Numerical and Statistical Methods for Lagrangian Actinometry

Eric M. Cox

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Lagrangian actinometry (LA) is an experimental method that allows for direct measurement of a UV dose distribution through the use of UV-sensitive dyed microspheres. While this method has been successfully demonstrated to yield accurate microbial inactivation predictions, a thorough treatment of the numerical and statistical aspects of LA had not been investigated. This research involves the application of numerical and statistical methods for the purposes of improving the LA method and data analysis.

To identify appropriate numerical methods for the LA problem, the properties of the LA least-squares problem were studied in terms of the singular value decomposition (SVD). This investigation illustrated that the LA problem has characteristics typical of ill-posed inverse problems. This outcome motivated an examination of methods that are used in the literature to handle such problems.

Two types of methods were applied to an LA test problem, namely, constrained least-squares methods and regularization methods. The results of the test problem revealed that truncated SVD (TSVD) could be effective for the LA problem. TSVD was applied to reactor data and compared against the solver that had been used previously used for computing LA dose distributions, FMINCON. It was found that TSVD solutions must be constrained, and this observation resulted in the development of a hybrid scheme, TSVD-FMINCON. TSVD-FMINCON was applied to large-scale reactor data, and in some cases outperformed FMINCON.

Due to the application of constraints and experimental error in LA, the bootstrap method for computing $1-\alpha\%$ confidence intervals about UV dose distributions and mircobial inactivation predictions was examined. This method showed that $1-\alpha\%$ confidence intervals were able to be computed for LA predictions of microbial inactivation for large-scale UV reactor data. In some cases, measured inactivation values were within the $1-\alpha\%$ bootstrap confidence intervals developed for LA predictions of microbial inactivation.

Future needs of this research include: development of improved methods for choosing truncation thresholds for the TSVD-FMINCON algorithm, a study to determine patterns in the data when TSVD-FMINCON outperforms FMINCON, and the development of a truncation method for TSVD-FMINCON when weighted least-squares methods are used.