CONSTRUCTION OF A POINT-SOURCE EMISSION FROM ATMOSPHERIC CONCENTRATION MEASUREMENTS USING INVERSE MODELLING

AMIT KUMAR SINGH

CENTRE FOR ATMOSPHERIC SCIENCES
INDIAN INSTITUTE OF TECHNOLOGY DELHI
OCTOBER 2019

Construction of a Point-Source Emission from Atmospheric Concentration Measurements using Inverse Modelling

by

Amit Kumar Singh

Centre for Atmospheric Sciences

Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the

Indian Institute of Technology Delhi

October 2019

Dedicated to My Parents

Certificate

This is to certify that the thesis entitled **"Construction of a Point-Source Emission from Atmospheric Concentration Measurements using Inverse Modelling"** being submitted by **Mr. Amit Kumar Singh** to the Indian Institute of Technology Delhi for the award of the degree of **DOCTOR OF PHILOSOPHY** is a record of the original bonafide research carried out by him. He has worked under my guidance and supervision and has fulfilled the requirements for the submission of the thesis. The results presented in this thesis have not been submitted in part or full to any other University or Institute for award of any degree or diploma.

New Delhi
October 2019

Professor Maithili Sharan
Centre for Atmospheric Sciences
Indian Institute of Technology Delhi
Hauz Khas, New Delhi-110016, India

Acknowledgements

The work presented in this thesis would not have been possible without my close association with many people. I take this opportunity to extend my sincere gratitude and appreciation to all those who made this Ph.D. thesis possible.

To commence with, I pay my obeisance and thank to The Almighty Lord Shiva, the limitless, the destroyer of negative emotions, the Guardian, and to whom I owe my very existence. I believe that whenever I chant the “Om Namah Shivaya” mantra, it calms my mind and brings spiritual insight and knowledge.

First and Foremost, I would like to express my sincere gratitude to my advisor Prof. Maithili Sharan for his valuable guidance, constructive criticism, scholarly inputs and consistent encouragement that I received throughout the research work. I always ended up with confidence and full of energy after the discussions with him. I feel privileged to be associated with a person like him during my life. The knowledge and wisdom I have gained from him will forever guide me in education and life.

I would like to extend my sincere gratitude to my SRC members; Prof. A. D. Rao Prof. R. K. Sharma (Department of Mathematics), Dr. K. AchutaRao and Dr. H. C. Upadhyaya, for generously sharing their knowledge and time. I would also like to thank Prof. (Mrs.) Manju Mohan, Head, CAS, IIT Delhi for providing all the essential facilities in the Centre. I am also grateful to all the faculty members of the Centre including Prof. (Mrs.) P. Goyal, Prof. O. P. Sharma and Prof. S. K. Dash for their help and suggestions.

I am truly indebted to Dr. Sarvesh Kumar Singh for the long discussions that helped me sorting out the technical details of my work. He generously gave his time to offer me valuable comments toward improving my work. I wish to express my sincerest thanks and appreciation to Dr. Jean-Pierre Issartel (University of Evry, France), for fruitful discussion and his encouragement. I wish to thank Dr. Pramod, Dr. Gregory Turbelin, Dr. Amir-Ali Feiz, Dr. Pierre Ngae, Prof. A. Chpoun (University of Evry, France) for their helpful discussions and suggestions during my stay in France.

I gratefully acknowledge the financial support received from CSIR, IIT Delhi, J C Bose fellowship to Prof. Maithili Sharan from DST-SERB. I am also extremely gratefull to the institute for providing me an oppurtuinity to visit Laboratory of Mechanics and

Energetics (LMEE), University of Evry, France for a period of three months under the Indo-French project between IIT Delhi and University of Evry, France with aegis of Indo- French Centre for Applied Mathematics (IFCAM).

I would like to thank my friends and colleagues Abhishek, Dr. Abhisekh Lodh, Dr. Anikender, Ankur, Dr. Dhirendra, Dr. Ram, Dr. Ragi, Dr. Raj Rani, Sathiya, Dr. Saurabh, Sourabh and Dr. Subhra for their active cooperation. The nice company made my stay at IIT pleasant and memorable. I also thank the whole staff of Centre for Atmospheric Sciences especially Mr. L. S. Negi, Mr. V. K. Kaushik, Mr. Madan Lal, Mr. Narender, Namita, Mr. Dataram and Vikas for their help and support.

I convey special thanks to my best friends Dr. Gavendra Pandey and Dr. Piyush Srivastava, with whom I shared my joy and sorrows during the long period of the research work. In many ways, I have dependent on both of them and they have given support and comfort whenever needed. Also, they provided me constructive criticism and inspiring discussions, which helped me to develop a broader perspective to my thesis.

I owe a lot to my parents, who encouraged and helped me at every stage of my personal and academic life, and longed to see this achievement come true. I would like to thank my parents, sister Ashmita, brother Amarjeet, brother-in-law Chitranjan, sister-in-law Sadhya, niece Pranjal and my nephew; Abhinav and Abhigyan for their life-long support, everlasting love, and sacrifices, which sustained my interest in research and motivated me towards the successful completion of this study. I would also like my sincere gratitude and a very special thanks to my parents-in-law, sisters-in-law and brother-in-law; Shashank for their love and unconditional support.

I owe thanks to a very special person, my wife Shweta for her love, constant support, unwavering belief, care and dedicated efforts which contributed a lot for completion of my thesis. But most of all, thank you for being my best friend. I would also like to thank with love to my son Aadvik. Words would never say how grateful I am to have such a lovely and caring family.

New Delhi Amit Kumar Singh

Abstract

The identification of source parameters of the unknown tracer emissions is a prerequisite in the contexts of various Chemical, Biological or Radiological airborne releases for an improved assessment and an effective emergency preparedness program during these accidental or deliberate dispersion events. Such problems are challenging and practically important due to its direct influence on human health and environment. The releases are unexpected, and may not be feasible to observe or measure directly on-site. Also, in such incidents a priori information about the contaminants or the releases is limited. The efficiency of emergency responses is subjected to the quality of information that can be obtained about the source of release. Thus, it is required to develop a methodology within the framework of data assimilation techniques for the source term estimation.

The primary aim of the thesis is to describe the inverse modelling techniques for the identification of an elevated point-source emission from a finite number of atmospheric concentration measurements. As a part of it, least square and renormalization inversion techniques, utilizing the concept of adjoint operator, are adopted for the identification of a point-source. These techniques are evaluated with the concentration measurements obtained from the diffusion experiments in low wind stable conditions conducted at Idaho Falls (Idaho, USA).

The construction of source is highly variable due to instrumental errors/noise involved in observational data as well as representativity errors associated with the dispersion model. The treatment of representativity errors in source inversion problems is difficult and has not been undertaken extensively. In view of this, the thesis explores the

further understanding of the effect of observation and model representativity errors. An approach based on regression is described for minimizing the model representativity errors to improve the source estimation. This approach is utilized within the framework of renormalization and least square inversion techniques to quantify the effect of minimization of model errors on the estimation of source characterstics.

The studies carried out so far are concerned with the estimation of the source (location and its intensity) of known height. Reckoning the height of a release in the source term estimation is also very important since a ground level approximation of the release leads to errors in capturing the actual extent of a plume. The release height is relatively more difficult to estimate from both technical as well as meteorological points of view. Technically, the computational cost and inversion complexity increase when number of unknown parameters increase. Meteorologically, the sensitivity of contaminant dispersion with the source height restricts the feasibility or quality of inversion. Also, in low wind stable conditions, the diffusion of pollutant is irregular and stagnated near to the release. The techniques, namely least squares and renormalization, are extended for the identification of the height of release along with its projected release location on the ground and intensity.

In addition, the thesis addresses the inadequacies in the source construction due to the approximation (to the ground level or negligence) of the height of the release and receptors. The sensitivity of source parameters is carried out for the requirement of the minimum number of measurements and also with respect to the measurement noise for the source estimation. The limitations and meteorological issues related to the inversion of an elevated release are also highlighted.

सार

अज्ञात ट्रैसर उत्सर्जन के स्रोत मापदंडों की पहचान इन आकस्मिक या इच्छित फैलाने वाली विभिन्न रासायनिक, जैविक या रेडियोलॉजिकल एयरबोर्न रिलीज़ घटनाओं के दौरान, एक बेहतर मूल्यांकन और एक प्रभावी आपातकालीन कार्यक्रम के संदर्भों में एक पहली शर्त है। मानव स्वास्थ्य और पर्यावरण पर इसके प्रत्यक्ष प्रभाव के कारण ऐसी समस्याएं चुनौतीपूर्ण और व्यावहारिक रूप से महत्वपूर्ण हैं। रिलीज अप्रत्याशित होते हैं तथा, और सीधे साइट पर निरीक्षण कर पाना संभव नहीं है। इसके अलावा, ऐसी घटनाओं में दूषित पदार्थों या रिलीज के बारे में एक प्राथमिक जानकारी सीमित है। आपातकालीन प्रतिक्रियाओं की दक्षता सूचना की गुणवत्ता के अधीन है जो रिलीज के स्रोत के बारे में प्राप्त की जा सकती है। इस प्रकार, स्रोत अवधि के आकलन के लिए डेटा आत्मसात तकनीकों के ढांचे के भीतर एक पद्धति विकसित करना आवश्यक है।

थीसिस का प्राथमिक उद्देश्य वायुमंडलीय कंसंट्रेशन माप की एक सीमित संख्या से एक ऊंचा बिंदु-स्रोत उत्सर्जन की पहचान के लिए इनवर्स मॉडलिंग तकनीकों का वर्णन करना है। इसके एक भाग के रूप में, लीस्ट स्क्वायर और रेनोर्मालिज़ेशन इनवर्जन तकनीक, समीपवर्ती ऑपरेटर की अवधारणा का उपयोग करते हुए, एक बिंदु-स्रोत की पहचान के लिए अपनाया गया है। इन तकनीकों का मूल्यांकन इडाहो फॉल्स (इडाहो, यूएसए) में आयोजित कम पवन स्थिर स्थितियों में प्रसार प्रयोगों से प्राप्त कंसंट्रेशन के माप से किया गया है।

स्रोत की खोज कंसंट्रेशन संबंधी डेटा के साथ-साथ मॉडल से जुड़े उपकरण संबंधी त्रुटियों के कारण अत्यधिक परिवर्तनशील है। स्रोत इनवर्जन तकनीक में निरूपण त्रुटियों का उपचार कठिन है और बड़े पैमाने पर नहीं किया गया है। इसे देखते हुए, थीसिस अवलोकन और मॉडल अभ्यावेदन त्रुटियों के प्रभाव की आगे की समझ की पड़ताल करता है। प्रतिगमन पर आधारित दृष्टिकोण को स्रोत आकलन में सुधार करने के लिए मॉडल प्रतिनिधित्वशीलता त्रुटियों को कम करने के लिए वर्णित किया गया है। स्रोत की विशेषताओ के अनुमान पर मॉडल त्रुटियों को कम करने के प्रभाव को निर्धारित करने के लिए इस दृष्टिकोण का उपयोग रेनॉर्मलाइजेशन और लीस्ट स्क्वायर इनवर्जन तकनीकों के अंतर्गत किया जाता है।

अब तक किए गए अध्ययन ज्ञात ऊंचाई के स्रोत (स्थान और इसकी तीव्रता) के अनुमान से संबंधित हैं। स्रोत की अवधि के अनुमान में एक रिलीज की ऊंचाई को पुनरावर्ती करना भी बहुत महत्वपूर्ण है क्योंकि रिलीज के एक जमीनी स्तर का अनुमान प्लूम की वास्तविक सीमा निर्धारण करने में त्रुटियों की ओर जाता है। रिलीज की ऊंचाई दोनों तकनीकों और साथ ही मौसम के दृष्टिकोण से अनुमान लगाना अधिक कठिन है। तकनीकी रूप से, कम्प्यूटेशनल लागत और व्युत्क्रम जटिलता बढ़ जाती है जब अज्ञात मापदंडों की संख्या बढ़ जाती है। मौसम की दृष्टि से, स्रोत की ऊंचाई के साथ दूषित फैलाव की संवेदनशीलता इनवर्जन की व्यवहार्यता या गुणवत्ता को प्रतिबंधित करती है। इसके अलावा, कम हवा की स्थिर परिस्थितियों में, प्रदूषक का प्रसार अनियमित है और रिलीज के पास स्थिर है। तकनीक, अर्थात् कम से कम वर्ग और पुनर्संरचना, जमीन पर इसकी अनुमानित रिलीज स्थान और तीव्रता के साथ रिलीज की ऊंचाई की पहचान के लिए विस्तारित हैं।

इसके अलावा, थीसिस रिलीज और रिसेप्टर्स की ऊंचाई के सन्निकटन (जमीनी स्तर) के कारण स्रोत निर्माण में अपर्याप्तता को संबोधित करता है। स्रोत मापदंडों की संवेदनशीलता माप की न्यूनतम संख्या की आवश्यकता के लिए और स्रोत अनुमान के लिए माप शोर के संबंध में भी की जाती है। ऊंचा रिलीज के इनवर्जन से संबंधित सीमाएं और मौसम संबंधी मुद्दे भी उजागर होते हैं।

Contents

Certificate

Acknowledgments

Abstract

Contents **(i)**

List of Figures **(v)**

List of Tables **(viii)**

1 General Introduction **1**

1.1 Introduction 2

1.2 Preliminary Background 4

1.3 Atmospheric Dispersion Model 5

1.4 Uncertainties of the Parameters in the Model 6

1.5 Inversion Technique 8

1.5.1 Source-Receptor Relationship 9

1.5.1.1 Adjoint Modelling 9

1.5.2 Least Square Technique 12

1.5.3 Renormalization Technique 14

1.5.4 Genetic Algorithm (GA) 15

1.5.5 Particle Swarm Optimization 16

1.5.6 Variational Assimilation 17

1.5.7 Bayesian Method 19

1.5.8 Maximum Entropy on Mean (MEM) 20

1.5.4 Organization of the Thesis 21

2 Identification of Point Source using Least Square Technique **28**

2.1 Introduction 29

2.2 Inversion Methodology 32

2.3 Source-receptor Relationship 33

2.4 Covariance Matrix 35
2.5 Diffusion Experiment 36
2.6 Atmospheric Dispersion Model 38
2.7 Numerical Computations 39
2.8 Source Estimation 41
2.9 Results and Discussion 42
2.9.1 Covariance matrix as an Identity Matrix 42
2.9.2 Intercomparison with various forms of error covariance matrix 45
2.10 Conclusions 48

3 Minimization Of Model Representativity Errors 49

3.1 Introduction 50
3.2 Methodology 54
3.3 Renormalization Technique 55
3.3.1 Estimation of point source 57
3.4 Least Square Technique 58
3.5 Regression Relationship 60
3.5.1 Modification of Adjoint Functions 62
3.6 Diffusion Experiment 63
3.6 Numerical Computations 63
3.8 Results and discussion 67
3.8.1 Renormalization Technique 67
3.8.2 Least-Squares Technique 73
3.9 Issues and Limitations 76
3.10 Conclusions 77

4 Reconstructing Height of an Unknown Point Release 79

4.1 Introduction 80
4.2 Inversion Technique 82
4.2.1 Adjoint Source-Receptor Correspondence 83
4.2.2 Cost Function Formulation 85
4.2.3 Point-Source Estimation 86

4.3 Experimental Observations 87
4.4 Numerical Computations 88
4.4.1 Adjoint or Backward Dispersion Model 90
4.4.2 Source Estimation 90
4.5 Results and Discussion 91
4.5.1 Synthetic Data 93
4.5.2 Real Data 93
4.5.3 Posterior errors (or variance) in the source parameters 93
4.5.4 Factors influencing the retrieval of the source parameters 95
4.5.5 Contour representation, Plots and Reconstruction Features 97
4.5.6 Measure of Errors in the Inversion 103
4.6 Sensitivity Analysis 104
4.6.1 Effect of neglecting the receptor's height 104
4.6.2 Measurement Noises 105
4.6.3 Minimum Number of Required Receptors 108
4.7 Advantages and limitations 109
4.7.1 Advantages 110
4.7.2 Assumptions 110
4.7.2 Issues and Limitations 110
4.6 Conclusions 111

5 Source Reconstruction using Renormalization Technique 114

5.1 Introduction 115
5.2 Renormalization Technique 117
5.3 Field Experiments 119
5.3.1 Idaho Diffusion Experiment 120
5.3.2 IIT Diffusion Experiment 121
5.4 Numerical Computations 122
5.4.1 Computational Domain 122
5.4.2 Renormalization: Discrete form 124
5.5 Results and Discussion 125
5.4.1 Idaho Diffusion Experiment 126

5.4.2 IIT Diffusion Experiment 130
5.6 Quantification of Posterior Uncertainty in Source Retrieval 133
5.7 Comparison with Least Square Technique 134
5.8 Conclusions 136
6 Conclusions and Future Perspectives 137
7.1 Conclusions 137
7.2 Limitations and Future Perspectives 142
References 147
Bio-Data 160

List of Figures

Figure 1.1	Flow diagram of a source term estimation (STE) algorithm (Redwood, 2011).	3
Figure 1.2	Representation of adjoint functions with respect to each detector (Issartel et al., 2012).	4
Figure 2.1	Layout of the computational domain (adopted from Sharan et al., 2012b). Black dots represent the samplers, located on the circular arcs of radii 100 m, 200 m and 400 m. The number of samplers is counted from north in a clockwise direction. S' refers to the point source located at the centre of the circular arcs. Meteorological information is provided by the meteorological tower (61 m) located on the 200 m arc.	41
Figure 2.2	Impact of covariance matrix in source reconstruction. Location and intensity errors in the estimated source based on least square technique using observation error covariance matrix as identity, diagonal, covariance, Gram and Toeplitz matrix in various runs. (a) Location error (m) and (b) Intensity error (%).	47
Figure 3.1	Outlines of methodology for minimization of model representativity.	55
Figure 3.2	Location and intensity errors in the estimated source based on renormalization approach in various runs. The symbols denote the errors with and without minimization of model representativity errors. (a) Location error (m) and (b) Intensity error (%).	70
Figure 3.3	Variation of normalized concentrations of observed, modeled predicted and modified concentration in run 8 at 100, 200 and 400 m respectively from top to bottom.	72
Figure 3.4	Same as in Fig 3.2 but for least square approach.	75
Figure 4.1	Layout of the computational domain. The size of the computational	89

domain is 1596m×1596m×50m.

Figure 4.2 Layout of the computational domain in the x-y plane. Black dots represent the samplers, located on the circular arcs of 100m, 200m and 400m. The number of samplers is counted from north in the clockwise direction. S' refers to the point source located at the centre of the circular arcs. Meteorological observations are provided by the tower (61m) located on the 200m arc. 90

Figure 4.3 Isopleths of with both (b) synthetic and (c) real data in the horizontal x-y plane taken at estimated release height above the ground. The panel (a) represents observed sensitivity information of emissions with respect to the measurements from the fixed monitoring network. The receptors in the form of black triangles are located at the height of 0.76m above the ground and are included in the figures for the reference of the operating monitoring network in the respective run. 100

Figure 4.4(a) Variation of with respect to the z axis (in meters) (up to 5m) in representative runs 6, 7, 8 and 10 with synthetic data for fixed estimated source grids in the horizontal x-y plane taken at (i) x=400, y=400 (Run 6), (ii) x=400, y=400 (Run 7), (iii) x=400, y=400 (Run 8) and (iv) x=400, y=400 (Run 10). 101

Figure 4.4(b) Variation of with respect to the z axis (in meters) (up to 5 m) in representative runs 6, 7, 8 and 10 with real data for fixed estimated source grids in the horizontal x-y plane taken at (i) x=395, y=399 (Run 6), (ii) x=397, y=403 (Run 7), (iii) x=410, y=388 (Run 8) and (iv) x=394, y=377 (Run 10). 102

Figure 5.1 Layout of the computational domain in the x-y plane (adapted from Sharan et al., (2012a)). Black dots represent the samplers, located on the circular arcs of 100 m, 200 m and 400 m. The number of samplers is counted from north in a clockwise direction. S' refers to the point source located at the centre of the circular arcs. 120

Meteorological information is provided by the meteorological tower (61 m) located on the 200 m arc.

Figure 5.2 Layout of the site for the IIT Delhi tracer diffusion experiment in the x-y plane (adapted from Sharan et al., (2009)). S' refers to the source in central position and S''to the source in shifted position. The samplers were arranged on circles of radius 50, 100 and 150 m, with regular angular spacing of 45^{o}. 121

Figure 5.3 Layout of the computational domain for Idaho experiment. The size of the computational domain is 1596m×1596m×50m. 123

Figure 5.4 Layout of the computational domain for IIT Delhi experiment. The size of the computational domain is 990m×990m×10m. 124

Figure 5.5 Isopleths of the weight functions (in panel a) and the source estimate (in panel b) in a horizontal plane corresponding to the estimated effective source height (h) in case of Idaho experiment for runs 4, 6, 8 and 9. The receptors in the form of black triangles are located at the height of 0.76 m above the ground and are included in the figures for the reference of the operating monitoring network in the respective run. 130

Figure 5.6 Location (m) and intensity errors (%) in the estimated source for (a) Idaho (b) IIT experiment. 132

Figure 5.7 Bar plots for (i) estimated height and (ii) intensity in case of Idaho experiment. The corresponding uncertainties are represented by the error bars. 134

Figure 5.8 Comparison of the source estimation obtained from renormalization approach with that computed using least square technique in Idaho experiment. 135

List of Tables

Table 2.1 Source identification using the real concentration measurements in the various runs of Idaho experiment. The estimated and experimental point releases are indicated in terms of location in grid units and intensity in μg s-1. The error (EL in meters) in the estimated location and the deviation in source strengths (EI in %) from the experimental value is shown. The +\- " sign shows over (under) estimation. The table is divided into two panels (a) for runs 4, 5, 6, 7, 8 and (b) for 9, 10, 11, 13 and 14. 43

Table 3.1 Continuous regression curves $f_{\beta_0}(r)$ and $f_{\beta_1}(r)$ (function of radial distance from centre of monitoring network) for runs 4-14 for renormalization approach. 65

Table 3.2 Same as in Table 3.1 but for least square approach. 65

Table 3.3 Comparison of source identification computed from with and without minimization of model errors using the real concentration measurements in the various runs. (The experimental point release and those estimated are indicated in terms of location in grid units and intensity in μg s-1. The error (EL in meters) in the estimated location from their experimental value is given in fifth and ninth rows. In seventh and eleventh rows, the deviation in source strengths (EI in %) from the experimental value is shown. The '+(-)' sign shows over(under) estimation. The table is divided into two panels (a) for runs 4, 5, 6, 7, 8 and (b) for 9, 10, 11, 13 and 14. 69

Table 3.4 Same as in Table 3.3 but for least square approach. 74

Table 4.1 Source reconstruction results with the real data in runs (4-14). The table is divided into two parts (a) runs 4, 6, 7, 8 and (b) runs 9, 10, 11, 13, 14. The experimental point releases (second row) with least-squares estimates (third row) are indicated in terms of location (x, y, 92

z) (in grid units), equivalent height of release (m) and intensity ($\mu g\,s^{-1}$). The location error (in meters) and the angular departure (in degrees) are shown in fourth and fifth rows respectively.

Table 4.2 Posterior errors in the estimated source parameters in all the runs. In the second column, the Euclidean distance of the estimated source from the true source (on the ground) is mentioned in terms of mean ± standard deviation (sd). The mean values refer to the estimated parameters given in table 4.1. The coefficient of variation (CV= sd/mean) for the release height and source intensity is shown in third and fourth columns respectively. 93

Table 4.3 Effect of neglecting receptor's height ($z_r = 0$) on the estimation of source parameters using real data. The retrieved source location (x, y, z) (second column) in grid units, source height (third column) in meters, intensity (fourth column) in $\mu g\,s^{-1}$ and angular departure error (fifth column) in degrees are presented corresponding to the each run (first column). 105

Table 4.4 Influence on the source parameters with respect to the proportion of noise in the synthetic measurements. The retrieved horizontal source location coordinates (x, y) (third column) in grid units, source height (fourth column) in meters and intensity (fifth column) in are presented in each run (first column). The release parameters (location, height, intensity) and angular departure are represented in the form of mean ± standard deviation. 107

Table 4.5 Minimum number of measurements required to achieve a reasonable source reconstruction with the real data. The number of measurements (second column), retrieved source location (x, y, z) (third column) in grid units, source height (fourth column) in meters and intensity (fifth column) in are presented corresponding to the each run (first column). 109

Table 5.1 Source identification using the real concentration measurements in 127

the various runs of Idaho experiment. The estimated and experimental point releases are indicated in terms of location in grid units and intensity in μg s-1. The error (EL in meters) in the estimated location, retrieved source height (h in meters) and the deviation in source strengths (EI in %) from the experimental value is shown. The +\- " sign shows over (under) estimation. The table is divided into two panels (a) for runs 4, 6, 7, 8 and (b) for 9, 10, 11, 13 and 14.

Table 5.2 Same as in Table1 but for IIT experiment. The table is divided into two panels (a) for runs 1, 6, 7 and 8 (b) for runs 11, 12 and 13. 131