Model function approach in the modified L-curve method–case study: identification of heat transfer in pool boiling process

Yi Heng[1], Shuai Lu[2,⋆], Adel Mhamdi[1], Sergei V. Pereverzev[2]

Supported by the Austrian National Science Foundation, FWF Grant P20235-N18

[1] AVT-Process Systems Engineering, RWTH Aachen University, Germany
[2] Johann Radon Institute for Computational and Applied Mathematics, Austria

Workshop IP-TA 2010, Warsaw, February 9–12, 2010

Pool boiling process background

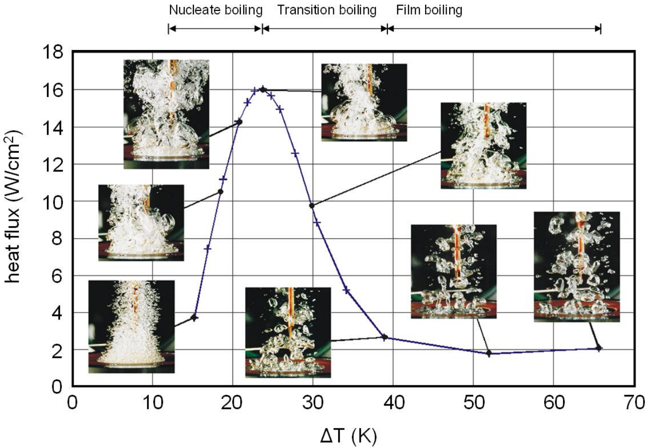


Figure: Analyze the properties of heat flux in pool boiling process.

Pool boiling process background

Pool boiling experiments

Figure: Left: Small number of sensors (Average information, TU Berlin);
Right: High resolution measurements (Local information, TU Darmstadt)

Pool boiling process background

Unmeasurable local heat flux on the boiling surface (up surface) = ?

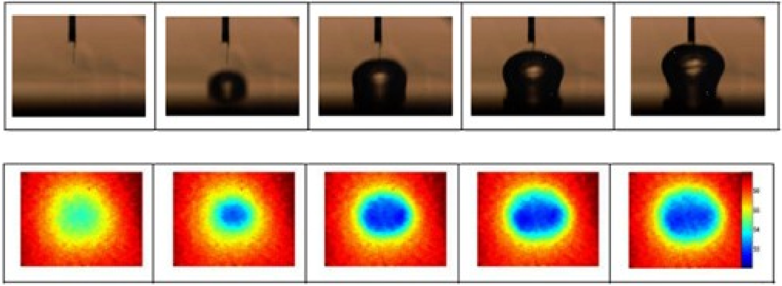


Figure: Up: Direct observation of bubble;
Down: Corresponding high-resolution temperature measurements (Lower boundary layer, TU Darmstadt)

Pool boiling process background

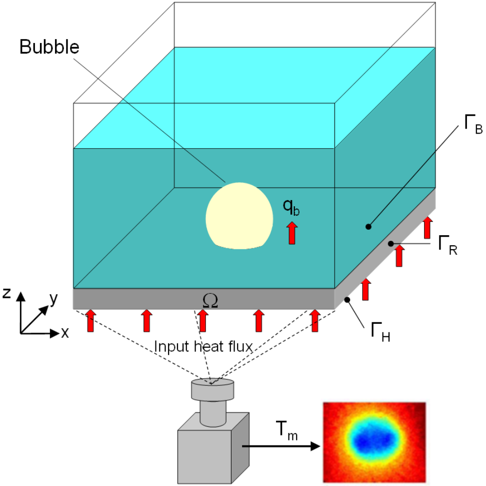


Figure: Schematic representation of a single-bubble nucleate boiling experiment

Linear ill-posed problem formulation

Original system

$$\mathbb{S} = \begin{cases} \frac{\partial T(\mathbf{x},t)}{\partial t} = a\Delta T(\mathbf{x},t), & (\mathbf{x},t) \in \Omega \times [0,t_f], \\ T(\mathbf{x},0) = T_0(\mathbf{x}), & \mathbf{x} \in \Omega, \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = q_h(\mathbf{x},t), & (\mathbf{x},t) \in \Gamma_H \times [0,t_f] \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = q_b(\mathbf{x},t), & (\mathbf{x},t) \in \Gamma_B \times [0,t_f] \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = 0, & (\mathbf{x},t) \in \Gamma_R \times [0,t_f]. \end{cases}$$

The system $\mathbb{S}$ provides a direct operator: $\mathbb{S}$ maps $(T_0,\, q_h,\, q_b) \rightarrow T_m$.

Linear ill-posed problem formulation

The original system $\mathbb{S}$ can be reformulated into two system

$$\mathbb{S}1 = \begin{cases} \frac{\partial T(\mathbf{x},t)}{\partial t} = a\Delta T(\mathbf{x},t), & (\mathbf{x},t) \in \Omega \times [0,t_f], \\ T(\mathbf{x},0) = T_0(\mathbf{x}), & \mathbf{x} \in \Omega, \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = q_h(\mathbf{x},t), & (\mathbf{x},t) \in \Gamma_H \times [0,t_f], \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = 0, & (\mathbf{x},t) \in \Gamma_B \times [0,t_f], \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = 0, & (\mathbf{x},t) \in \Gamma_R \times [0,t_f], \end{cases}$$

and

$$\mathbb{S}2 = \begin{cases} \frac{\partial T(\mathbf{x},t)}{\partial t} = a\Delta T(\mathbf{x},t), & (\mathbf{x},t) \in \Omega \times [0,t_f], \\ T(\mathbf{x},0) = 0, & \mathbf{x} \in \Omega, \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = 0, & (\mathbf{x},t) \in \Gamma_H \times [0,t_f], \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = q_b(\mathbf{x},t), & (\mathbf{x},t) \in \Gamma_B \times [0,t_f], \\ -\lambda \frac{\partial T(\mathbf{x},t)}{\partial n} = 0, & (\mathbf{x},t) \in \Gamma_R \times [0,t_f]. \end{cases}$$

Linear ill-posed problem formulation

Define the linear operator $\mathbb{S}2 = A$ (denote as A for simplicity), we can write the exact operator equation as

$$Aq_b(\mathbf{x},t) = T2_m(\mathbf{x},t) = T_m(\mathbf{x},t) - T1_m(\mathbf{x},t).$$

T_m is the data from system $\mathbb{S}$ and $T1_m$ is the data from $\mathbb{S}1$. So the linear ill-posed problem that we need to handle will be

$$Aq_b(\mathbf{x},t) = T2_m^{\delta}(\mathbf{x},t) = T_m^{\delta}(\mathbf{x},t) - T1_m(\mathbf{x},t).$$

Problem set-up

1. X, Y are real infinite-dimensional Hilbert spaces;
2. $A : X \to Y$, $Range(A) \neq \overline{Range(A)}$;
3. $x_0, y_0 : Ax_0 = y_0$;
4. $y_\delta : \|y_0 - y_\delta\|_Y \leq \delta$, δ is unknown.

Ill-posed operator equation

$$Ax = y_\delta.$$

Regularization and parameter choice rules

Tikhonov regularization

$$\min J(\alpha, x), \quad J(\alpha, x) := \|Ax - y_\delta\|^2 + \alpha \|x\|^2.$$

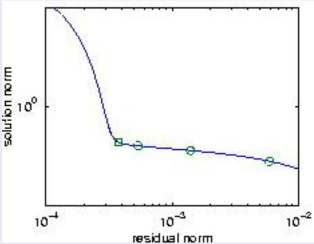
Parameter choice rules

- *a priori* parameter choice
- *a posteriori* parameter choice
  - δ-dependent criteriae: discrepancy principle, monotone error rule, balancing principle;
  - δ-independent criteriae: quasi-optimality, GCV, L-curve, Hanke-Raus rule, modified L-curve.

L-curve and modified L-curve method

L-curve [Hansen and O'Leary 1993]

Let $x(\alpha) = \arg\min J(\alpha, x)$. Plot $\|x(\alpha)\|$ versus $\|Ax(\alpha) - y_\delta\|$ in a log-log scale for a large range of α values. The choice of a regularization parameter is focused on the corner, where the vertical line turns to be a horizontal one.



L-curve and modified L-curve method

Modified L-curve [Regińska 1996]

If the curvature of the L-curve is maximized at $\alpha = \alpha^*$, and if the tangent value of the L-curve at $\left(\log \|Ax(\alpha^*) - y_\delta\|^2, \log \|x(\alpha^*)\|^2\right)$ has a slope $-1/\mu$, then the function

$$\Psi_\mu(\alpha) = \|Ax(\alpha) - y_\delta\|^2 \|x(\alpha)\|^{2\mu}, \qquad \mu > 0$$

has a minimum value at the same point $\alpha = \alpha^*$.

Preliminary results: model function approach

We define a function $J(\alpha)$ with respect to α such that

$$J(\alpha) := \|Ax(\alpha) - y_\delta\|^2 + \alpha\|x(\alpha)\|^2 = \|y_\delta\|^2 - \|Ax(\alpha)\|^2 - \alpha\|x(\alpha)\|^2.$$

Lemma (Kunisch and Zou 1998)

The first derivative of $J(\alpha)$ with respect to α is given by

$$J'(\alpha) = \|x(\alpha)\|^2.$$

Preliminary results: model function approach

For a fixed α, we locally approximate the term $\|Ax(\alpha)\|^2$ by $T\|x(\alpha)\|^2$, where T is a positive constant to be determined. It gives us

$$J(\alpha) + \alpha J'(\alpha) + TJ'(\alpha) \approx \|y_\delta\|^2.$$

By a model function we mean a function $m(\alpha)$, for which this formula is exact, that is, $m(\alpha)$ should solve differential equation

$$m(\alpha) + (\alpha + T)m'(\alpha) = \|y_\delta\|^2.$$

Preliminary results: model function approach

Model functions

A simple parametric family of the solutions is given as

$$m(\alpha) = \|y_\delta\|^2 + \frac{C}{\alpha + T}.$$

where C, T are constants to be determined.

Residual and solution norms

The first derivative of the model function $m(\alpha)$ can be used to approximate the first derivative of $J(\alpha)$, i.e.,

$$J'(\alpha) = \|x(\alpha)\|^2 = m'(\alpha) = -\frac{C}{(\alpha + T)^2}.$$

The approximated residual norm $\|Ax(\alpha) - y_\delta\|^2$ can also be given in terms of the model function $m(\alpha)$ as

$$\|Ax(\alpha) - y_\delta\|^2 \approx m(\alpha) - \alpha m'(\alpha).$$

Preliminary results: modified L-curve

Modified L-curve

In the modified L-curve method, the original function Ψ_μ is defined as

$$\Psi_\mu(\alpha) = \|Ax(\alpha) - y_\delta\|^2 \|x(\alpha)\|^{2\mu}.$$

Model function approach

By introducing a model function $m(\alpha)$, Ψ_μ can be (locally) approximated by the function $\Psi_{C,T,\mu}$ as

$$\begin{aligned}\Psi_\mu(\alpha) \approx \Psi_{C,T,\mu}(\alpha) \quad &:= \quad (m(\alpha) - \alpha m'(\alpha))(m'(\alpha))^\mu \\ &= \quad \left(\|y_\delta\|^2 + \frac{C}{\alpha + T} + \frac{\alpha C}{(\alpha + T)^2}\right)\left(\frac{-C}{(\alpha + T)^2}\right)^\mu.\end{aligned}$$

Preliminary results: modified L-curve

Constants C and T

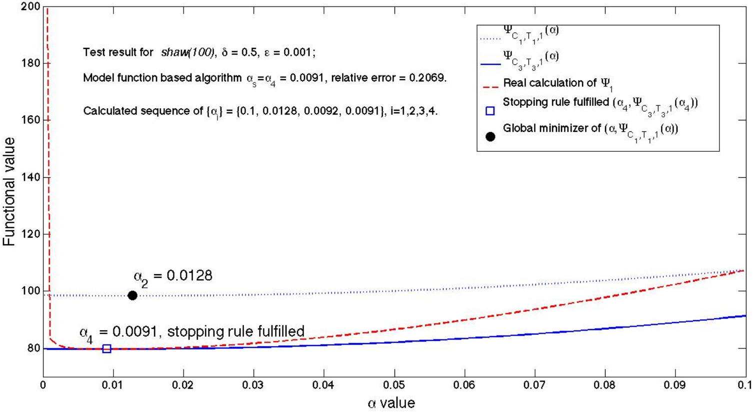
In the vicinity of any $\alpha = \alpha_k$ the constants can be easily calculated using the knowledge of residual norm and regularized solution norm, i.e.,

$$\begin{cases} m(\alpha_k) = \|y_\delta\|^2 + \frac{C_k}{\alpha_k + T_k} = J(\alpha_k) = \|Ax(\alpha_k) - y_\delta\|^2 + \alpha\|x(\alpha_k)\|^2; \\ m'(\alpha_k) = -\frac{C_k}{(\alpha_k + T_k)^2} = J'(\alpha_k) = \|x(\alpha_k)\|^2; \end{cases}$$

or more precisely,

$$C_k = -\frac{(\|Ax(\alpha_k)\|^2 + \alpha_k\|x(\alpha_k)\|^2)^2}{\|x(\alpha_k)\|^2}, \qquad T_k = \frac{\|Ax(\alpha_k)\|^2}{\|x(\alpha_k)\|^2}.$$

Performance of the Basic Algorithm



Basic Algorithm

Algorithm 1: Model function approach in modified L-curve

Input: $\varepsilon > 0$, y_δ, A, $\mu > 0$.

1: Choose initial guess $\alpha_1 > \alpha_*$, and set $k = 1$.

2: **Do**

3: Solve $(A^T A + \alpha_k I)x = A^T y_\delta$ to find $x = x(\alpha_k)$

4: Update C_k and T_k, construct the corresponding model function

$$m_k(\alpha) = \|y_\delta\|^2 + \frac{C_k}{\alpha + T_k}.$$

5: Insert $m_k(\alpha)$ into modified L-curve, update α_{k+1} as the minimizer of $\Psi_{C_k,T_k,\mu}(\alpha)$, set $k := k+1$ (this step is equivalent to solving a quadratic equation).

6: **While** $\left|\frac{\alpha_{k+1}-\alpha_k}{\alpha_k}\right| \leq \varepsilon$.

7: If the stopping rule is fulfilled return x, α_k as the regularized solution x_S and α_S.

Numerical examples

We compare the model function approach in the modified L-curve method (Algorithm 1) with the original L-curve method. The L-curve method will be performed with the use of the *Regularization toolbox* and its updated large-scale descendant *Moore tools*.

We consider the conjugate gradient least square (CGLS) method in later computation to solve some linear systems appearing in the Tikhonov regularization.

Numerical examples

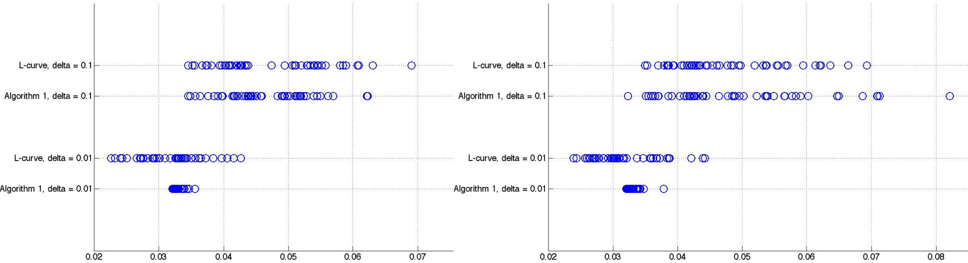


Figure: ($Shaw(1000)$ with noisy data simulated 50 times) In each picture, the first two lines from above correspond to the noise level $\delta = 0.1$ while the other two lines are for $\delta = 0.01$. Each circle in the figures indicates the relative error for one reconstruction by means of L-curve method or by the Algorithm 1 (with $\mu = 1$ on the left picture, and $\mu = 1/2$ on the right picture).

Numerical examples

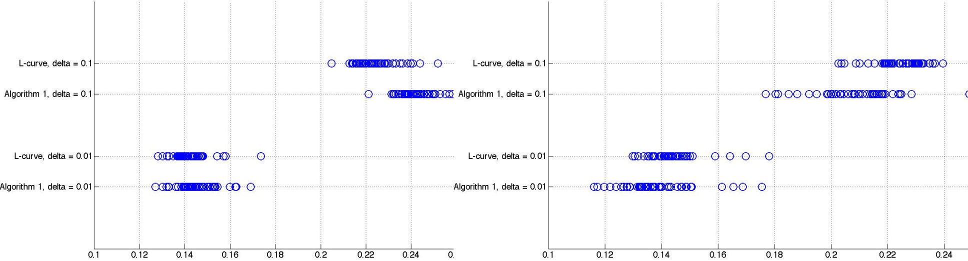


Figure: ($baart(1000)$ with noisy data simulated 50 times) In each picture, the first two lines from above correspond to the noise level $\delta = 0.1$ while the other two lines are for $\delta = 0.01$. Each circle in the figures indicates the relative error for one reconstruction by means of L-curve method or by the Algorithm 1 (with $\mu = 1$ on the left picture, and $\mu = 1/2$ on the right picture).

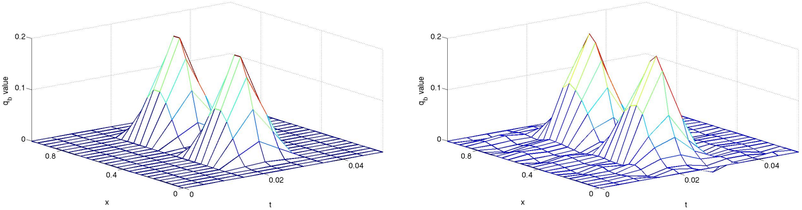
Numerical examples

Table: Comparison of the Algorithm 1 with the L-curve method in terms of the amount of computations. (Average data over 50 tests; Comp Time means the computational time, units in seconds)

	Noise Level	A1 Iteration	A1 Comp Time	L-curve Comp Time
$Shaw(1000)$				
$\mu = 1$	$\delta = 0.1$	3	2.1656	27.2446
	$\delta = 0.01$	4	2.6524	26.6567
$\mu = 1/2$	$\delta = 0.1$	3	2.2133	27.9781
	$\delta = 0.01$	4	2.6663	26.9823
$Baart(1000)$				
$\mu = 1$	$\delta = 0.1$	3	1.9712	29.3494
	$\delta = 0.01$	4	2.3736	28.0244
$\mu = 1/2$	$\delta = 0.1$	3	1.9368	28.5860
	$\delta = 0.01$	3.16	1.9980	28.3343

Case study: academic example

$q_b(x,t) = q^1(t)q^2(x)$ where $q^1(t) = 0.1\sin(100\pi(t-0.02)) + 0.1$ for $t \in [0.015, 0.035]$, zero elsewhere, and $q^2(x) = 0.5\sin(5\pi(0.3 - |x-0.5|)) + 0.5$ for $|x-0.5| \le 0.4$, zero elsewhere. Space discretization level is 25 and time discretization level is 10.



Case study: real data

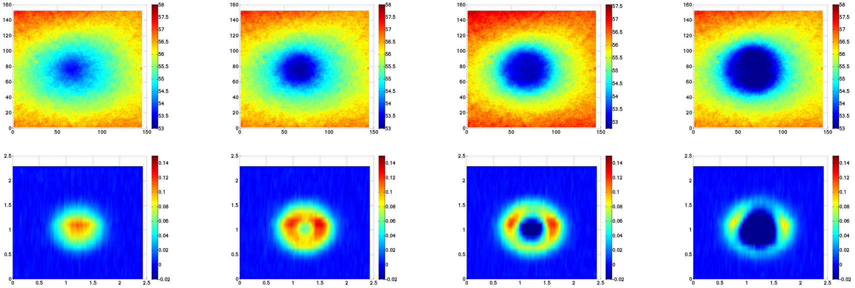


Figure: Upper: Measured temperature field on the heating boundary of the layer, Frame 24–27; Lower: Reconstructed surface boiling heat flux, Frame 24–27.

References

Hansen P. C. and O'Leary D. P. (1993)
The use of the L-curve in the regularization of discrete ill-posed problems
SIAM J. Sci. Comput. 14, 1487-1503

Regińska T. (1996)
A regularization parameter in discrete ill-posed problems
SIAM J. Sci. Comput. 17, 740-749

Hansen P. C.
Moore tools
http://www2.imm.dtu.dk/∼pch/

Ito K. and Kunisch K. (1992)
On the choice of the regularization parameter in nonlinear inverse problems
SIAM J. Optim. 2, 376-404

References

- Kunisch K. and Zou J. (1998)
  Iterative choices of regularization parameters in linear inverse problems
  Inverse Problems 14, 1247-1264

- LS, Pereverzev S. V. and Tautenhahn U. (2008)
  Dual regularized total least squares and multi-parameter regularization
  Comput. Meth. Appl. Math. 8, 253-263

- Heng Y., LS, Mhamdi A. and Pereverzev S. V. (2009)
  Model function approach in the modified L-curve method for the choice of the regularization parameter
  RICAM report 2009-08, submitted

- LS and Mathe P. (2009)
  Heuristic parameter selection based on functional minimization: Optimality and model function approach
  WIAS report 1413, submitted

Thank you for your attention!