Solution of Inverse Thermal Problem for Assessment of Thermal Parameters of Engineered H$_2$ Storage Materials

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Presented at the COMSOL Conference, Boston October 14$^{th}$, 2011
Fabrication and measurement

New materials for $H_2$ storage requires accurate estimation of thermal parameters.
Inverse problem

Find PDE parameters that match solution of forward problem

\[
\rho_{\text{sensor}} \cdot C_{\text{sensor}} \cdot d_{\text{sensor}} \cdot \frac{\partial T_{\text{sensor}}}{\partial t} + \nabla(-d_{\text{sensor}} \cdot k_{\text{sensor}} \cdot \nabla T_{\text{sensor}}) = d_{\text{sensor}} \cdot q + h \cdot (T_{\text{sample}} - T_{\text{sensor}})
\]

\[
\rho_{\text{sample}} \cdot C_{\text{sample}} \cdot \frac{\partial T_{\text{sample}}}{\partial t} + \nabla(-k_{\text{sample}} \cdot \nabla T_{\text{sample}}) = 0
\]

\[
- \mathbf{n} \cdot (-k_{\text{sample}} \cdot \nabla T_{\text{sample}}) = h \cdot (-T_{\text{sample}} + T_{\text{sensor}})
\]

7 seconds to solve on 4 processor computer

2560 hexahedral elements with exponentially changing density
Inverse problem as optimization task

Forward problem: Comsol; Backward problem: Matlab Global Optimization Toolbox

Objective = \((\text{Experiment}_{\text{axial}} - \text{Comsol}_{\text{axial}})^2 + (\text{Experiment}_{\text{radial}} - \text{Comsol}_{\text{radial}})^2\)

Matalb optimization routine \texttt{patternsearch} implements derivative free direct search algorithm

- Fast to converge to vicinity of minimum
- Does not require derivatives
- Very robust
- Allows for work with different norms
- Very slow in vicinity of minimum
- Very slow in the long shallow valleys

Kolda, Tamara G., Robert Michael Lewis, and Virginia Torczon.
Optimization by direct search: new perspectives on some classical and modern methods.
• Smoothed parameter dynamics allows for parametric reconstruction of objective function manifold for each parameter;
• The size of the leap step is computed from the smooth parametric reconstruction of error plot;
• The step is made for each parameter;
• The procedure is repeated until parameters stop changing.
• The length of direct search run is the algorithm adjustable parameter.
Optimization algorithm

Smooth local parametric representation of objective function manifold

Step n:
• run direct search for \( \ell \) steps; slow
• calculate smooth curve for each parameter as a function of step \( n \); fast
• run line search along the smooth parametrically represented line to find the minimum of objective function at the end of the line; fast
• Repeat at Step \( n+1 \)
Results

Thermal parameters for 3 new materials have been reconstructed using Comsol Matlab combination.

The first 0.2 [s] of experimental data have been discarded to keep complexity of the sensor model to minimum.