Constrained Regularization for Lagrangian Actinometry

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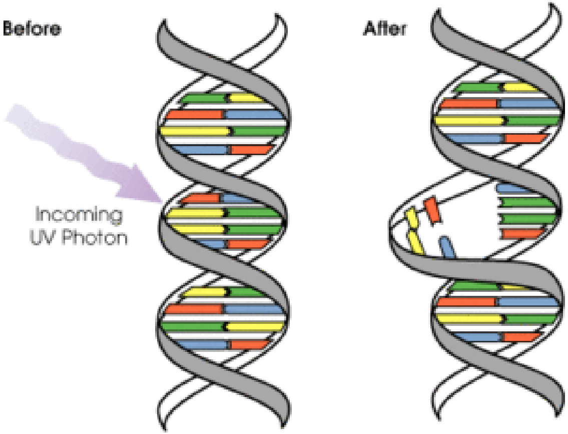
September 21, 2010

UV Irradiation and Disinfection: UV Reactors

http://water-techology.net/projects/sharjah

UV Irradiation and Disinfection



http://em.wikipedia.org/wiki/Pyrimidine_dimers

UV Dose: Master Variable (Lagrangian = Particle Specific)

Integral

$$\text{Dose} = \int_0^t I(t) \cdot dt$$

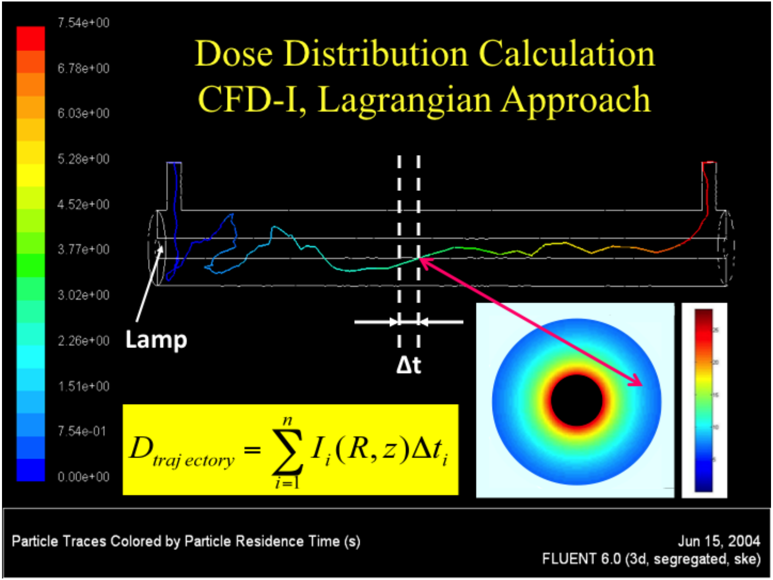
Discrete

$$\text{Dose} \approx \sum_{j=1}^{n} I_j(R, z) \cdot \Delta t_j$$

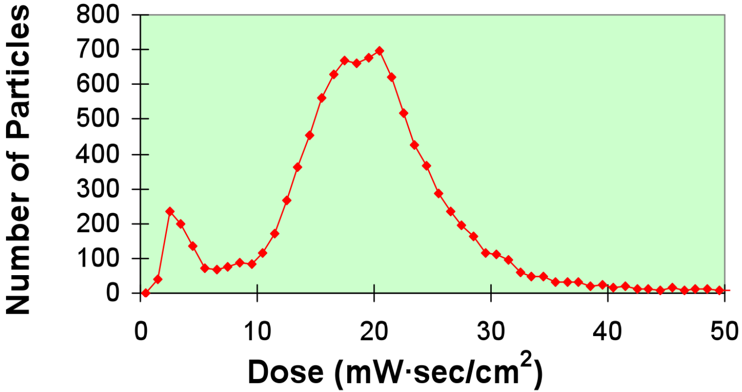
- Exposure Time
- Intensity Field
- Intensity History
- Particle Trajectory

UV Dose Distributions: CFD-I Models

- Chiu, *et al.* [1] (Particle Tracking)
- Lyn and Blatchley [2] (CFD models for UV disinfection)
- J. Ducoste *et al.* [3] (Lagrangian vs. Eulerian)

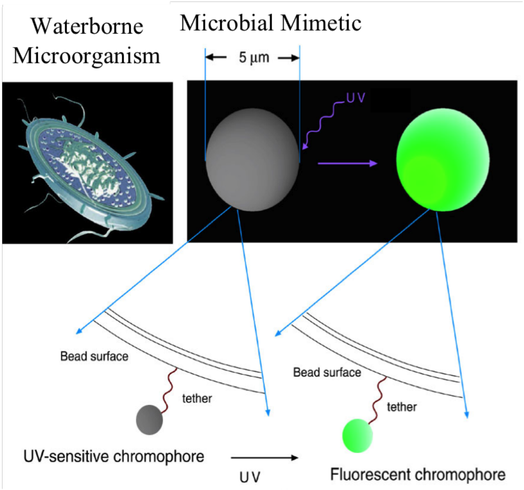


Dose Distribution (Chiu *et al.* 1999 [1])

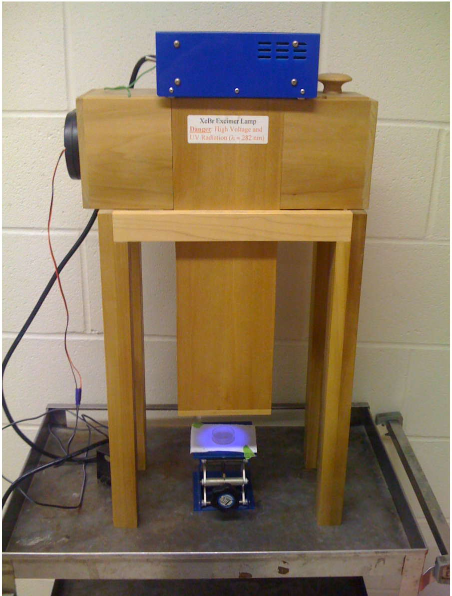


Lagrangian Actinometry (LA): Dyed Microspheres

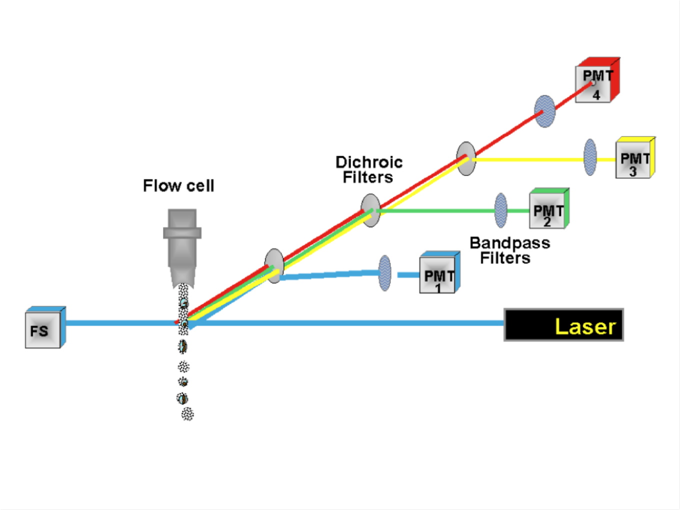
- Blatchley *et al.* [4]



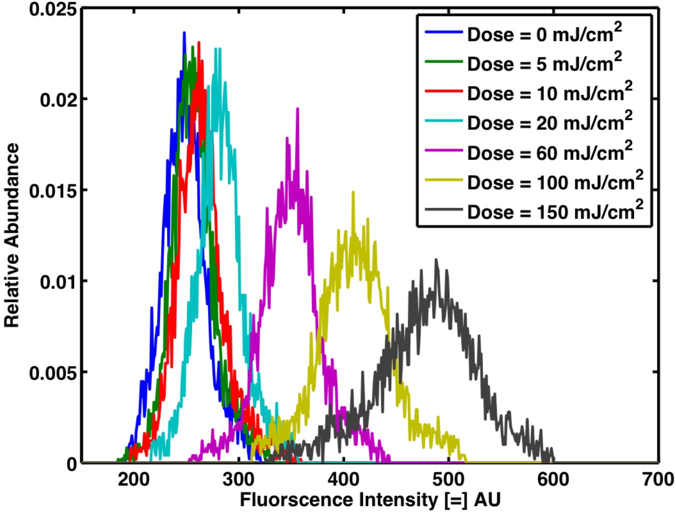
Lagrangian Actinometry (LA): Dose-Response Calibration



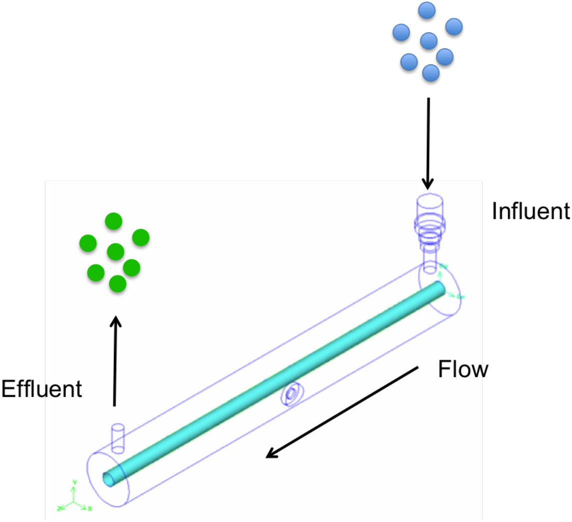
Lagrangian Actinometry (LA): Flow Cytometry [5]



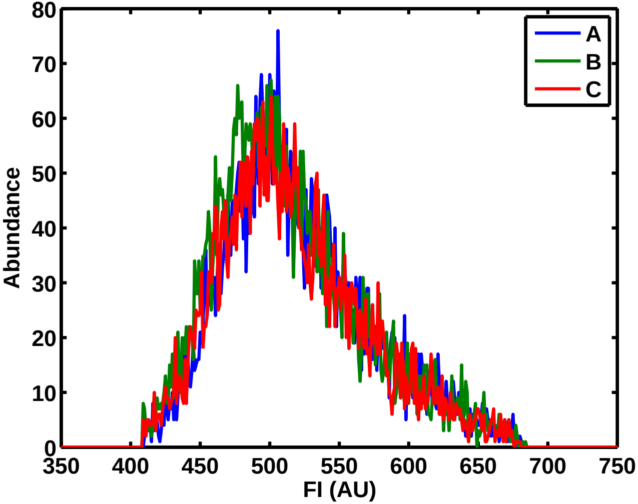
Lagrangian Actinometry (LA): Dose-Response Calibration



Lagrangian Actinometry (LA): UV Reactor Experiment



Lagrangian Actinometry (LA): UV Reactor FI Distributions

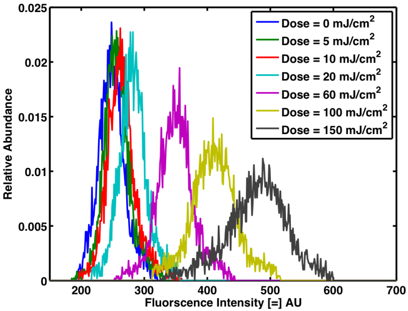


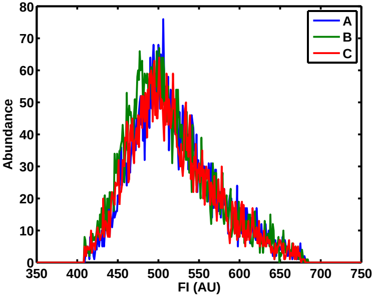
Lagrangian Actinometry (LA): Linear Equations

Linear Combination [4]

$$k_{i1}x_1 + k_{i2}x_2 + \cdots + k_{in}x_n = y_i \tag{1}$$

with, $i = 1, 2, \cdots, m$, FI channels. UV dose $j = 1, 2, \cdots, n$



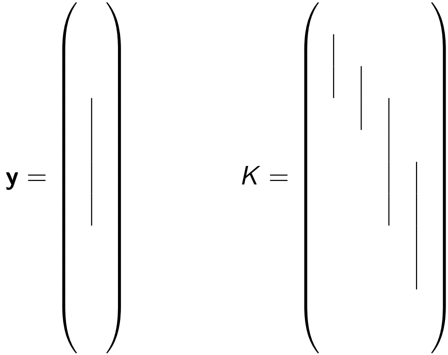


Lagrangian Actinometry: Linear Equations

Linear Least-Squares Problem (linear model)

$$\mathbf{y} = K\mathbf{x} + \epsilon \tag{2}$$

with $\mathbf{y} \in \mathbb{R}^m$, measured reactor FI distribution, $K \in \mathbb{R}^{m \times n}$, dose-response calibration matrix, $\mathbf{x} \in \mathbb{R}^n$ dose distribution, $\epsilon \sim N(0, S^2)$ vector of measurement errors.



Historical Method

Regularization Method

Truncated SVD

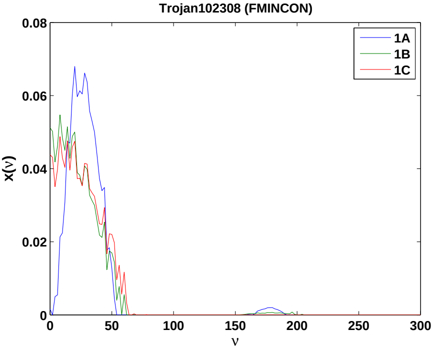
Constrained Regularization

Application to Large-scale UV reactors

Constrained Minimization Method (FMINCON)

Constrained Minimization Problem (FMINCON)

$$\min_{\mathbf{x}} \varphi(\mathbf{x}) = \|\mathbf{y} - K\mathbf{x}\|_2^2 \quad \text{subject to} \begin{cases} B\mathbf{x} = \mathbf{d} \rightarrow \sum_i x_i = 1 \\ 0 \leq \mathbf{x} \leq 1 \end{cases} \tag{3}$$



- **As of 2006, This Summarizes the Extent of Knowledge on Numerical Methods for LA.**

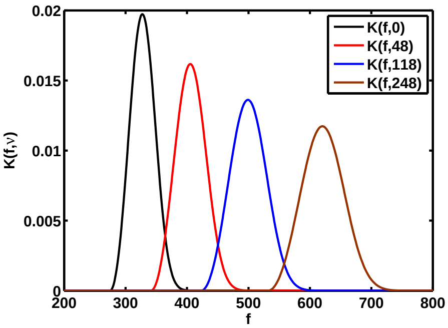
Constrained Minimization Test Problem

Objective: Determine if Solution is Stable Under Small Perturbations to $\mathbf{y}_{tr} = K\mathbf{x}^*$

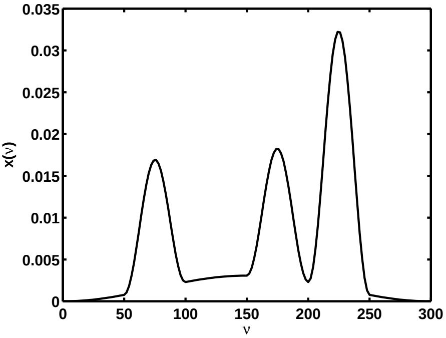
Definitions

- $\mathbf{y}_{tr} = K\mathbf{x}^*$, with $\mathbf{x}^*$ is a "true solution"
- $\mathbf{y} = K\mathbf{x}^* + \epsilon$, with ϵ being the perturbation to $\mathbf{y}_{tr}$

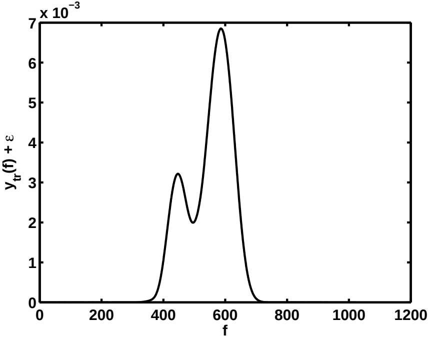
K matrix



$\mathbf{x}^*$ "true solution"



Constrained Minimization Test Problem: Right-Hand Side



Data Generation

$$\mathbf{y} = K\mathbf{x}^* + \epsilon \tag{4}$$

$$\epsilon \sim N(0, S^2) \tag{5}$$

with, $S^2 = \mathrm{diag}(s_1^2, s_2^2, \cdots, s_m^2)$

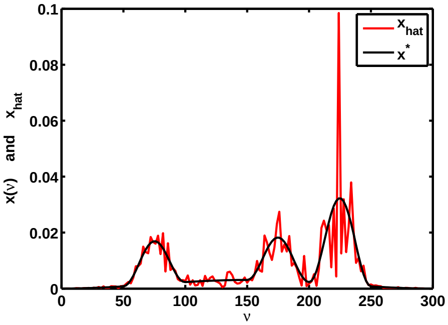
$$s_i = 10^{-5}\sqrt{y_{tr,i}} \tag{6}$$

Scaled Solutions

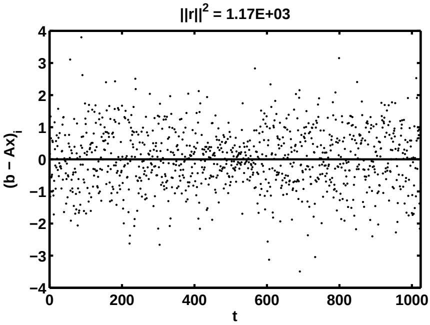
Constrained Weighted Least-Squares

$$\min_{\mathbf{x} \geq 0} \varphi = \|S^{-1}(\mathbf{y} - K\mathbf{x})\|_2^2, \qquad \mathbf{w}^T\mathbf{x} = 1 \tag{7}$$

Computed Solution, $\hat{\mathbf{x}}$



Residuals



Singular Value Decomposition (SVD) Characteristics

Characteristics of Ill-Posed Problems (SVD) [10], [11]

1. The right singular vectors $\mathbf{v}_j$ become more oscillatory as j increases.
2. The singular values σ_j of A gradually decay to zero without a noticeable gap.
3. The discrete Picard condition occurs.

- For problems with SVD characteristics above, truncated SVD is effective

Singular Value Decomposition: SVD

SVD

$$A = U\hat{\Sigma}V^T \tag{8}$$

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T, \quad \Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n) \tag{9}$$

$A \in \mathbb{R}^{m\times n}$, $U \in \mathbb{R}^{m\times m}$, $\Sigma \in \mathbb{R}^{m\times n}$, and $V \in \mathbb{R}^{n\times n}$.

SVD Properties

- $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$, and
- $$U^TU = I_m = UU^T, \quad V^TV = I_n = VV^T \tag{10}$$

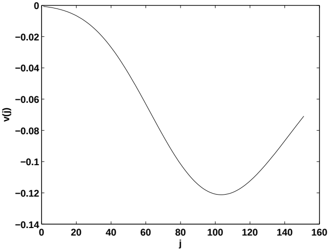
SVD Least-Squares Solution

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2^2 = \min_{\mathbf{x}\in\mathbb{R}^n} \left\| \begin{pmatrix} U_1^T \\ U_2^T \end{pmatrix} \mathbf{b} - \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T\mathbf{x} \right\|_2^2, \tag{11}$$

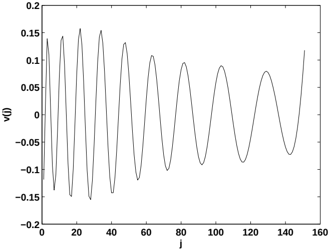
Note: $U_1 \in \mathbb{R}^{n\times m}$, $U_2 \in \mathbb{R}^{m-n\times m}$.

$$V^T\hat{\mathbf{x}} = \Sigma^{-1}U_1^T\mathbf{b}, \quad \therefore \hat{\mathbf{x}} = V\mathbf{z} \tag{12}$$

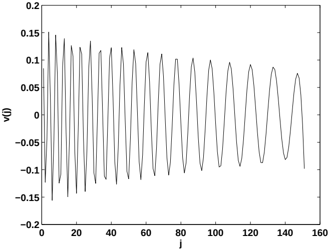
Right Singular Vectors, V



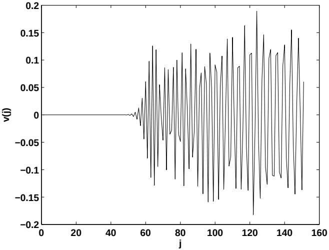
(a) $\mathbf{v}_1$



(b) $\mathbf{v}_{20}$

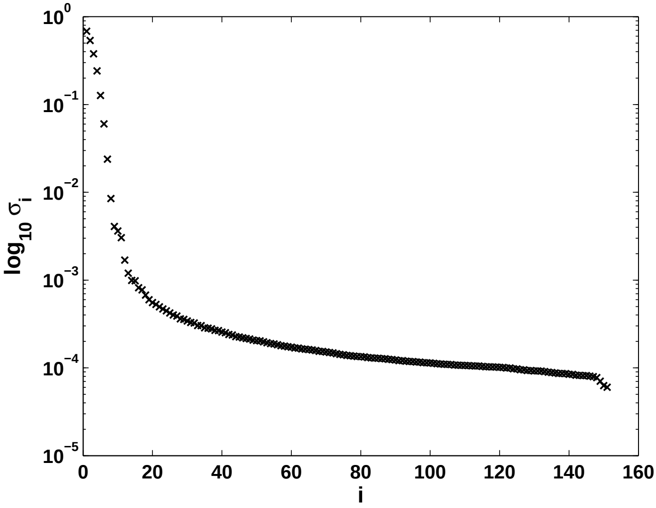


(c) $\mathbf{v}_{40}$

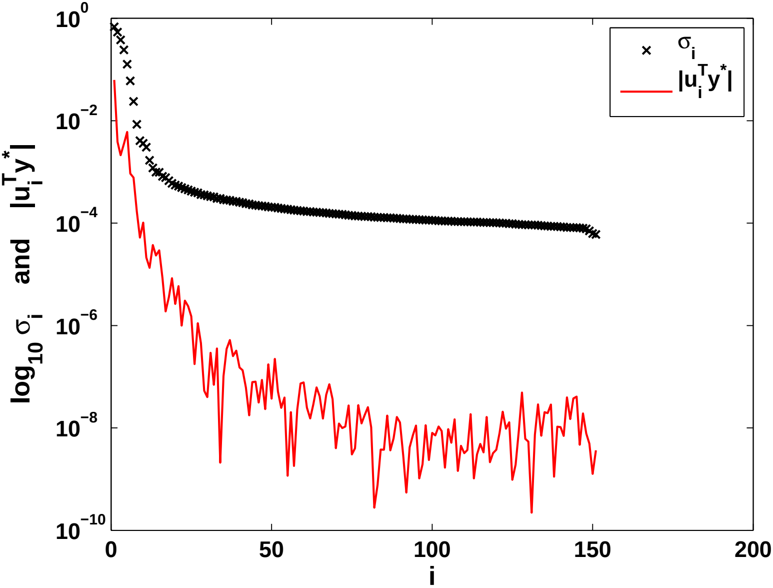


(d) $\mathbf{v}_{120}$

Singular Values, σ_j



The Discrete Picard Condition



Truncated Solution $V^T\mathbf{x} = \mathbf{z}$ (Rust and O'Leary, [8], [9])

SVD Least-Squares Solution

From SVD solution,

$$V^T\hat{\mathbf{x}} = \Sigma^{-1}U_1^T\mathbf{b}, \quad \therefore \hat{\mathbf{x}} = V\mathbf{z} \tag{13}$$

Truncated SVD Equation

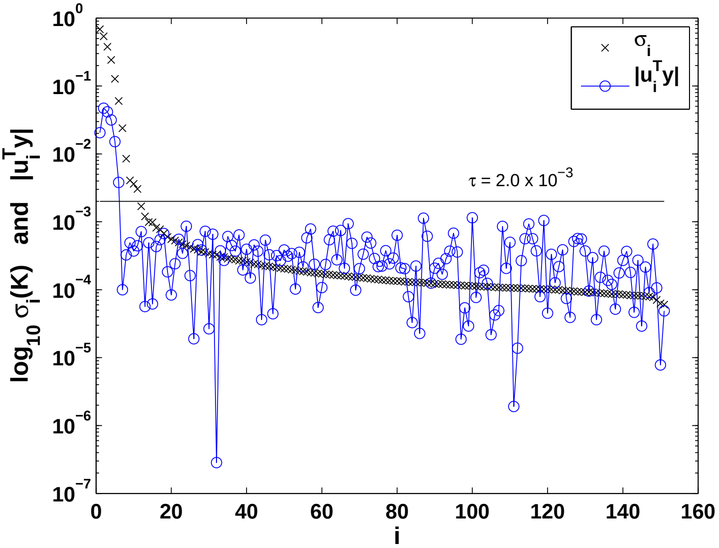
$$(V^T\tilde{\mathbf{x}})_i = \begin{cases} \frac{(\mathbf{u}_i^T\mathbf{b})}{\sigma_i}, & \text{if} \quad |\mathbf{u}_i^T\mathbf{b}| > \tau \\ 0, & \text{otherwise,} \end{cases} \tag{14}$$

$i = 1, 2, \ldots, n$

Truncated SVD Solution

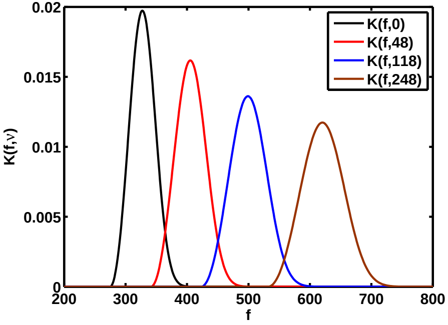
$$V^T\tilde{\mathbf{x}} = \Sigma^{-1}\widetilde{U_1}^T\mathbf{b} \tag{15}$$

Truncating $|U^T \mathbf{b}|$

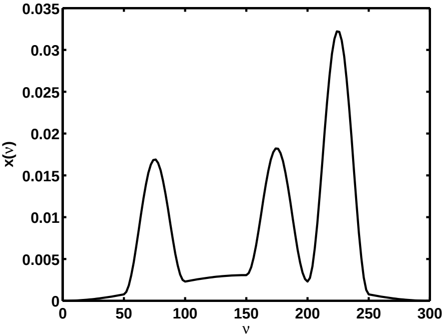


TSVD for Test Problem

K matrix

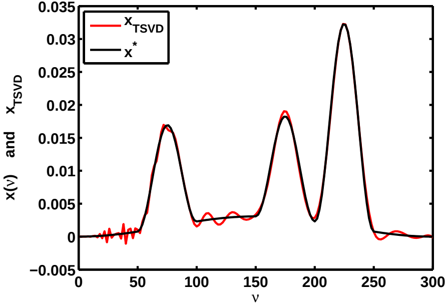


$\mathbf{x}^*$ "true solution"

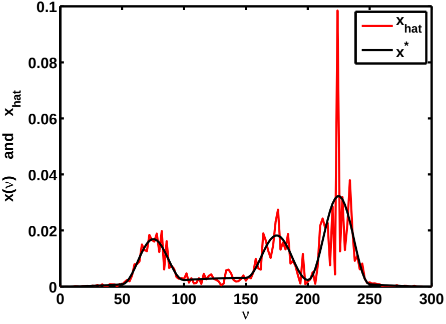


Truncated SVD vs Constrained Minimization (FMINCON) solutions

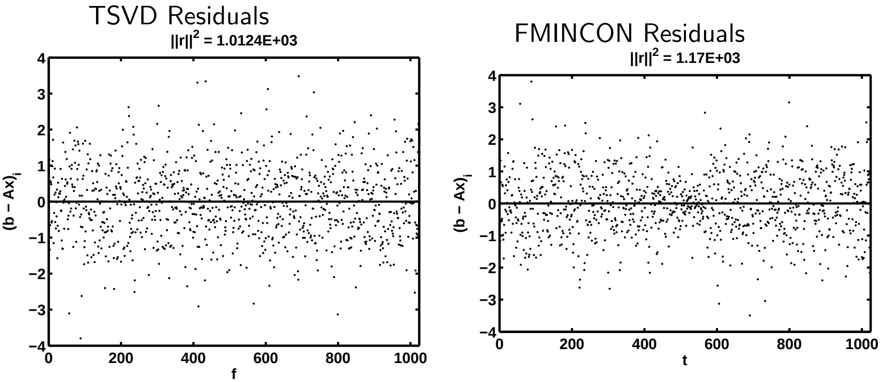
TSVD solution



FMINCON Solution

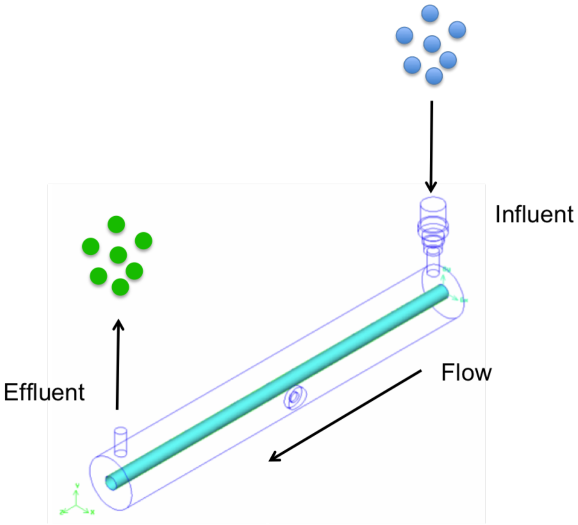


Residual Comparison for truncated SVD and FMINCON Solns.



Recall: $m = 1024$, $\|\mathbf{b} - A\hat{\mathbf{x}}\|_2^2 \in [978.7, 1069.2]$

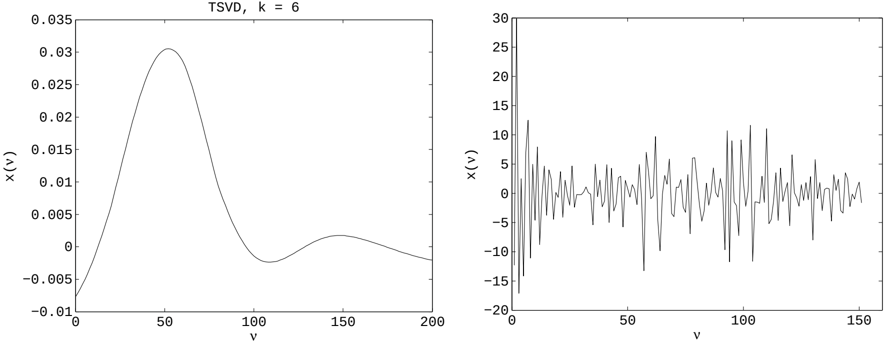
Reactor Data



TSVD vs Full SVD Solution: UV Reactor Data

SVD Least-Squares Solution

$$V^T \hat{\mathbf{x}} = \Sigma^{-1} U_1^T \mathbf{b}, \quad \therefore \hat{\mathbf{x}} = V\mathbf{z} \tag{16}$$



Background for Constrained TSVD

After Truncation

$$V^T \tilde{\mathbf{x}} = \Sigma^{-1} \widetilde{U}_1^T \mathbf{b}, \tag{17}$$

if $\tilde{\mathbf{z}} := \Sigma^{-1} \widetilde{U}_1^T \mathbf{b}$ then one obtains an $n \times n$ linear system,

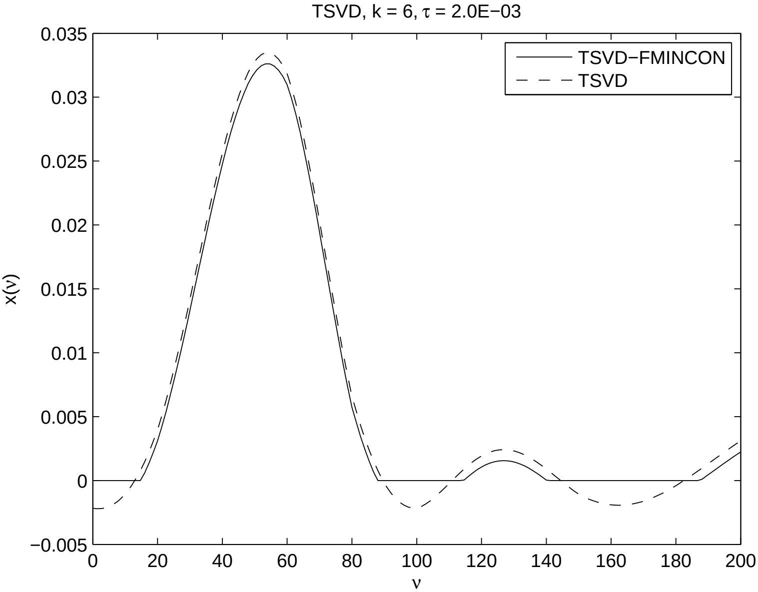
$$V^T \tilde{\mathbf{x}} = \tilde{\mathbf{z}} \tag{18}$$

New Minimization Problem

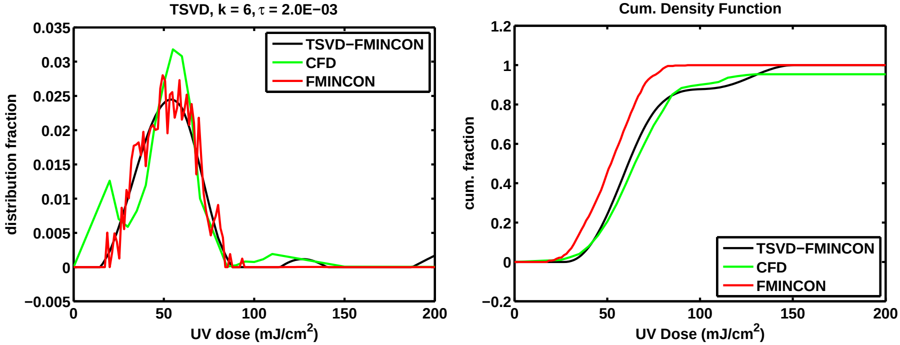
$$\varphi = \min_{\bar{\mathbf{x}} \geq 0} \|\tilde{\mathbf{z}} - V^T \bar{\mathbf{x}}\|_2^2, \quad \text{subject to} \quad \mathbf{e}^T \bar{\mathbf{x}} = 1, \tag{19}$$

Since Eqn. was solved by FMINCON, Constrained TSVD scheme is TSVD-FMINCON

TSVD-FMINCON Solution



Bench Scale Reactor: TSVD-FMINCON vs. CFD-I and FMINCON

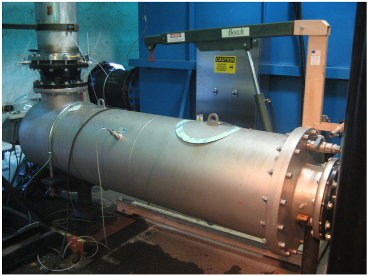


Large Scale Reactors Tested

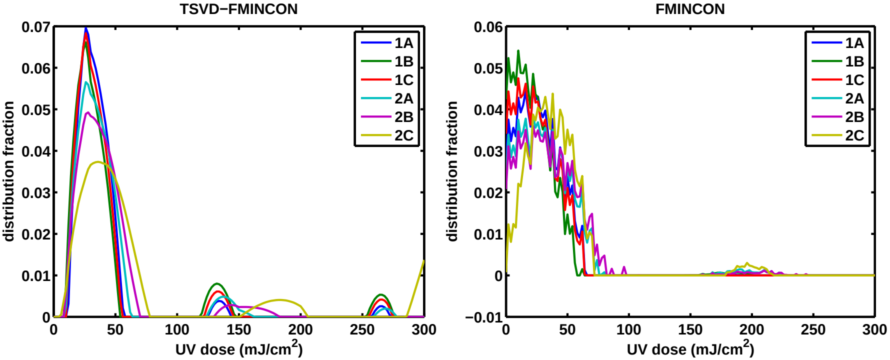
Matrix	Operating Conditions, **y**
TROJAN_102308	1 (A, B, C) - 9 (A, B, C)
WEDECO_111307	1 (A, B, C) - 5 (A, B, C)

Trojan Reactor

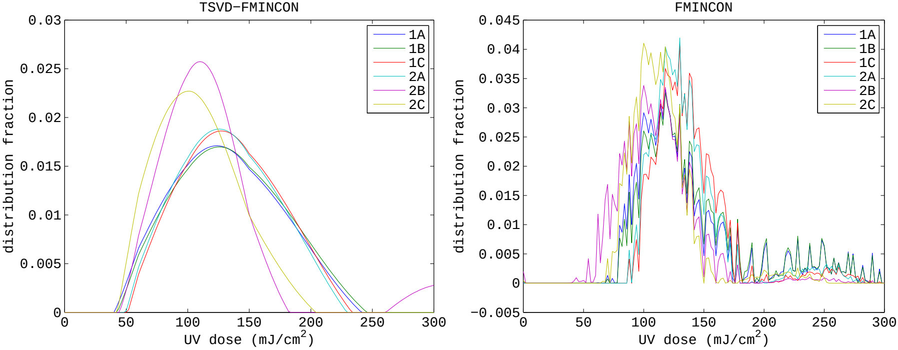
Wedeco Reactor



TROJAN102308: TSVD-FMINCON vs. FMINCON Dose Distributions

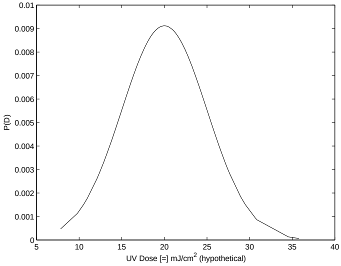


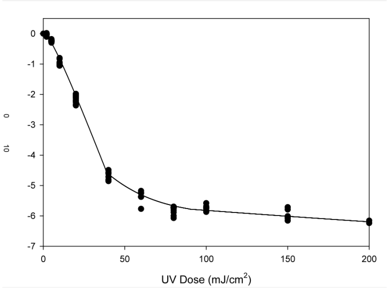
WEDECO111307: TSVD-FMINCON vs. FMINCON



LA: Prediction of Microbial Inactivation

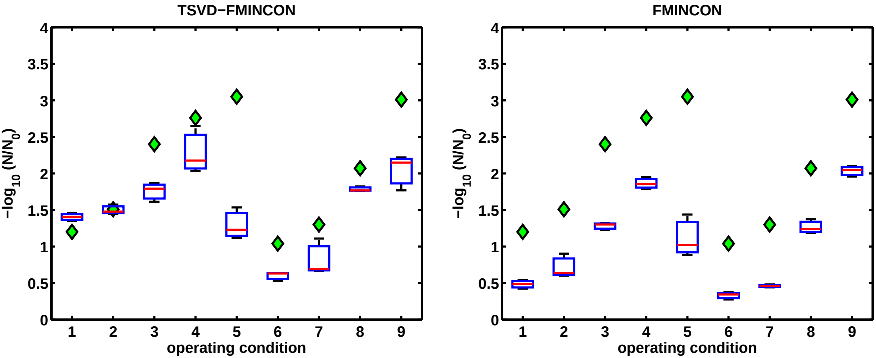
- For disinfection purposes microbial inactivation predictions are used...



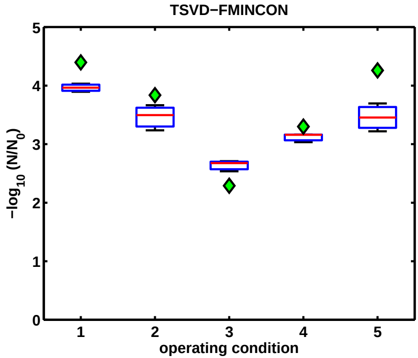


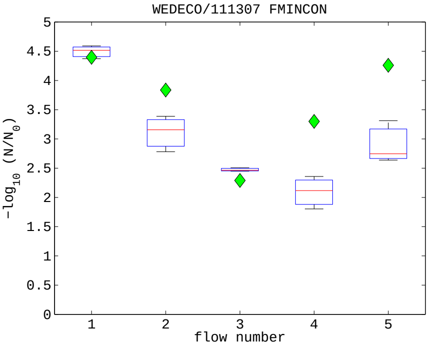
$$\left(\frac{N}{N_0}\right)_{Reactor} \approx \sum_{j=1}^{n} \left(\frac{N}{N_0}\right)_{batch,j} \cdot P_j(D_j) \cdot \Delta D_j$$

TROJAN102308: Log inactivation predictions MS2



WEDECO111307: Log inactivation predictions MS-2





Summary

- SVD leads to the verification that the LA problem shared characteristics common to ill-posed problems.
- The constrained truncated SVD (TSVD-FMINCON) scheme reduced noise in dose distributions, spurious zero-dose contributions, and for most reactor tests it provided better microbial inactivation predictions when compared to the "historical" method.

Acknowledgments

- Partial Funding: NYSERDA, WRF
- Data provided by HydroQual, Inc. UV Validation Research Center (C. Shen, and K. Scheible)

Questions

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