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A PROTOCOL FOR MODEL IDENTIFICATION IN FOOD THERMAL PROCESSING

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Computer-aided simulation offers a powerful, rational and systematic way to explain complex phenomena, evaluate hypotheses and guide new operation conditions.

AEs, ODEs, PDEs.

$$\Psi\left(\boxed{\mathbf{x}}, \mathbf{x}_{\xi}, \mathbf{x}_{\xi\xi}, \mathbf{x}_{t}, \mathbf{v}_{t}, \boxed{\mathbf{v}}, \boxed{\mathbf{u}}, \boxed{\boldsymbol{\theta}}, \boxed{\xi}, \boxed{t}\right) = 0$$

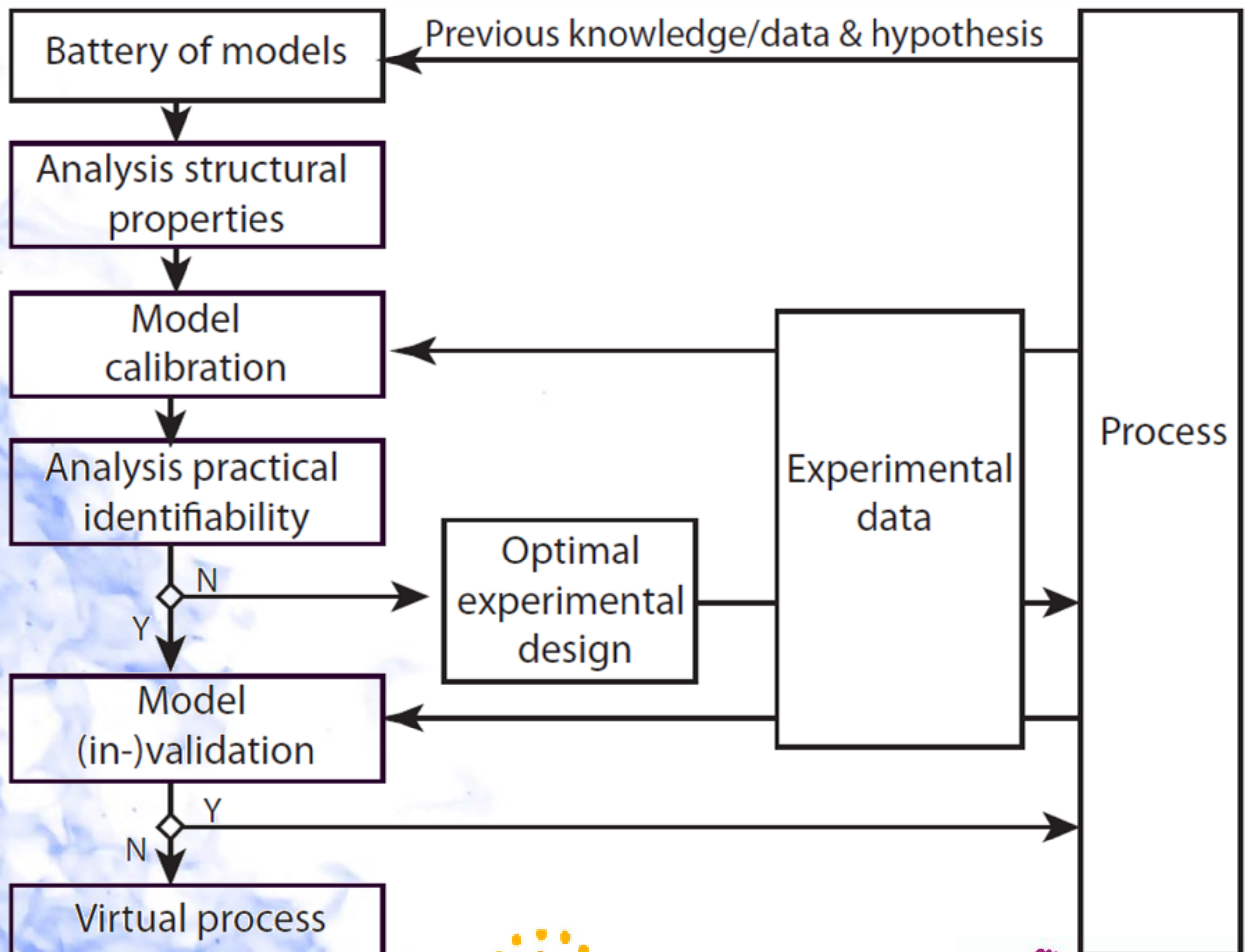
Distributed State **Lumped State** **Controls** **Parameters** **Space** **Time**

Initial conditions + Boundary conditions

How do we reconcile models with experimental data?
How can we improve model predictive capabilities?

Model identification protocol

Proposed protocol for model identification



Challenges

- Structural properties: indistinguishability, lack of identifiability

Re- formulation

Re-parameterisation

Iterative procedure

- Nonlinear models
- Large scale dynamics – Computational cost
- Medium - Large number of parameters
- The order of magnitude may be unknown
- Multimodal character of the NLP

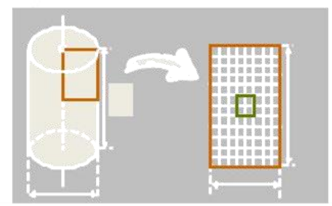
Use of efficient and robust simulation and global optimisation

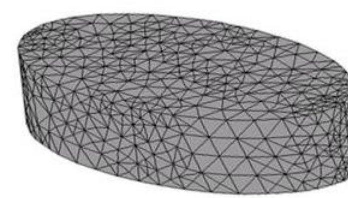
- Quantity, Quality and Variety of data
- Practical identifiability problems

Optimal experimental design

Simulation

- Typically: spatial discretisation techniques.
- Finite elements or finite differences.
- **Reduced order modelling** offers a way to capture the essential features of the systems dynamics, with a reduced computational effort.





Model calibration

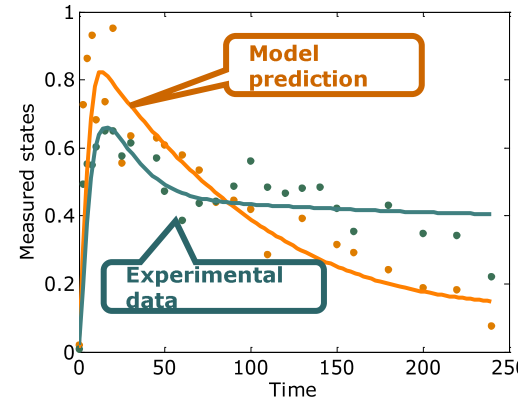
System dynamics:

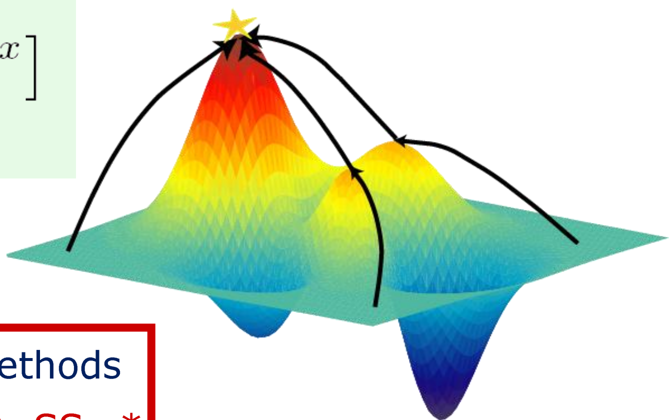
$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{v}, \boldsymbol{\theta}, t)$$

$$\mathbf{y}(t_s^k, \mathbf{u}, \mathbf{v}, \boldsymbol{\theta}) = \mathbf{g}(\mathbf{x}(\mathbf{u}, \mathbf{v}, \boldsymbol{\theta}, t_s^k), \boldsymbol{\theta}, t_s^k)$$

Find θ and x_0 to minimise:

$$J(\boldsymbol{\theta}) = \sum_{ix=1}^{n_{exp}} \sum_{i=1}^{n_{obs}} \left[\Delta Y_i^{ix}\right]^T \mathbf{Q}_i^{ix} \left[\Delta Y_i^{ix}\right]$$





- Local direct search and gradient based methods
- Global methods: Evolutionary (DE, SRES), SSm*

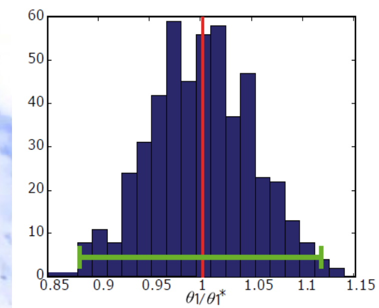
*Egea, J.A., et al (2007). J. Global Optimization 37(3):481-503.

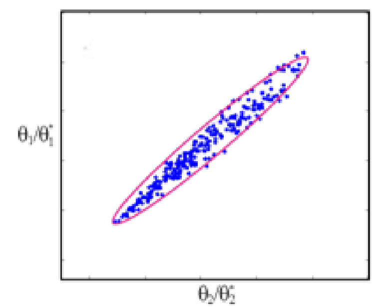
Practical identifiabilty

To asses the uncertainty of the parameter estimates

Confidence regions

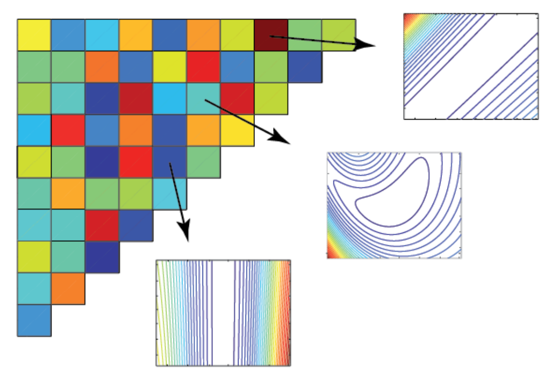
Monte-Carlo based approaches





Fisher Information Matrix

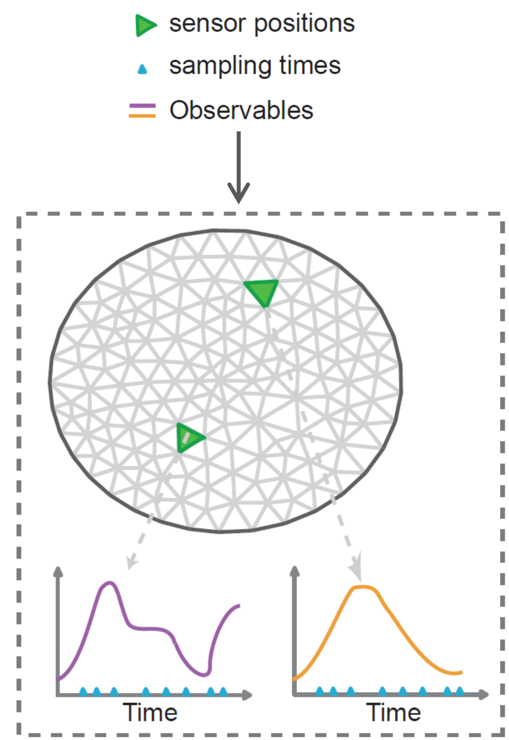
$$\mathcal{F} = E_{|_{y_m,\boldsymbol{\theta}^*}}\left\{\left[\frac{\partial \mathcal{J}_{PE}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right]\left[\frac{\partial \mathcal{J}_{PE}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right]^T\right\}$$



Optimal experimental design

Calculate the dynamic scheme of measurements so as to generate the maximum amount and quality of information for model calibration purposes.

$$J_{OED} = \phi(\mathcal{F})$$



Subject to the system dynamics:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{v}, \boldsymbol{\theta}, t)$$

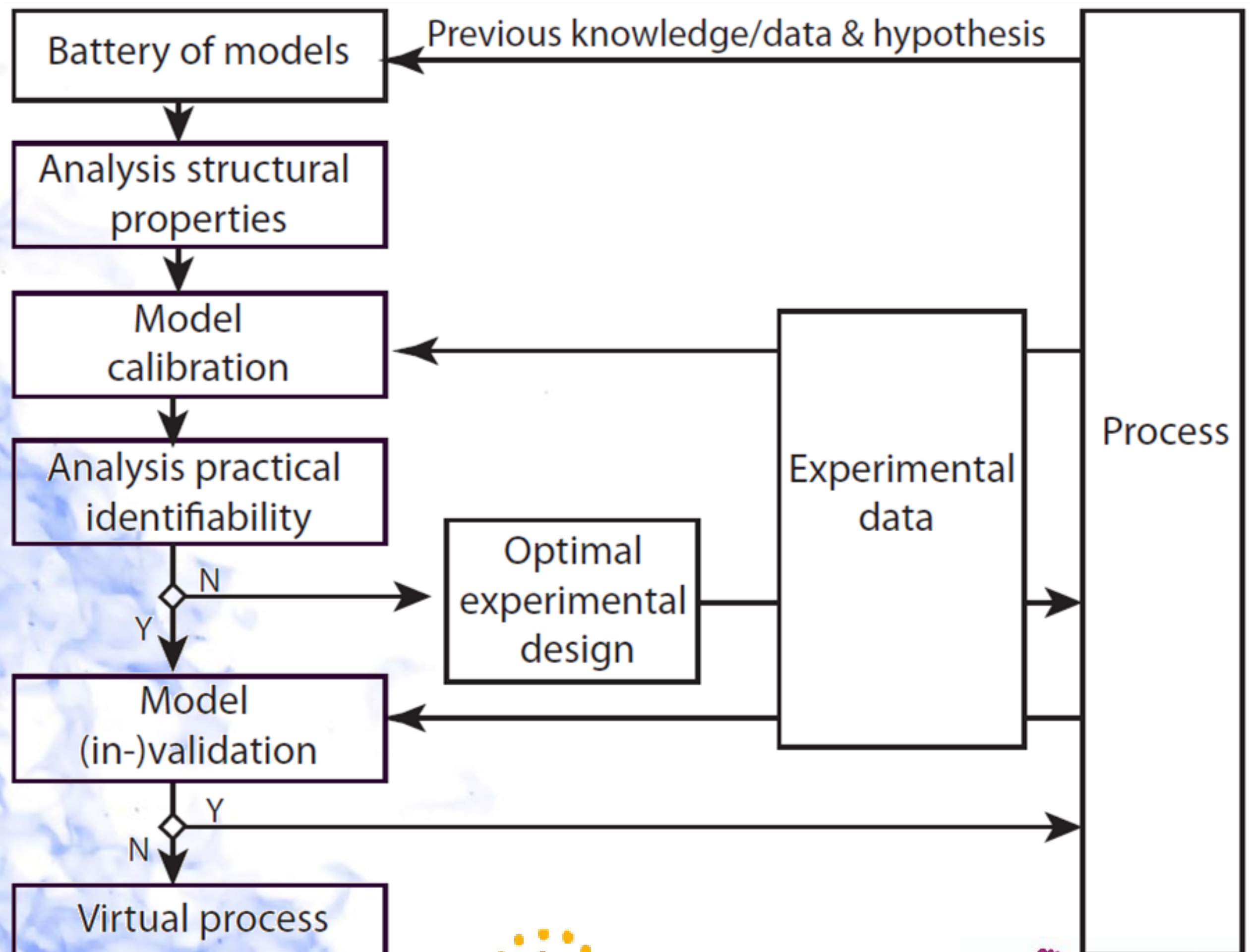
$$\mathbf{y}(t_k, \mathbf{u}, \mathbf{v}, \boldsymbol{\theta}) = \mathbf{g}(\mathbf{x}(\mathbf{u}, \mathbf{v}, \boldsymbol{\theta}, t), \boldsymbol{\theta}, t)$$

And experimental constraints:

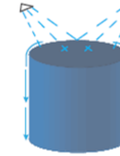
$$\mathbf{u}^L(t) \leq \mathbf{u}(t) \leq \mathbf{u}^U(t)$$

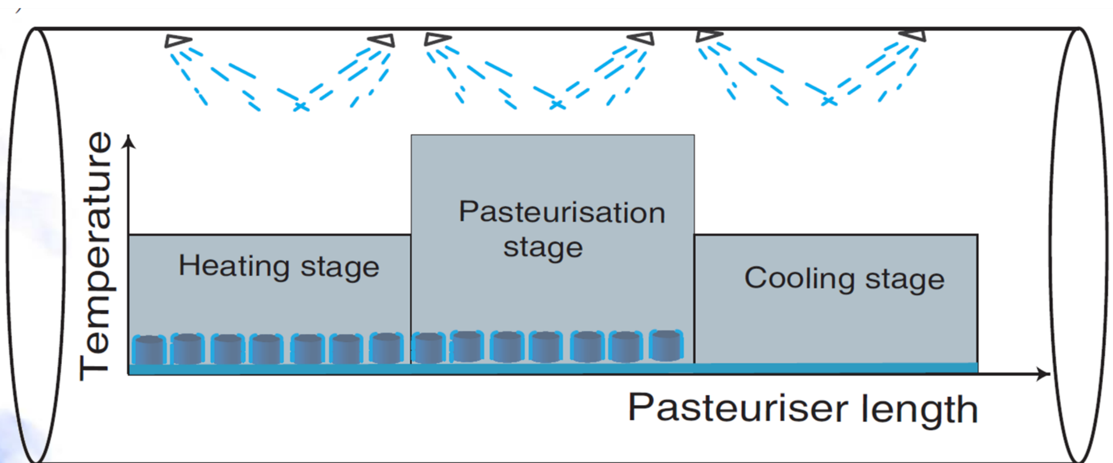
$$\mathbf{v}^L \leq \mathbf{v} \leq \mathbf{v}^U$$

Proposed protocol for model identification



Example I: Tunnel pasteurisation



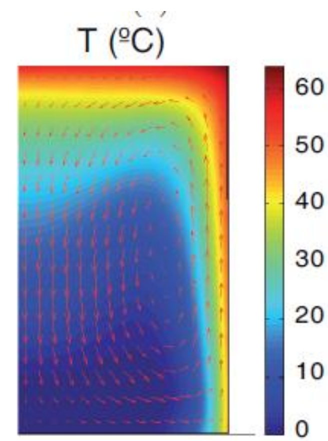


$$\nabla \vec{u} = 0.$$

$$\frac{\partial T}{\partial t} = \alpha \triangle T - \vec{u}\nabla T,$$

$$\rho\frac{\partial u}{\partial t} = \mu\triangle u - \rho\vec{u}\nabla u - \nabla P,$$
$$\rho\frac{\partial v}{\partial t} = \mu\triangle v - \rho\vec{u}\nabla v - \nabla P + \rho g\beta(T - T_0),$$

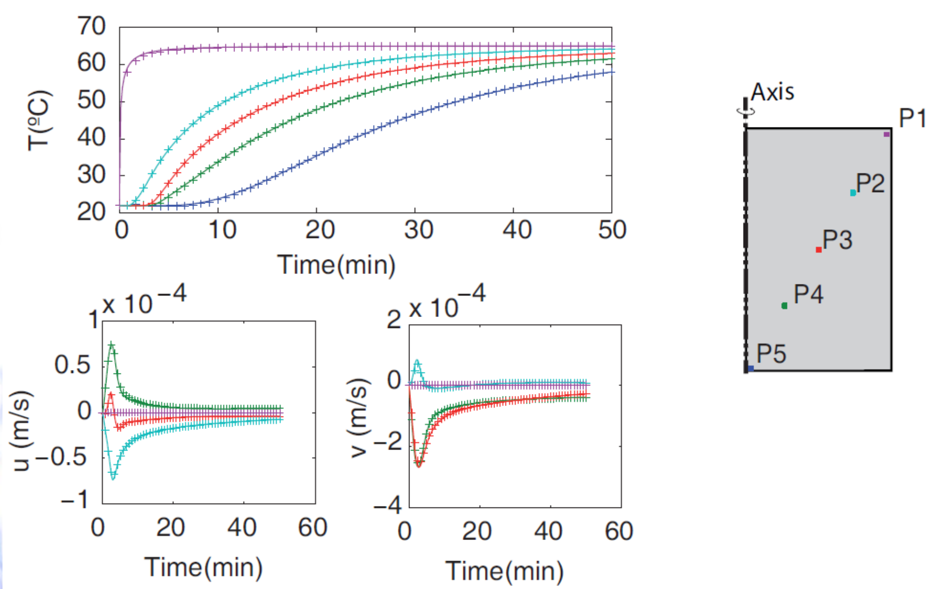
$$\frac{dP^m}{dt} = 10^{\frac{\bar{T}(t)-T_{ref}}{z_{ref}}}$$



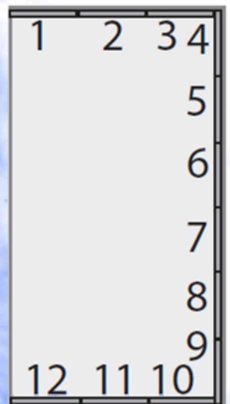
Problem I: Model simulation

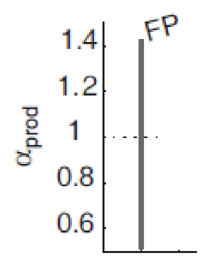
PE and OED with AMIGO linked to ROM obtained by POD

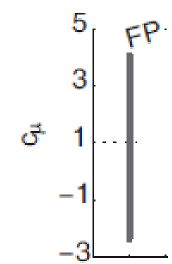
Simulation method	Number of ODEs	Mean error T [%]		Mean error $\|\vec{u}\|$ [%]		Simulation time [s]
		Exp 1	Exp 2	Exp 1	Exp 2	
FEM	2900	-	-	-	-	25
ROM	10	1.08	0.75	4.3	2.61	3.1
	20	0.7	0.46	2.7	1.9	3.5
	40	0.47	0.12	1.82	0.65	4.2
	100	0.47	0.08	1.58	0.53	6.5



Problem I: Sensor calibration

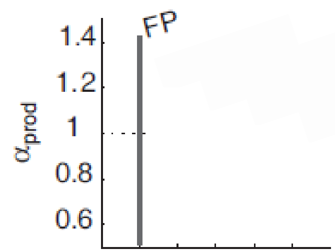


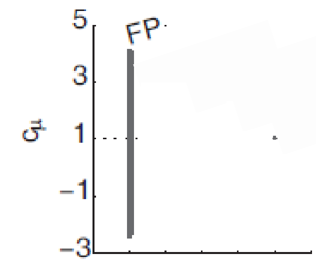




	h_{jar} $[\frac{W}{m^2K}]$	α_{prod} $[m^2/s]$	β [ ]	a_μ [ ]	b_μ [ ]	c_μ [ ]	mean CI	max CI
FP	0.92	0.97	1.33	0.84	0.94	0.87	251%	545%

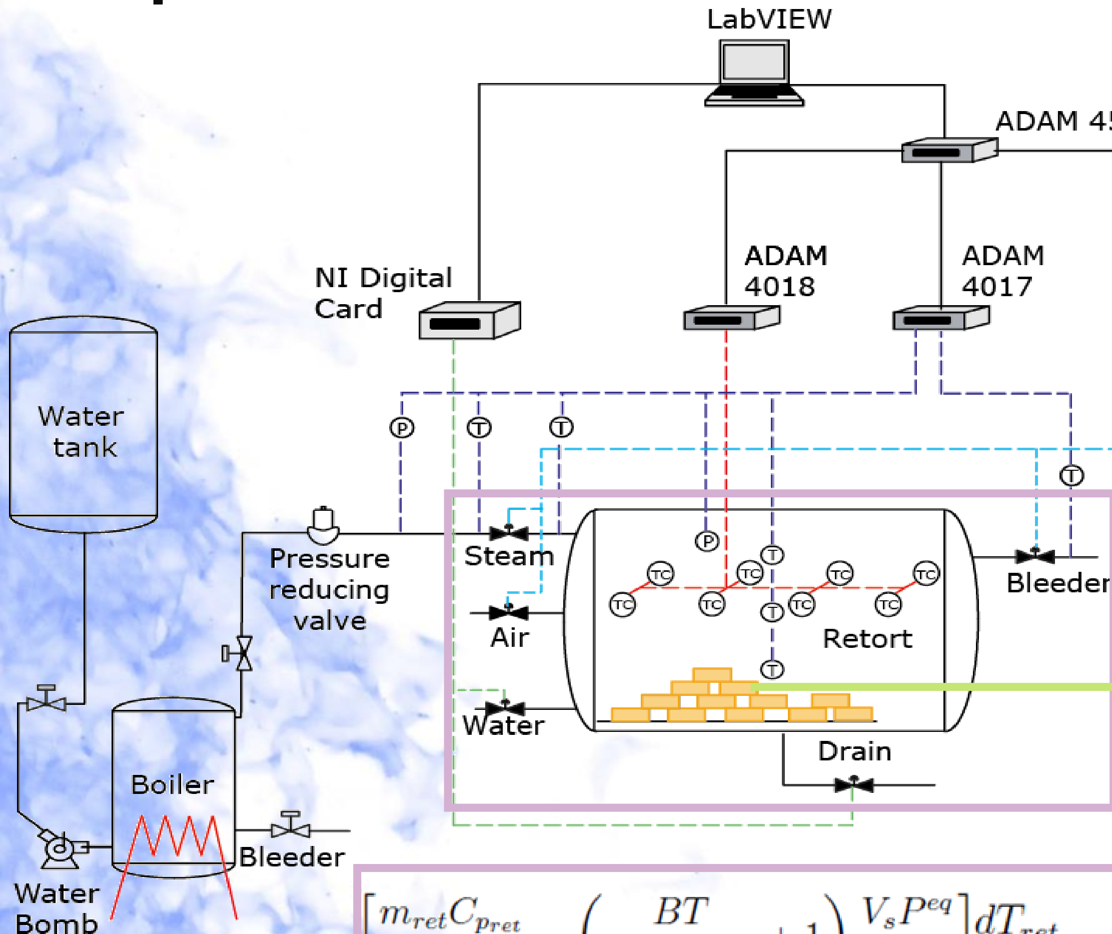
Problem I: Sensor calibration





	h_{jar} $[\frac{W}{m^2K}]$	α_{prod} $[m^2/s]$	β [ ]	a_μ [ ]	b_μ [ ]	c_μ [ ]	mean CI	max CI
FP	0.92	0.97	1.33	0.84	0.94	0.87	251%	545%
FP+1OD	1.02	0.88	2.74	1.19	0.81	1.20	94%	210%
FP+2OD	1.01	0.97	1.55	1.17	0.81	1.03	45%	104%
FP+3OD	1.01	0.98	1.47	0.96	0.85	1.07	12%	27%
FP+4OD	1.01	0.99	1.02	1.08	1.00	1.01	1%	2.3%

Example II: Retort sterilisation



$$\rho_{prod} c_{p_{prod}} \frac{\partial T}{\partial t} = \kappa_{prod} \nabla T$$

$$\frac{dlog(C_i)}{dt} = -\frac{1}{D_{i,ref}} 10^{\left(\frac{T_s - T_{i,ref}}{Z_{i,ref}}\right)}$$

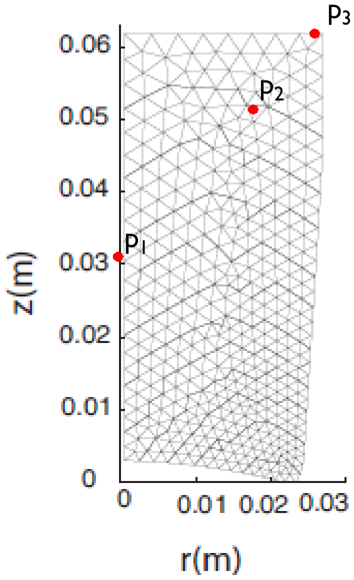
$$\left[\frac{m_{ret} C_{p_{ret}}}{\lambda} - \left(\frac{BT}{(T-C)^2} + 1\right) \frac{V_s P^{eq}}{R T_{ret}^2}\right] \frac{dT_{ret}}{dt} = F_s - F_b - \frac{Q_{rad} + Q_{conv}}{\lambda},$$

$$F_s = 3.4 \cdot 10^{-8} \delta_s(u_s) C_f P_{in} \sqrt{G_f} (w_s - 0.148 w_s^3); \quad w_s = \frac{1.63}{C_f} \sqrt{\frac{P_{in} - P_r}{P_{in}}},$$

$$F_b = 3.4 \cdot 10^{-8} \delta_b(u_b) C_f P_r \sqrt{G_f} (w_b - 0.148 w_b^3); \quad w_b = \frac{1.63}{C_f} \sqrt{\frac{P_r - P_e}{P_r}},$$

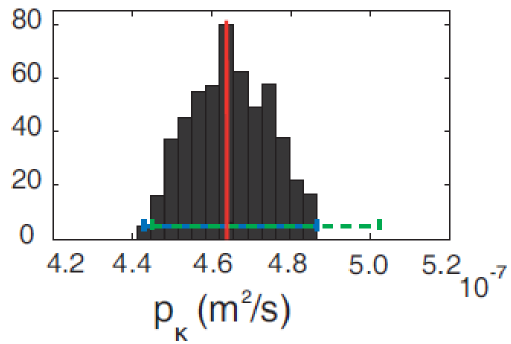
Problem II: Product model identification

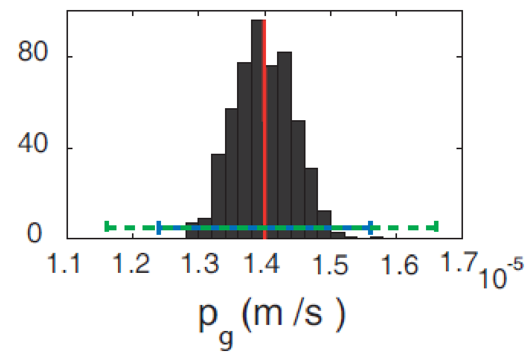
PE and OED with AMIGO linked to ROM obtained by POD



Thermo-physical properties of food product plus package heat transfer parameters

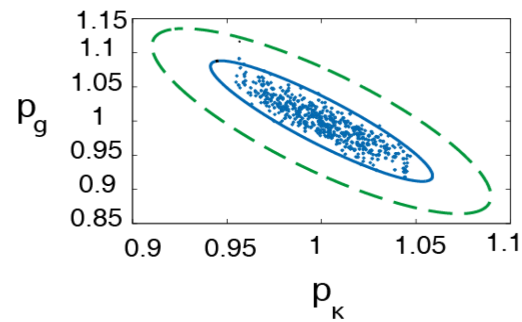
Problem II: Product model identification

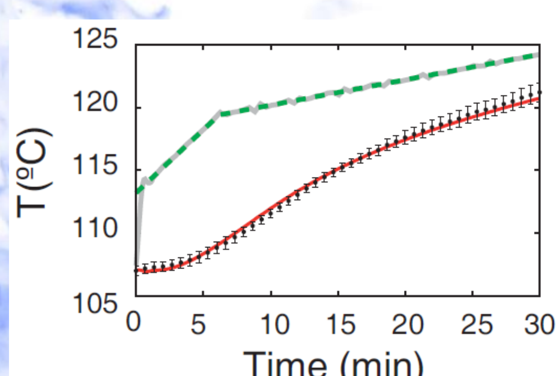


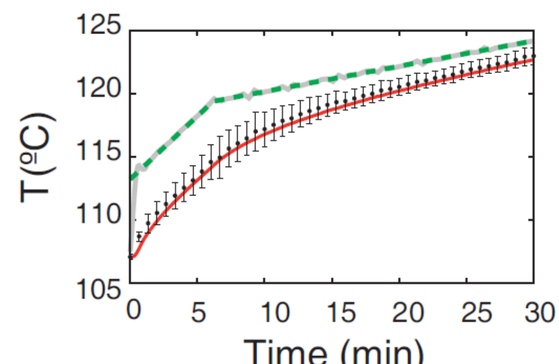


First 3 constant temperature experiments were carried out.

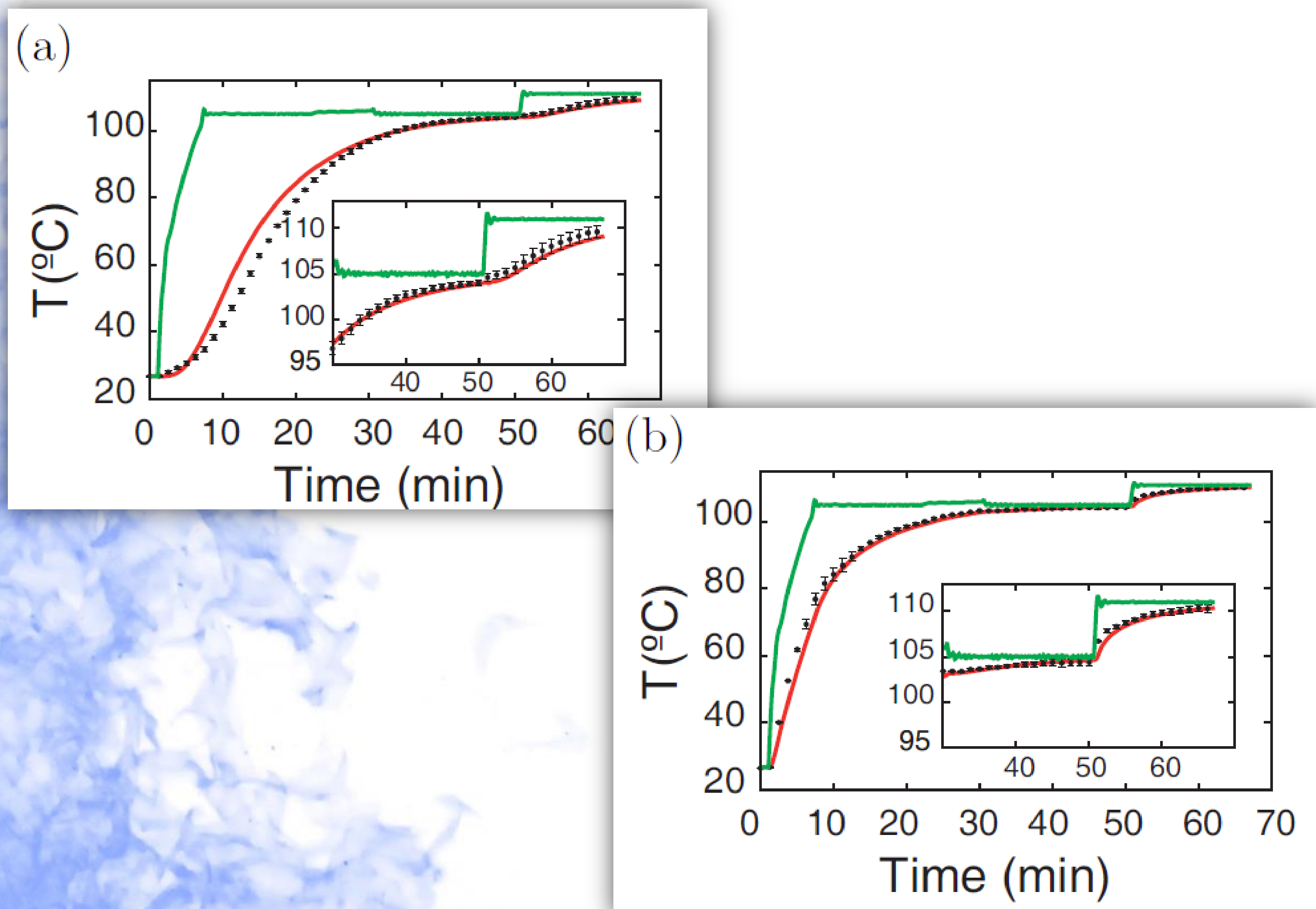
Optimally designed experiments







Problem II: Experimental validation in pilot plant



Conclusions

◈An iterative identification protocol for nonlinear dynamic models of food processes was presented and its performance evaluated with several examples.

◈The protocol is intended to iteratively improve predictive capabilities of models.

◈Key steps: Structural, practical identifiability analysis, parameter estimation and optimal experimental design.

◈ Key elements: Sensors + data

Reduced order model techniques

Global optimisation methods

Software: GenSSI + AMIGO

Acknowledgments

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Thank you !