\infty(t)$?
  - what amplitude ?
  - what frequency ?



Using the Optimal Experimental Design (OED)

Some references :

- FEDOROV 1972 [2],
- BECK and Arnold 1977 [3],
- WALTER et al. 1990 [4, 5],
- UCINSKI 2004 [6].

With applications in :

- ARTYUKHIN et al. 1985 [7],
- NENAROKOMOV et al. 2005 [8],
- KARALASHVILI et al. 2015 [9].

Searching the OED

Parameter estimation problem for $\boldsymbol{P} = \left[p_m \right], \forall m \in \{1, \ldots, M\}$

1. Compute the sensitivity functions :

$$\Theta_m(x,t) = \frac{\sigma_p}{\sigma_u} \frac{\partial u}{\partial p_m}, \qquad \forall m \in \{1, \ldots, M\}$$

2. Compute the FISHER information matrix :

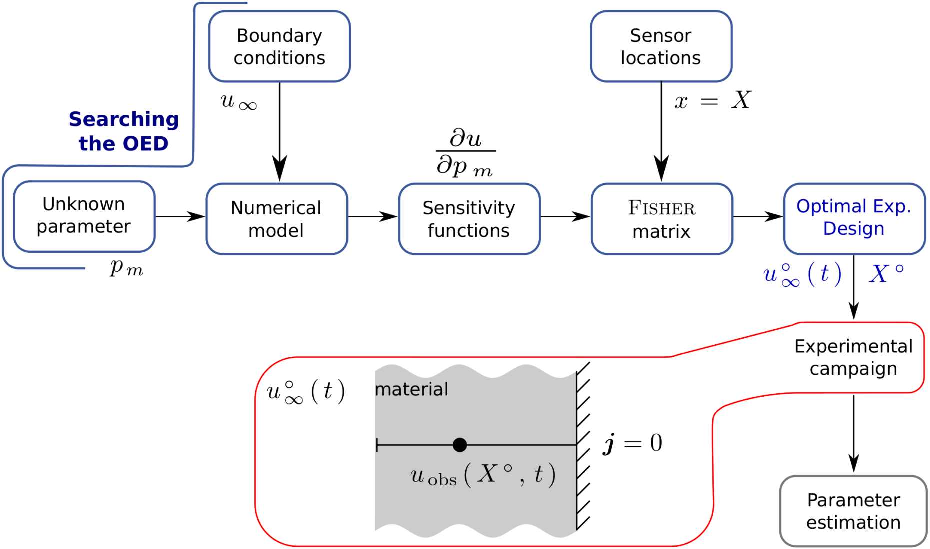
$$F = \left[\Phi_{ij} \right], \qquad \forall (i,j) \in \{1, \ldots, M\}^2,$$

$$\Phi_{ij} = \sum_{n=1}^{N} \int_0^{\tau} \Theta_i(X_n, t)\, \Theta_j(X_n, t)\, \mathrm{dt},$$

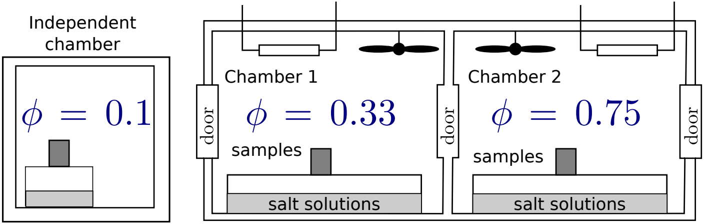
3. Maximize the criteria Ψ :

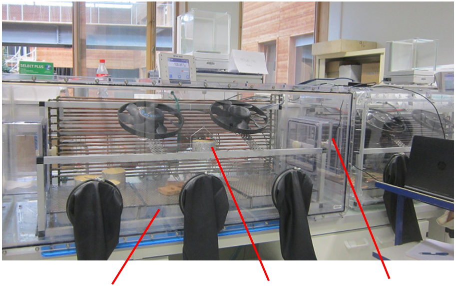
$\Psi = \det\left[F(\pi) \right]$, as a function of the design $\pi = \{ X, u_\infty \}$

Synthesis of the methodology



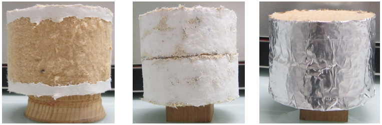
The facility





Salt solution Sample Airlock

Sensors



Samples

The physical model

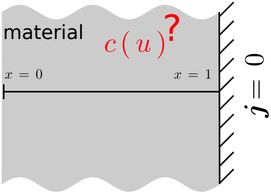
Vapor transfer in porous material [10]

$$c(u)\,\frac{\partial u}{\partial t} = \mathrm{Fo}\,\frac{\partial}{\partial x}\left(d(u)\,\frac{\partial u}{\partial x} - \mathrm{Pe}\,u\right),$$

and the boundary conditions :

$$d(u)\,\frac{\partial u}{\partial x} - \mathrm{Pe}\,u = \mathrm{Bi}\cdot(u - u_\infty), \qquad x = 0.$$

$u_\infty(t)$



Coefficient $c(u)$ is unknown and parameterized as : $c(u) = 1 + c_1\,u + c_2\,u^2$

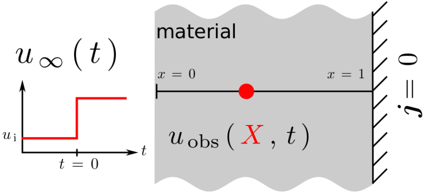
Parameters to be estimated : Fo, c_1 and c_2.

The possible designs : single step

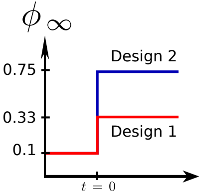
Configuration :

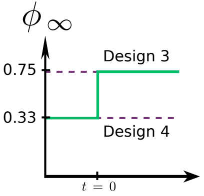
- single step of relative humidity,
- one sensor to place inside the material,
- estimation of one parameter among

  Fo, c_1 and c_2.

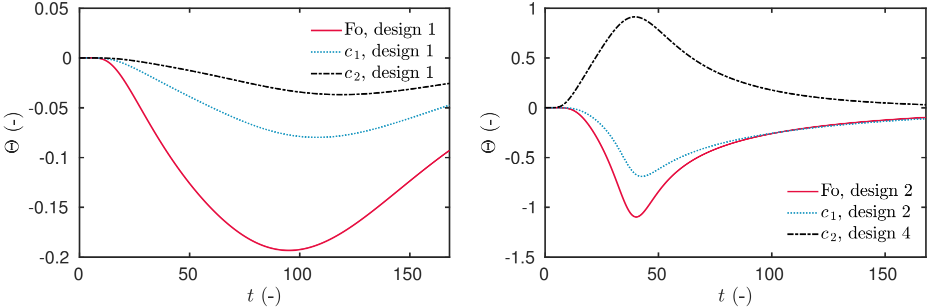


Design	Initial cond. ϕ_i	Boundary cond. ϕ_∞
1	0.1	0.33
2	0.1	0.75
3	0.33	0.75
4	0.75	0.33





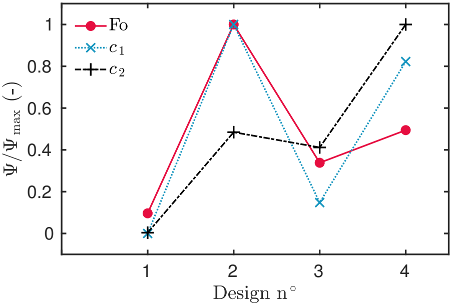
The sensitivity functions

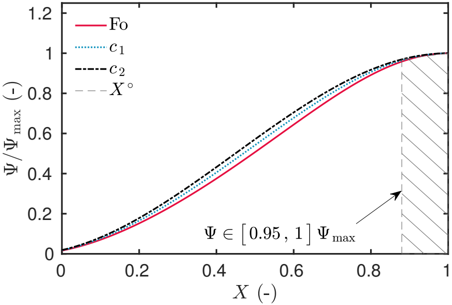


Design	$\phi_{\,\mathrm{i}}$	$\phi_{\,\infty}$
1	0.1	0.33
2	0.1	0.75
3	0.33	0.75
4	0.75	0.33

$$\Theta = \left(\frac{\partial u}{\partial \mathrm{Fo}} \,, \frac{\partial u}{\partial c_1} \,, \frac{\partial u}{\partial c_2} \right)$$

Searching the OED





Design	ϕ_{i}	ϕ_{∞}
1	0.1	0.33
2	0.1	0.75
3	0.33	0.75
4	0.75	0.33

OED :

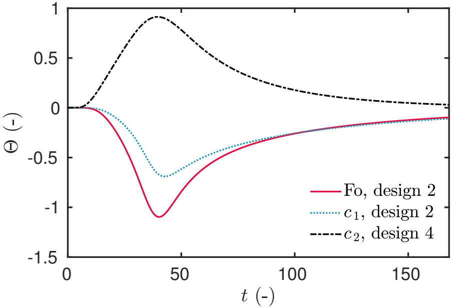
- Estimation of Fo and $c_1 \Rightarrow$ Design 2
- Estimation of $c_2 \Rightarrow$ Design 4
- Location of the sensor $\Rightarrow \ X \in [0.9\,,\,1]$.

Single step experiments

However,

- only for the estimation of one parameter,
- strong correlation of sensitivity functions :

$$\mathrm{Cor}\left(\mathrm{Fo}\,,\,c_1\right) \in \left[0.94\,,\,0.99\right],$$
$$\mathrm{Cor}\left(c_1\,,\,c_2\right) \in \left[0.92\,,\,0.99\right],$$
$$\mathrm{Cor}\left(\mathrm{Fo}\,,\,c_2\right) \in \left[0.71\,,\,0.95\right].$$



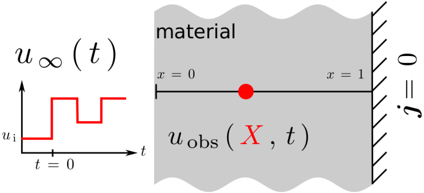
- for the estimation of the three parameters Fo, c_1 and c_2

$\Longrightarrow$ need other experimental data

The possible designs : multiple steps

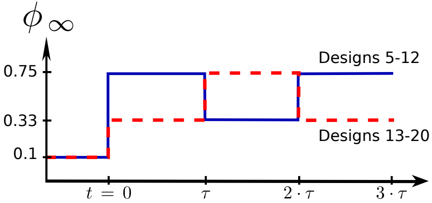
Configuration :

- multiple steps of relative humidity,
- variable duration of the step τ,
- one sensor to place inside the material,
- estimation of the two parameters $\left(\mathrm{Fo}, c_2 \right)$.

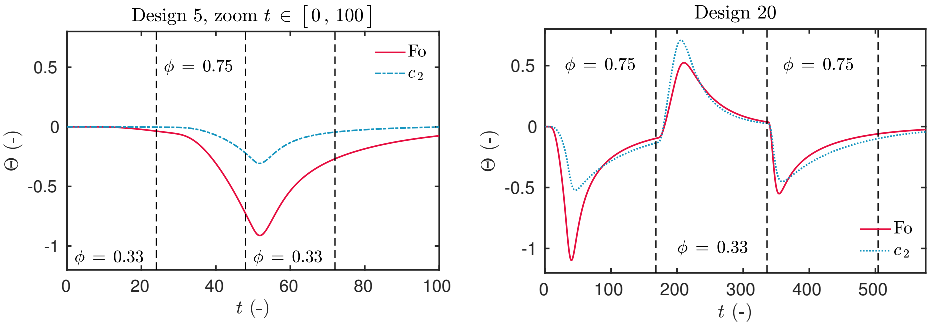


Des.	Initial cond.	Boundary cond.		
	ϕ_i	$\phi_{\infty,1}$	$\phi_{\infty,2}$	$\phi_{\infty,3}$
5-12	0.1	0.33	0.75	0.33
13-20	0.1	0.75	0.33	0.75

$\tau \in [1, 8]$ days

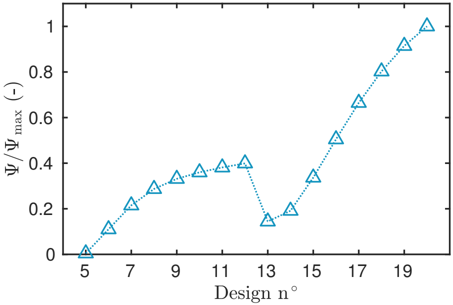


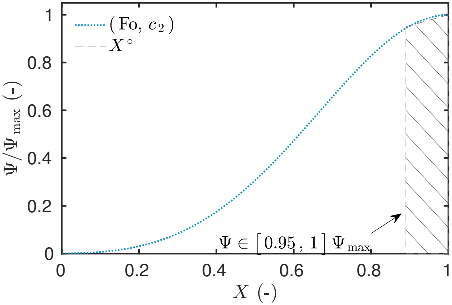
The sensitivity functions



Design	ϕ_{i}	$\phi_{\infty,1}$	$\phi_{\infty,2}$	$\phi_{\infty,3}$	τ (days)
5	0.1	0.33	0.75	0.33	1
20	0.1	0.75	0.33	0.75	8

Searching the OED





OED :

- Estimation of $\left(\mathrm{Fo} \,,\, c_2 \right) \Rightarrow$ Design 20
- Location of the sensor $\Rightarrow \ X \in \left[0.9 \,,\, 1 \right]$.

Design	$\phi_{\,\mathrm{i}}$	$\phi_{\,\infty\,,\,1}$	$\phi_{\,\infty\,,\,2}$	$\phi_{\,\infty\,,\,3}$	τ (days)
20	0.1	0.75	0.33	0.75	8

Solving the parameter estimation problem

Performing the experiments :

- one sensor located at $X = 1$.
- OED for single step of relative humidity

$\Rightarrow$ estimation of c_1

Single step

Design	ϕ_{i}	ϕ_{∞}
OED	0.1	0.75

- OED for multiple steps of relative humidity,

$\Rightarrow$ estimation of $\left(\mathrm{Fo}, c_2\right)$

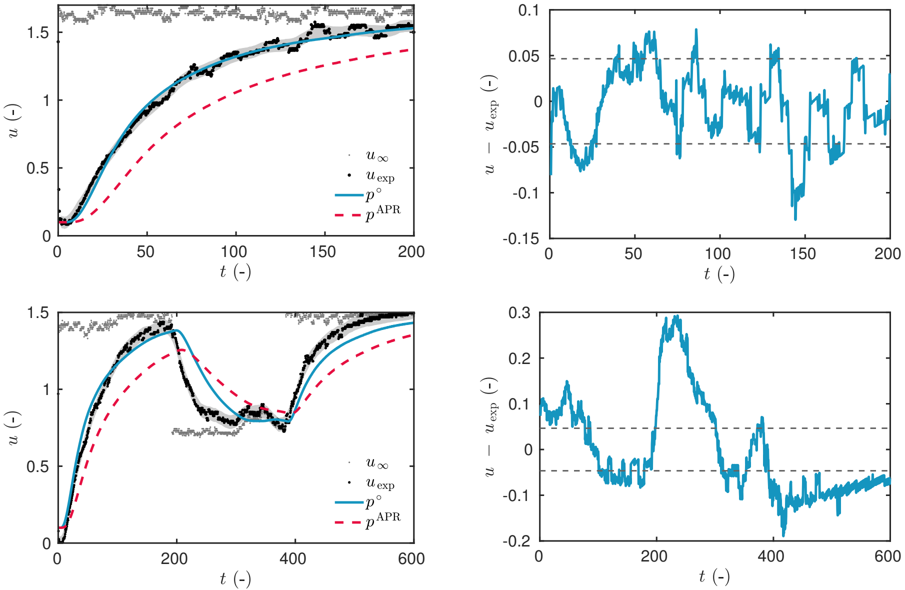
Multiple steps

Design	ϕ_{i}	$\phi_{\infty,1}$	$\phi_{\infty,2}$	$\phi_{\infty,3}$	τ (days)
OED	0.1	0.75	0.33	0.75	8

Solving the parameter estimation problem :

- demonstration of the formal identifiability (Strucutral Global Identifiability),
- interior point algorithm with `fmincon` `Matlab`$^{\mathrm{TM}}$ function.

Solving the parameter estimation problem

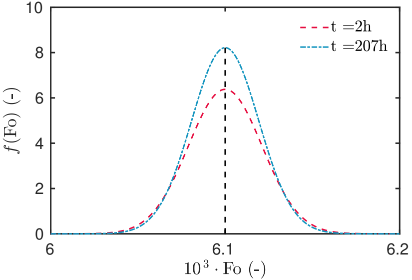


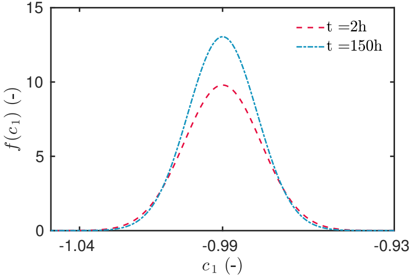
Solving the parameter estimation problem

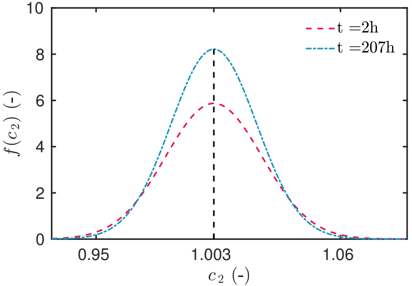
The importance of sensitivity functions :

- the probability of the unknown parameter p_m can be approximated :

$$F(\bar{p}_m) = \mathcal{P}\left\{ p_m \leqslant \bar{p}_m \right\}$$
$$= F\left(u + \Theta_m \cdot \left(\bar{p}_m - p_m^{\circ} \right) \right).$$







Conclusion

Optimal Experimental Design approach :

- within parameter estimation problem context,
- numerical method for the definition of experimental design,
- the importance of the sensitivity functions.

Limitations :

- depends on the physical model,
- depends on the *a priori* parameters values.

Outlooks :

- taking into account hysteresis effects in the physical model.

Merci pour votre attention

Validation OED

Problem :

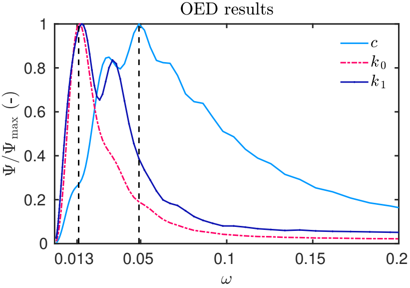
$$c \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\left(k_0 + k_1 u \right) \frac{\partial u}{\partial x} \right),$$

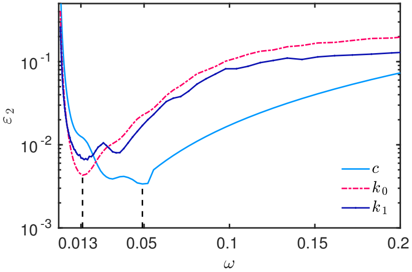
$$- k\left(u \right) \frac{\partial u}{\partial x} = A \sin\left(2 \pi \omega t \right), \quad x = 0.$$

Validation :

- for a fixed ω,
- for a given $p_m^\circ \in \left\{ c, k_0, k_1 \right\}$,
- observation generated numerically with a noise u_{obs},
- $N_e = 100$ inverse problem solved to estimate p_m,
- computation of the error :

$$\varepsilon_2 = \sqrt{\frac{1}{N_e} \sum \left(p_m - p_m^\circ \right)}$$





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