IMPROVING THE ACCURACY OF 3D GEOLOGIC SUBSURFACE MODELS

IMPROVING THE ACCURACY OF 3D GEOLOGIC SUBSURFACE MODELS

By

KELSEY ELAINE MACCORMACK, B.Sc. (Hons), M.Sc.

A Thesis

Submitted to the School of Graduate Studies

in Partial Fulfilment of the Requirements

for the Degree

Doctor of Philosophy

McMaster University

© Copyright by Kelsey Elaine MacCormack, June 2010

Doctor of Philosophy (2010) McMaster University

(Geography and Earth Sciences) Hamilton, Ontario,
Canada

TITLE: **IMPROVING THE ACCURACY OF 3D GEOLOGIC SUBSURFACE MODELS**

AUTHOR: Kelsey Elaine MacCormack B.Sc. (Hons)
(McMaster University, Hamilton, Canada, 2001)

M.Sc.
(McMaster University, Hamilton, Canada, 2005)

SUPERVISOR: Dr. Carolyn H. Eyles

NUMBER OF PAGES: xv, 186

ABSTRACT

This study investigates ways to improve the accuracy of 3D geologic models by assessing the impact of data quality, grid complexity, data quantity and distribution, interpolation algorithm and program selection on model accuracy. The first component of this research examines the impact of variable quality data on 3D model outputs and presents a new methodology to optimize the impact of high quality data, while minimizing the impact of low quality data on the model results. This 'Quality Weighted' modelling approach greatly improves model accuracy when compared with un-weighted models.

The second component of the research assesses the variability and influence of data quantity, data distribution, algorithm selection, and program selection on the accuracy of 3D geologic models. A series of synthetic grids representing environments of varying complexity were created from which data subsets were extracted using specially developed MATLAB scripts. The modelled data were compared back to the actual synthetic values and statistical tests were conducted to quantify the impact of each variable on the accuracy of the model predictions. The results indicate that grid complexity is the predominant control on model accuracy, more data do not necessarily produce more accurate models, and data distribution is particularly important when relatively simple environments are modelled. A major finding of this study is that in some situations, the software program selected for modelling can have a greater influence on model accuracy than the algorithm used for interpolation. When modelling spatial data

there is always a high level of uncertainty, especially in subsurface environments where the unit(s) of interest are defined by data only available in select locations. The research presented in this thesis can be used to guide the selection of modelling parameters used in 3D subsurface investigations and will allow the more effective and efficient creation of accurate 3D models.

ACKNOWLEDGEMENTS

First and foremost I would like to thank my thesis supervisor, Dr. Carolyn Eyles for all of her support and encouragement over the years. I have learned so much and I will forever appreciate the friendship and guidance that I have received. She has always been incredibly supportive and constantly encourages her students to focus their research in areas they are truly interested. I cannot thank her enough for going above and beyond her responsibilities as a supervisor and encouraging me, even when I subtly switched my research focus from sediments to statistics. I can't even begin to express my gratitude to her for inspiring me become the 'computer geek' I never knew I wanted to be!!

I would also like to thank Dr. Jeff Harris and Dr. Antonio Paez for agreeing to be on my committee. You both have been incredibly helpful and supportive and have had such a positive influence on my research. I am very appreciative for all your positive comments and suggestions – they have helped to inspire many great ideas. I would also like to thank Dr. Harvey Thorleifson for agreeing to be the external examiner for my thesis defence. I really appreciate all the time he took to read my thesis and provide very interesting and valuable comments.

I also need to thank all the amazing people that I have had the opportunity to work with in the lab over the years. Carolyn often talks about the importance of having a 'sense of community' at McMaster. However in doing so, managed to create a sense of 'family' within our lab. Over the years there have been many additions to our 'lab family', who have all contributed in some way to this research. I would like to thank Mark Radomski, Luke Hunt, Aislyn Trendall, and Sean Fletcher for their friendship and support during the early years of my PhD. I would also like to thank Stacey Puckering, Jessica Slomka, Riley Mulligan, Paul Durkin, and Prakteek Gupta for all their help (especially over this past week!). I cannot thank Stacey enough for the week she spent helping me track down and properly reference every journal article I had read during the past 4 years! Jessica, for somehow making hours upon hours of core logging fun! I definitely need to thank Paul and Riley for all the repetitious button clicking required to run all those models - as well as for keeping a straight face when I asked to talk about the results! I would also like to thank Prateek, who managed to teach me more about the English language in the past two weeks than I ever learned in grade school. And finally John, who I must owe hundreds of dollars to for all the coffees he's bought me – especially over these past few weeks. I am truly fortunate to have had the opportunity to get to know and work with you all!

I also owe a special thanks to Jason Brodeur for all of his help with MATLAB. He always willing to come over to the lab when MATLAB was giving me grief – which happened more often than I would like to admit!!

Finally, I would like to acknowledge my family. My parents have been too helpful for words. I can't thank them enough for putting their dreams aside so that I could pursue mine. They have been more helpful than they can ever imagine and I truly appreciate all of their support and encouragement. I also thank my three beautiful children, Tyler, Ashleigh and Carter for being the best children anyone could ask for. They are the reason that I enjoy every day. Last but never least, I would like to thank my wonderful husband Mike, whose love and support has made this all possible. I am eternally grateful for having each one of them in my life.

I truly love my research and couldn't imagine being happier doing anything else. I acknowledge that without the tremendous support from all of these people, it would not have been possible, and therefore I thank them all!!

TABLE OF CONTENTS

ABSTRACT iii

ACKNOWLEDGEMENTS v

LIST OF FIGURES x

LIST OF TABLES xv

CHAPTER 1: INTRODUCTION 1

Objectives of this research 4

Thesis Structure 7

Reference List 10

CHAPTER 2: ENHANCING THE RELIABILITY OF 3D SUBSURFACE MODELS THROUGH DIFFERENTIAL WEIGHTING AND MATHMATICAL RECOMBINATION OF VARIABLE QUALITY DATA 17

Abstract 17

2.1 Introduction 18

2.2 Sources of Data and Data Classification 26

2.3 Data Modelling 32

2.3.1 Creating a differential 'Quality Weighting' mechanism 37

2.4 Testing the Method: Model Outputs 43

2.4.1 Visual Comparison of Model Outputs 45

2.4.2 Grid Math 45

2.4.3 Volumetrics 53

2.4.4 Impact of the Quality Weighting method on Predicted Grid Node Values 56

2.4.5 Impact on the Standard Deviation of the Output Models 57

2.5 Validation of the Quality Weighting Method 58

2.5.1 Comparison of Model Output with Proxy Data 59

2.6 Conclusion 63

Acknowledgments 65

Reference List 66

CHAPTER 3: EVALUATING THE IMPACT OF DATA QUANTITY, DISTRIBUTION, AND ALGORITHM SELECTION ON THE ACCURACY OF 3D SUBSURFACE MODELS USING SYNTHETIC GRID MODELS OF VARYING COMPLEXITY 70
Abstract 70
3.1 Introduction 71
3.2 Methods 73
3.2.1 Synthetic Surface Development 74
3.2.2 Extracting Sample Data from each Model 78
3.2.3 Grid Interpolation and Comparison 83
3.3 Results and Discussion 88
3.3.1 Number of Data Points 89
3.3.2 Data Point Distribution 102
3.3.3 Algorithm Comparison 105
3.3.4 Bias Error Analysis 109
3.5 Conclusions 115
Reference List 119
APPENDIX 3.1: GRID COMPARISON DATA 123
CHAPTER 4: ASSESSING THE IMPACT OF PROGRAM SELECTION ON THE ACCURACY OF 3D GEOLOGIC MODELS 128
Abstract 128
4.1 Introduction 129
4.2 Methods 130
4.2.1 Grid Creation 134
4.2.2 Data Extraction 135
4.2.3 Data Formatting 139
4.2.4 Establishing Unbiased Interpolation Settings 139
4.2.5 Comparing the Output Models 140
4.3 Results and Discussion 142
4.3.1 Influence of Grid Complexity 143

4.3.2 Influence of Data Point Distribution 152
4.3.3 Impact of Data Quantity 156
4.3.4 Influence of Algorithm Selection 158
4.3.5 Bias Error Analysis 159
4.4 Conclusions 163
Reference List 165
APPENDIX 4.1: RMSE RESULTS 168
APPENDIX 4.2: ANOVA DESCRIPTION 172
APPENDIX 4.3: ANOVA RESULTS 174
CHAPTER 5: SUMMARY AND CONCLUSIONS 178
Future Work 183
References 185

LIST OF FIGURES

Figure 2.1: A) & B) Maps showing the location of McMaster Campus in Southern Ontario. Photos courtesy of Google Earth and Hamilton Maps. 22

Figure 2.2: Georeferened airphoto of the McMaster campus showing the location of the borehole data classified according to the quality of the data. High quality data points are shown as circles, low quality data points by squares, and erroneous data points (outliers) are shown as stars. 24

Figure 2.3: The data were separated into 4 datasets based on quality and then used to model the thickness of the sand and gravel aquifer using ROCKWORKS 2006. The dataset containing all the available data (the Original Dataset; a) was split into two separate datasets; one containing only high quality data (b) and the other containing only low quality data (c). The outliers were removed from the Low Quality Dataset to create a Refined Dataset (d). 30

Figure 2.4: Diagram to show how data points located in space (A) are overlain by a grid (B) populated by grid nodes which are values calculated by the selected interpolation algorithm (C). 33

Figure 2.5: Diagram to show how the weights are determined for gridding algorithms. Typical algorithm weights are based on the distance of the data points (circles & stars) from the node of interest (hexagon)..... 35

Figure 2.6: Flow chart showing how the grids created by the high and low quality datasets were then multiplied by a 'weighting factor' to either enhance or decrease the influence of the respective data on the final output model. The weighted grids were then mathematically recombined with one another using a grid math process. Assigning a larger relative weighting factor to the grid created by the high quality data allows it to have a greater influence on the final model output..... 38

Figure 2.7: Map showing the difference in thickness of the sand and gravel unit between the model generated with Low Quality Dataset and Refined Dataset. The greatest difference in thickness occurs in the area of the outliers which were removed from the Refined Dataset. Areas where the two grids are very similar appear as purples and blues, the green areas of the grid indicate where there are small differences, whereas areas of reds and yellows and black highlight the areas where the greatest differences occur..... 47

Figure 2.8: Map of the Quality Weighted [High (0.7) + Refined (0.3)] minus the High Quality grids shows that there is little change in the model output for areas where the high quality data are present. The greatest difference is along the north-west perimeter of the study area where the Quality Weighted grid was able to utilize the lower quality data to constrain the model where high quality data are sparse. 49

Figure 2.9: Map of the Original Dataset model – High (0.7) + Low (0.3) model showing how the Quality Weighting method has reduced the impact of the extreme outliers. The greatest difference in unit thickness occurs in the area of the outliers (which are present in both grids) however their influence has been greatly reduced using the Quality Weighted method. 51

Figure 2.10: Voxel models of the sand and gravel aquifer unit produced by the a) Original, b) High Quality, c) Low Quality, and d) Refined Datasets. 54

Figure 2.11: The thickest portions of the subsurface aquifer identified on the isopach map generated from the Quality Weighted [High (0.7) + Refined (0.3)] model (a) more closely correlates with the mapped contaminant plume pathways (transparent overlay) determined independently by Conestoga Rovers and Associates (1996) than the model created by the un-weighted Original Dataset (b). 61

Figure 3.1: Synthetic grids created to represent realistic geologic environments from which the data points for modeling were extracted. a) Grid 1 forms a gently sloping surface that may represent one element of a basin system or gently dipping bedrock valley wall, b) Grid 2 consists of two linear 'highs' separated by a central trough and represents a simple valley form, c) Grid 3 shows a series of interconnecting troughs separated by linear 'highs' and may represent an eroded bedrock surface or a braided river system, and d) Grid 4 consists of a flat surface incised by a highly sinuous channel and represents an incised meandering river system. 76

Figure 3.2: Data points were extracted from the synthetic grids in 4 spatial distribution patterns a) clustered, b) random, c) regular, and d) sparse. Sample distribution patterns for the 676 point dataset are shown. 79

Figure 3.3: Flow diagram showing how the four synthetic grids (a.) were sampled to create the individual data subsets, which were then interpolated and modelled. Each synthetic grid (a.) was created with 6400 data points which were then sampled using 100, 676, and 1600 points in clustered, random, regular and sparse distribution patterns (b.). Visualizations of grid 2 were modelled using either IDW or OK with various amounts of data, in a variety of distributions (clustered, random, regular, and sparse) are also shown (c.). 90

Figure 3.4: Graphs showing the Root Square Mean Error (RMSE) associated with models constructed for the four grids using each sampling distribution. The RMSE values were analyzed for models interpolated using a) 100, b) 256, c) 676, and d) 1600 data points. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 92

Figure 3.5: Graphs showing how the RMSE values calculated for the four synthetic grids (a) grid 1, b) grid 2, c) grid 3, and d) grid 4) vary according to data distribution pattern (clustered, random, regular, and sparse), number of data points and algorithm used for interpolation (OK and IDW). RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. Note change of scale for grids 3 and 4. 94

Figure 3.6: Graphs showing decline of RMSE values as the number of randomly distributed data points available for interpolation increases using either the a) IDW, or b) OK algorithms. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 97

Figure 3.7: Bias Error Analysis a) graph showing the decrease in the range of average bias errors calculated for the IDW and OK algorithms as the number of data points included in the modelling process increases. Note that the average errors are all negative and suggest that the models represent under-estimations of actual values. b) Bias errors for models of grid 3 using different numbers of data points, data distribution patterns and algorithm. c) Bias errors for models of grids 1 - 4 using 256 data points modelled with IDW and OK in clustered, random, regular and sparse distributions. Note: Bias error values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 111

Figure 4.1: Synthetic grids created with 6400 known data points represent realistic geologic environments from which the data points for modelling were extracted. a) Grid 1 forms a gently sloping surface that may represent one element of a basin system or gently dipping bedrock valley wall, b) Grid 2 consists of two linear 'highs' separated by a central trough and represents a simple valley form, c) Grid 3 shows a series of interconnecting troughs separated by linear 'highs' and may represent an eroded bedrock surface or a braided river system, and d) Grid 4 consists of a flat surface incised by a highly sinuous channel and represents an incised meandering river system. 131

Figure 4.2: Data points were extracted from the four synthetic grids in 3 spatial distribution patterns a) random, b) regular, and c) clustered. Sample distribution patterns for the 256 point dataset are illustrated 137

Figure 4.3: Graphs of RMSE results for datasets modelled with 256 data points in a) random, b) regular, and c) clustered distributions. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 146

Figure 4.4: Graphs showing the change in RMSE produced by the software programs (X, Y, Z) using algorithms IDW and OK, as increasing numbers of regularly distributed data a) 100, b) 256, and c) 676 were modelled. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 150

Figure 4.5: Graphs showing the change in RMSE values produced by the software programs (X, Y, Z) as increasing numbers (100, 256, 676) of data points in random (a,d,g,j), regular (b,e,h,k), and clustered (c,f,i,l) distributions are used to interpolate synthetic grids 1 (a,b,c), 2 (d,e,f), 3 (g,h,i) and 4 (j,k,l). RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 153

Figure 4.6: Graphs showing the change in the absolute sum of the bias errors (ABBE) and the average bias errors (AVBE) produced by the software programs (X, Y, Z) to interpolate Grids 1, 2, 3, and 4 using 100 (a), 256 (b) and 676 (c) data points. Bias error values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. 161

LIST OF TABLES

Table 2.1: Actual (observed) and interpolated grid thickness node values with corresponding volumes and standard deviations for the sandy gravel aquifer unit for both the weighted and unweighted datasets..... 44

Table 3.1: RMSE results for randomly distributed data points used to model the 4 synthetic grids with IDW and OK, using various quantities of data points. The cells highlighted in green indicate the point at which the rate of RMSE declined in relation to the inclusion of additional data points. The cells highlighted in orange identify the point at which RMSE values began to increase with the inclusion of additional data points. ... 99

Table 4.1: Summary ANOVA results for RMSE values averaged for all model simulations. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3..... 144

Table 4.2: Summary ANOVA table of RMSE results for grid 1 showing the influence of individual variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3. 144

Table 4.3: Summary ANOVA table of RMSE results for grid 2 showing the influence of individual variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3. 144

Table 4.4: Summary ANOVA table of RMSE results for grid 3 showing the influence of individual variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3. 145

Table 4.5: Summary ANOVA table of RMSE results for grid 4 showing the influence of individual and selected combinations of variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3..... 145

CHAPTER 1
INTRODUCTION

Three-dimensional (3D) modelling has been used in the field of geosciences for many years. The oil industry has been using 3D models in some capacity since the 1930s (Berg & Keefer, 2004), but only recently (in the past 20 years) have 3D models become an important element in geological and hydrogeological studies (Berg & Keefer, 2004). Today, 3D geological models are used for a wide variety of applications including resource (mineral, oil, gas, and groundwater) exploration (Jessel, 2001; Gong et al., 2004; Parks et al., 2005; Rawling et al., 2006; Pranter et al., 2007; Kaufmann & Martin, 2008; Sech et al., 2009), identification of source protection areas (Ross et al., 2005; Burt, 2007; Zwiers et al., 2008; Bajc et al., 2009), predicting contaminant migration pathways (Birken & Versteeg, 2000; Saito & Goovaerts, 2002; Culshaw, 2005), and the reconstruction of past geologic events and processes (MacCormack et al., 2005; Logan et al., 2006; Zanchi et al., 2009; Keller et al., 2009; Susini & De Donatis, 2009)

A relatively recent application of 3D models is to aid with studies and investigations designed to protect human health and safety, such as groundwater source protection (Sharpe & Russell, 2005; Burt & Bajc, 2007), and natural hazard risk assessment (Kemec & Duzgun, 2006; Deparis et al., 2007; Hengxing et al., 2007; Ongaro et al., 2008; Frattini et al., 2008). After the fatal Walkerton tragedy in 2000, a key recommendation of the subsequent inquiry was for every municipality in Ontario to develop groundwater source protection plans in which 3D subsurface models play a key

role (Sharpe & Russell, 2005; Burt & Bajc, 2007). The purpose of groundwater source protection plans is to protect sources of drinking water from potential contaminants by accurately identifying sensitive areas at high risk of contamination and potential contaminant transport routes (O'Connor, 2000; Sharpe and Russell, 2002). 3D subsurface models are used to analyze and visualize the geometry and extent of geological units that serve as either aquifers (allowing effective transmission of water and/or contaminants) or aquitards (that retard fluid flow), and are critical to the understanding of the overall groundwater system. Failing to address uncertainty in such models could have fatal repercussions; ensuring that 3D model results are as reliable and accurate as possible is therefore of great importance (O'Connor, 2002; Sharpe & Russell, 2005).

The technology and computational software required to produce 3D models is now readily accessible to a wide range of users. Unfortunately, not all users are aware of the limitations and potential inaccuracies of the model outputs and apply these models inappropriately (Goodchild & Haining, 2004). All models are simply approximations of what exists in reality and it has even been stated by Box (1976) that all models are wrong, but some are useful. This raises the issue of model accuracy and the need to identify and quantify uncertainty in model predictions (Jackson, 2007). The accuracy and reliability of 3D subsurface models being generated for a range of applications is often questionable (Thorleifson & Berg, 2002; Keefer & Rittenhouse, 2005; Venteris, 2007). Reasons for this may be the simplistic perception that computer generated models, which are capable of calculating model estimations to multiple significant digits, are incredibly precise (Goodchild, 2006). This view of model accuracy (uncertainty) is drastically changing as

more people realize that 3D models are simply approximations/versions of reality and that it is the responsibility of the modeler (not the computer) to ensure the end result is as accurate and realistic as possible (Devillers & Jeansoulin, 2006). 3D models are frequently used as the basis for important and costly decisions, such as determination of the economic feasibility of mineral or oil extraction from a specific area (Milkereit et al., 2000; Eaton et al., 2003; Feltrin et al., 2009), identification of sufficient groundwater resources to support the future growth of rural cities (Howard, 1997; Howard & Livingstone, 2000; Sharpe et al., 2002), and the identification of contaminant migration pathways (Birken & Versteeg, 2000). Therefore, identifying potential sources of uncertainty within 3D models, and evaluating model accuracy and reliability is extremely important and can have costly implications (Isaaks & Srivistava, 1989; Englund, 1990; Weber & Englund, 1992; Brus et al., 1996; Zimmerman et al., 1999; Schloeder et al., 2001; Saito & Goovaerts, 2002; Costa, 2003; Dille et al., 2003; Jones et al., 2003; Jackson, 2007).

It is critical for any modeler or model user to be cognizant of the uncertainty and errors associated with 3D models (Weber & Englund, 1992; Weber & Englund, 1994; Zimmerman et al., 1999; Jones et al., 2003; Devillers & Jeansoulin, 2006; Tacher et al., 2006; Fisher et al., 2006). Unfortunately, many studies and even software companies avoid addressing the uncertainty associated with interpolating data (Houlding, 1994; Keefer, 2005; Devillers & Jeansoulin, 2006; Goodchild, 2006; Tacher et al., 2006; Keefer, 2007). Goodchild (2006) suggests that there has been little demand for methods to characterize and quantify uncertainty in 3D modelling studies conducted over the past

30 years. However studies are beginning to emerge that assess the impact of various interpolation algorithms on model output results (Weber & Englund, 1992; Weber & Englund, 1994; Brus et al., 1996; Walker & Loftis, 1997; Nalder & Wein, 1998; Zimmerman et al., 1999; Schloeder et al., 2001; Dille et al., 2003; Kravchenko, 2003; Lapen & Hayhoe, 2003). This is a promising start, although algorithm selection is only one variable that may affect model accuracy. Numerous other sources of uncertainty can be introduced into 3D models that relate to the quality, quantity and spatial distribution of input data, the geologic complexity of the area being modelled, and the software program selected for use. It is imperative to identify these potential sources of uncertainty and thoroughly understand how they impact the accuracy and reliability of 3D model results.

Objectives of this research

The overall objective of this study is to investigate ways to improve the accuracy of 3D geologic models by assessing the impact of data quality, grid complexity, data quantity and distribution, as well as interpolation algorithm and program selection on model accuracy.

In 1997, Strong et al. (1997) determined that the negative impact of low quality data used in studies employing 3D modelling techniques, on both the economy and society, was in the billions of dollars. There is no cost estimate on what this impact would be today, but it can be assumed that both the cost and impacts are likely increasing at an exceptional rate due to the increased accessibility and transferability of geospatial

data (Devillers et al., 2002). As the demand for 3D geological models has steadily increased, so too has the dependency on large, readily available digital databases for input data. A serious concern with the 'unedited' use of large digital databases as the primary source of data for 3D subsurface modelling is the variable quality of the data, which severely reduces the reliability of model outputs (Goodchild & Clarke, 2002; Burt, 2004; Dey et al., 2005; Carter & Castillo, 2006; Logan et al., 2006; Venteris, 2007). This presents a major problem when trying to create accurate 3D models as most modelling programs give equal weight to all input data, thus allowing relatively low quality data to override the influence of higher quality data, negatively impacting the output model accuracy and reliability. Despite recognition of the problem of including variable data quality in the modelling process, no studies have proposed methods to rectify the issue (Goodchild & Clarke, 2002; Keefer, 2005; Logan et al., 2006; Burt, 2007). Research reported in this thesis (Chapter 2) proposes an innovative 'Quality Weighting' methodology that allows the user to assign a differential weighting factor to data points of variable quality in the modelling process. This allows the 3D modelling program to maximize the use and effectiveness of data from all available sources while giving high quality data greater influence on the final model output.

A common saying in 3D modelling is that "you can never have enough data", which leads to the assumption that increased data quantity will lead to increased model accuracy. Some studies boast that their models were created with tens of thousands of data points (Bajc & Newton, 2005; Keller et al., 2005; Logan et al., 2006), to upwards of 370,000 data points (Gunnink, 2005). Other studies claim that they have developed 3D

models with what they consider to be 'minimal', 'insufficient', or 'sparse' numbers of data points, which raises questions concerning the accuracy of model results (Wu et al., 2005; de Kemp, 2006; Paulen et al., 2006; Bond et al., 2007). It has been suggested by Davis (2002) and Houlding (2000) that models should ideally be interpolated with regularly distributed data throughout the study area; however, in geological studies this is rarely the case. The vast majority of 3D geologic studies are interpolated with clustered data (Krajewski & Gibbs, 1996; Davis, 2002; Paulen et al., 2006; Bond et al., 2007; Keefer, 2007), and it is therefore important to understand the impact of data quality and distribution on model accuracy. Chapter 3 of this thesis presents a quantitative assessment of the impact of data quantity, distribution and algorithm selection on the accuracy of 3D models using synthetic grids surfaces.

The importance of understanding variability in modelling algorithms was identified by (Englund, 1990) as having significant effects on both the quality of the results and decisions based on the results. The impact of algorithm selection on the accuracy of model predictions has been tested in many studies (Weber & Englund, 1992; Weber & Englund, 1994; Brus et al., 1996; Walker & Loftis, 1997; Nalder & Wein, 1998; Zimmerman et al., 1999; Schloeder et al., 2001; Dille et al., 2003; Jones et al., 2003; Kravchenko, 2003; Lapen & Hayhoe, 2003). However none of these studies considered the impact of program selection upon model accuracy. The research presented in Chapter 4 assesses the impact of both model and program selection on the accuracy of 3D models generated by different algorithms and with different numbers and distributions of data points.

Identifying and quantifying the impact of the many variables that affect model accuracy is important and can have huge implications to a wide variety of geosciences applications (Isaaks & Srivistava, 1989; Englund, 1990; Weber & Englund, 1992; Weber & Englund, 1994; Brus et al., 1996; Zimmerman et al., 1999; Schloeder et al., 2001; Costa, 2003; Dille et al., 2003; Jones et al., 2003).

Thesis Structure

These objectives were addressed in the form of three chapters included in this thesis. These chapters are formatted for publication in scientific journals and summarized below.

Chapter 2 - Enhancing the Reliability of 3D Subsurface Models through Differential Weighting and Mathematical Recombination of Variable Quality Data

Input data used in 3D modelling can come from a variety of sources and may be categorized according to their reliability and/or quality. The output from the 3D model is a prediction of subsurface conditions based on these data and the reliability of the output model is highly dependent on both the quality of input data and the types of interpolation methods used.

This paper presents a new 'Quality Weighting' methodology that allows the user to assign a differential weighting factor to data points of variable quality in the modelling process. Input data are categorized into High and Low Quality Datasets which are then recombined using a grid math process in which a differential 'weighting' factor is

applied. This allows the 3D modelling program to maximize the use and effectiveness of data from all available sources while giving high quality data greater influence on the final model output and will result in the generation of more accurate and reliable 3D subsurface models.

Chapter 3 - Evaluating the impact of data quantity, distribution, and algorithm selection on the accuracy of 3D subsurface models using synthetic grid models of varying complexity.

Testing the accuracy of 3D modelling algorithms used for geological applications is extremely difficult as model results cannot be easily validated. This paper presents a new approach to the evaluation of the effectiveness of common interpolation algorithms used in 3D subsurface modelling, by using four synthetic grids that represent conditions of varying geologic complexity. Employing synthetic grids for this evaluation allows quantitative statistical assessment (root mean square error and bias error) of the accuracy of the two interpolation algorithms (inverse distance weighting and ordinary kriging) being tested.

The objective of this paper is to evaluate the effectiveness of the two algorithms to model the synthetic grids employing different input data density and spatial distribution patterns. This evaluation will provide valuable information that can be used to guide selection of the most appropriate algorithm, data quantity and data distribution pattern for interpolating subsurface units, and ultimately will lead to more effective and efficient means of modelling subsurface environments.

Chapter 4 – Assessing the Impact of Program Selection on the Accuracy of 3D Geologic Models

As the field of 3D subsurface geological modelling develops at an increasingly rapid rate, so too does the number of available software packages catering to these applications. Although most of these software programs offer very similar ensembles of algorithms for interpolating data, little consideration has been given to the assessment of differences in uncertainty and variability introduced into the model by software program selection. In this study, inverse distance weighted and ordinary kriging algorithms from three different software programs (ArcGIS, ROCKWORKS 2006, and VIEWLOG) were used to interpolate identical datasets. The objective of this paper is to determine if program selection has an impact on model accuracy, and if so, to identify the model conditions resulting in the greatest differences.

Chapter 5 – Conclusions and Recommendations for Future Work

This chapter summarizes the results and conclusions reported in this thesis and makes recommendations for future work.

Reference List

Bajc, A. F. & Newton, M. J. (2005). 3D Modelling of Quaternary Deposits in Waterloo Region, Ontario: A Case Study Using Datamine Studio Software. *Three-Dimensional Geologic Modelling for Groundwater Applications: Workshop Extended Abstracts, Geological Survey of Canada Open File 5048,* 5-10.

Bajc, A. F., Zwiers, W. G., Rainsford, D. R. B., Marich, A. S., & MacCormack, K. E. (2009). A geological investigation of the Dundas buried valley, southern Ontario, Canada. In *Geological Society of America Abstracts with Programs* (pp. 214).

Berg, R. C. & Keefer, D. A. (2004). Commentary - Three-dimensional geologic modeling: challenging our terminology and understanding of geologic maps. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Illinois State Geological Survey (ISGS) Open-File Series 2004-8,* 4-9.

Birken, R. & Versteeg, R. (2000). Use of four-dimensional ground penetrating radar and advanced visualization methods to determine subsurface fluid migration. *Journal of Applied Geophysics, 43,* 215-226.

Bond, C. E., Gibbs, A. D., Shipton, Z. K., & Jones, S. (2007). What do you think this is? "Conceptual uncertainty" in geoscience interpretation. *GSA Today, 17,* 4-10.

Box, G. E. P. (1976). Science and statistics. *Journal of the American Statistical Association, 71,* 791-799.

Brus, D. J., De Gruijter, J. J., Marsman, B. A., Visschers, R., Bregt, K. A., Breeuwsma, A. et al. (1996). The performance of spatial interpolation methods and choropleth maps to estimate properties at points: a soil survey case study. *Environmetrics, 7,* 1-16.

Burt, A. (2004). Three-dimensional mapping of Quaternary (surficial) deposits in the Barrie area, central Ontario. In Summary Field Work and Other Activities 2004. *Ontario Geological Survey,* 35-1-35-5.

Burt, A. (2007). Three-dimensional geological modelling of thick Quaternary deposits in the Barrie-Oro area, central Ontario: new modelling techniques. In Summary of field Work and Other Activities 2007. *Ontario Geological Survey, Open File Report 6145:* 35-1-35-5.

Burt, A. & Bajc, A. F. (2007). New products and advancements in 3-D modelling protocols based on studies in thick drift areas in Ontario, Canada. *Three*

Dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4, 9-13.

Carter, T. R. & Castillo, A. C. (2006). Three-dimensional mapping of Paleozoic bedrock formations in the subsurface of southwestern Ontario: A GIS application of the Ontario petroleum well database. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 435-450). St. John's: Geological Association of Canada.

Costa, J. F. (2003). Reducing the impact of outliers in ore reserves estimation. *Mathematical Geology, 35,* 323-345.

Culshaw, M. G. (2005). From concept towards reality: develiping the attributed 3D geological model of the shallow subsurface. *Quarterly Journal of Engineering Geology & Hydrogeology, 38,* 231-284.

Davis, J. C. (2002). *Statistics and data analysis and geology.* John Wiley and Sons.

de Kemp, E. A. (2006). 3-D interpretive mapping: An extension of GIS technologies for the geoscientist. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 591-612). St. John's: Geological Association of Canada.

Deparis, J., Garambois, S., & Hantz, D. (2007). On the potential of Ground Penetrating Radar to help rock fall hazard assessment: A case study of a limestone slab, Gorges de la Bourne (French Alps). *Engineering Geology, 94,* 89-102.

Devillers, R., Gervais, M., Bedard, Y., & Jeansoulin, R. (2002). Spatial Data Quality: from metadata to quality indicators and contextual end-user manual. In *2002 OEEPE/ISPRIS Joint Workshop on Spatial Data Quality Management* (pp. 45-55).

Devillers, R. & Jeansoulin, R. (2006). Spatial Data Quality: Concepts. In *Fundamentals of Spatial Data Quality.* (pp. 1-312). London: Wiley.

Dey, W. S., Davis, A. M., Abert, C. C., Curry, B. B., & Seiving, J. C. (2005). Three-dimensional geologic mapping of groundwater resources in Kane County, Illinois. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Geological Survey of Canada, Open File 5048,* 21-24.

Dille, J. A., Milner, M., Groeteke, J. J., Moretensen, D. A., & Williams, M. M. (2003). How good is your weed map? A comparison of spatial interpolators. *BioOne, 51,* 44-55.

Eaton, D., Milkereit, B., & Salisbury, M. (2003). Hardrock sesimic exploration: mature technologies adapted to new exploration targets. *The Leading Edge,* 580-585.

Englund, E. J. (1990). A variance of Geostatisticians. *Mathematical Geology, 22,* 417-455.

Feltrin, L., McLellan, J. G., & Oliver, N. H. S. (2009). Modelling the giant, Zn-Pb-Ag Century deposit, Queensland, Australia. *Computers & Geosciences, 35,* 108-133.

Fisher, P., Comber, A., & Wadsworth, R. (2006). Approaches to Uncertainty in Spatial Data. In R.Devillers & R. Jeansoulin (Eds.), *Fundamentals of Spatial Data Quality* (pp. 43-59). Wiley-ISTE.

Frattini, P., Crosta, G., Carrara, A., & Agliardi, F. (2008). Assessment of rockfall susceptibility by integrating statistical and physically-based approaches. *Geomorphology, 94,* 419-437.

Gong, J., Cheng, P., & Wang, Y. (2004). Three-dimensional modeling and application in geological exploration engineering. *Computers & Geosciences, 30,* 391-404.

Goodchild, M. F. (2006). Foreword. In R.Devillers & R. Jeansoulin (Eds.), *Fundamentals of Spatial Data Quality* (pp. 13-16). Wiley.

Goodchild, M. F. & Clarke, K. C. (2002). Data Quality in Massive Data sets. In J.Abello, P. M. Pardalos, & M. G. C. Resende (Eds.), *Handbook of Massive Data Sets* (pp. 643-659). Norwell, MA: Kluwer Academic Publishers.

Goodchild, M. F. & Haining, R. P. (2004). GIS and spatial data analysis: converging perspectives. *Papers in Regional Science, 83,* 363-385.

Gunnink, J. L. (2005). Geological mapping in the Netherlands: the case of the shallow subsurface (- 500 m). In *2005 Annual Meeting Geological Society of America* (pp. 27-30).

Hengxing, L., Martin, C. D., & Lim, C. H. (2007). RockFall analyst: A GIS extension for three-dimensional and spatially distributed rockfall hazard modeling. *Computers & Geosciences, 33,* 262-279.

Houlding, S. W. (1994). *3D Geoscience Modelling.* Hong Kong: Springer-Verlag Berlin Heidelberg.

Houlding, S. W. (2000). *Practical Geostatistics: Modeling and Spatial Analysis.* Germany: Springer-Verlag.

Howard, K. W. F. (1997). Do tills beneath urban Toronto provide adequate groundwater protection? In J.Chilton (Ed.), *Groundwater in the Urban Environment. Rotterdam Vol. 1* (pp. 433-438). AA Balkema.

Howard, K. W. F. & Livingstone, S. J. (2000). Transport of urban contaminants into Lake Ontario via subsurface flow. *Urban Water, 2,* 183-195.

Isaaks, E. H. & Srivistava, R. M. (1989). *An Introduction to Applied Geostatistics.* New York: Oxford University Press.

Jackson, I. (2007). So where do we go from here? *Three-dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4,* 19-22.

Jessel, M. (2001). Three-dimensional geological modelling of potential-field data. *Computers & Geosciences, 27,* 455-465.

Jones, N. L., Davis, R. J., & Sabbah, W. (2003). A comparison of Three-dimensional interpolation techniques for plume characterization. *Groundwater, 41,* 411-419.

Kaufmann, O. & Martin, T. (2008). 3D geological modeling from boreholes, cross-sections and geological maps, application over former natural gas storage in coal mines. *Computers & Geosciences, 34,* 278-290.

Keefer, D. A. (2005). A method for addressing variable data quality and clustered data. *Illinois State Geological Survey (IGSG) Open File Series 2004-8.*

Keefer, D. A. (2007). A framework and methods for characterizing uncertainty in geologic maps. *Three Dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4,* 23-26.

Keefer, D. A. & Rittenhouse, S. (2005). Estimating the uncertainty of 3D geologic maps. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Geological Survey of Canada, Open File 5048,* 31-35.

Keller, G., Matile, G., & Thorleifson, H. (2009). Progress in 3D geological mapping in the eastern prairies of Canada and the USA. In *2009 Annual Meeting Geological Society of America.*

Keller, G., Matile, G., Thorleifson, L. H., & Malolepszy, Z. (2005). 3D geological model of the Red River Valley, Central North America. *Three-Dimensional Geologic Mapping for Groundwater Applications: Workshop Extended Abstracts, Geological Survey of Canada Open File Report 5048,* 35-38.

Kemec, S. & Duzgun, H. S. (2006). Use of 3D visualization in natural disaster risk assessment for urban areas. In A.Abdul-Rahman, S. Zlatanova, & V. Coors (Eds.), *Innovations in 3D Geo Information Systems* (pp. 1-760). New York: Springer-Verlag Berlin Heidelberg.

Krajewski, S. A. & Gibbs, B. L. (1996). *Understanding Contouring*. Colorado: Gibbs Associates.

Kravchenko, A. N. (2003). Influence of spatial structure on accuracy of interpolation methods. *Soil Science Society of America Journal, 67,* 1564-1571.

Lapen, D. R. & Hayhoe, H. N. (2003). Spatial analysis of seasonal and annual temperature and precipitation normals in southern Ontario, Canada. *Journal of Great Lakes Research, 29,* 529-544.

Logan, C., Russel, H. A. J., Sharpe D.R., & Kenny, F. M. (2006). The role of GIS and expert knowledge in 3-D modelling, Oak Ridges Moraine, southern Ontario. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 519-542). St. John's: Geological Association of Canada.

MacCormack, K. E., MacLachlan, J. C., & Eyles, C. H. (2005). Viewing the subsurface in three dimensions: Initial results of modeling the Quaternary sedimentary infill of the Dundas Valley, Hamilton, Ontario. *Geosphere, 1,* 23-31.

Milkereit, B., Berrer, E. K., King, A. R., Watts, A. H., Roberts, B., Adam, E. et al. (2000). Development of 3-D seismic exploration technology for deep nickel-copper deposits - a case history from the Sudbury basin, Canada. *Geophysics, 65,* 1890-1899.

Nalder, I. A. & Wein, R. W. (1998). Spatial interpolation of climatic Normals: test of a new method in the Canadian boreal forest. *Agricultural and Forest Meteorology, 92,* 211-225.

O'Connor, D. R. (2002). *Report of the Walkerton Inquiry: Part 1 - The Events of May 2000 and Related Issues* Toronto.

Ongaro, T., Neri, A., Menconi, G., Vitturi, M., Marianelli, P., Cavazzoni, C. et al. (2008). Transient 3D numerical simulations of column collapse and pyroclastic density current scenarios at Vesuvius. *Journal of Volcanology and Geothermal Research, 178,* 378-396.

Parks, K., Andriashek, L., & Atkinson, N. (2005). Lowering barriers to public communication with 3D groundwater mapping at Alberta Geological Survey: Examples from Canada's Oil Sands Area. *Three-Dimensional Geological Mapping for Groundwater Applications: Workshop Extended Abstracts, Geological Survey of Canada Open File 5048,* 57-60.

Paulen, R. C., McClenaghan, M. B., & Harris, J. R. (2006). Bedrock topography and drift thickness models from the Timmins area, northeastern Ontario: An application of GIS to the Timmins overburden drillhole database. In J.R.Harris (Ed.), *GAC*

Special Paper 44: GIS for the Earth Sciences (pp. 413-434). St. John's: Geological Association of Canada.

Pranter, M. J., Ellison, A. I., Cole, R. D., & Patterson, P. E. (2007). Analysis and modeling of intermediate-scale reservoir heterogeneity based on a fluvial point-bar outcrop analog, Williams Fork Formation, Piceance Basin, Colorado. *AAPG Bulletin, 91,* 1025-1051.

Rawling, T. J., Schaubs, P. M., Dugdale, L. J., Wilson, C. J. L., & Murphy, F. C. (2006). Application of 3D models and numerical simulations as a predictive exploration tool in western Victoria. *Australian Journal of Earth Sciences, 53,* 825-839.

Ross, M., Parent, M., & Lefebvre, R. (2005). 3D geologic framework models for regional hydrogeology and land-use management: a case study from a Quaternary basin of southwestern Quebec, Canada. *Hydrogeology Journal, 13,* 690-707.

Saito, H. & Goovaerts, P. (2002). Accounting for measurment error in uncertainty modeling and decision-making using indicator kriging and p-field simulation: application to a dioxin contaminated site. *Environmetrics, 13,* 555-567.

Schloeder, C. A., Zimmerman, N. E., & Jacobs, M. J. (2001). Comparison of methods for interpolating soil properties using limited data. *Soil Science Society of America Journal, 66,* 479.

Sech, R. P., Jackson, M. D., & Hampson, G. J. (2009). Three-dimensional modeling of a shoreface-shelf parasequence reservoir analog: Part 1. Surface-based modeling to capture high-resolution facies architecture. *AAPG Bulletin, 93,* 1155-1181.

Sharpe, D. R., Hinton, M. J., & Russell, H. A. J. (2002). The need for basin analysis in regional hydrogeological studies: Oak Ridges Moraine, southern Ontario. *Geoscience Canada, 29,* 3-20.

Sharpe, D. R. & Russell, H. A. J. (2005). Basin analysis applied to modelling buried valleys in the Great Lakes basin. In *Geological Assoication of Canada/Mineralogic Association of Canada, 49th Annual Meeting.*

Strong, D. M., Lee, Y. W., & Wang, R. Y. (1997). Data Quality in Context. *Communications of the ACM, 40,* 103-110.

Susini, S. & De Donatis, M. (2009). 3D model of a sector of the South Scotia Ridge (Antarctica). *Computers & Geosciences, 35,* 83-91.

Tacher, L., Pomian-Srzednicki, I., & Parriaux, A. (2006). Geological uncertainties associated with 3-D subsurface models. *Computers & Geosciences, 32,* 212-221.

Thorleifson, L. H. & Berg, R. C. (2002). Introduction - The need for high-quality three-dimensional geological information for groundwater and other environmental applications. *Geological Survey of Canada, Open File 1449.*

Venteris, E. R. (2007). 3-D modeling of glacial stratigraphy using public water well data, geologic interpretation, and geostatistics. *Three-dimensional Geological Mapping for Groundwater Applications: Workshop Extended Abstracts, Minnesota Geological Survey Open-File Report 07-4,* 81-84.

Walker, D. D. & Loftis, J. C. (1997). Alternative spatial estimators for ground-water and soil measurements. *Groundwater, 35,* 593-599.

Weber, D. & Englund, E. J. (1992). Evaluation and comparison of spatial interpolators. *Mathematical Geology, 24,* 381-391.

Weber, D. & Englund, E. J. (1994). Evaluation and comparison of spatial interpolators II. *Mathematical Geology, 26,* 589-603.

Wu, Q., Xu, H., & Zou, X. (2005). An effective method for 3D geological modeling with multi-source data integration. *Computers and Geosciences, 31,* 35-43.

Zanchi, A., Francesca, S., Stefano, Z., Simone, S., & Graziano, G. (2009). 3D reconstruction of complex geological bodies: Examples from the Alps. *Computers & Geosciences, 35,* 49-69.

Zimmerman, D., Pavlik, C., Ruggles, A., & Armstrong, M. P. (1999). An experimental comparison of Ordinary and Universal Kriging and inverse distance weighting. *Mathematical Geology, 31,* 375-390.

Zwiers, W. G., Rainsford, D. R. B., & Bajc, A. F. (2008). Project Unit 06-026: investigation of the Dundas Buried Bedrock Valley. *Summary of Field Work and Other Activities 2008, Ontario Geological Survey, Open File Report 6226,* 33-1-33-7.

CHAPTER 2

ENHANCING THE RELIABILITY OF 3D SUBSURFACE MODELS THROUGH DIFFERENTIAL WEIGHTING AND MATHMATICAL RECOMBINATION OF VARIABLE QUALITY DATA

Abstract

One of the first stages of the 3D subsurface modelling process involves collation and analysis of available borehole and/or outcrop data to identify individual subsurface units, usually distinguished by the grain size of the sediment, and the elevation of their bounding contacts. Input data can come from a variety of sources and may be categorized according to their reliability and/or quality. The output from the 3D model is a prediction of subsurface conditions based on these data and the reliability of the output model is highly dependent on both the quality of input data and the types of interpolation methods used.

This paper presents a new 'Quality Weighting' methodology that allows the user to assign a differential weighting factor to data points of variable quality in the modelling process. Input data are categorized into High and Low Quality Datasets which are then recombined using a grid math process in which a differential 'weighting' factor is applied. This allows the 3D modelling program to maximize the use and effectiveness of data from all available sources while giving high quality data greater influence on the

final model output and will result in the generation of more accurate and reliable 3D subsurface models.

2.1 Introduction

Three-dimensional (3D) models are now being used by both private industry and government agencies to visualize subsurface geological characteristics as they readily communicate complex concepts to both specialists and the general public (EarthFX, 2004; Jackson, 2004; Kessler et al,. 2005; Parks et al., 2005; RockWare, 2006; Jackson, 2007; Zwiers et al., 2008). The versatility and effectiveness of 3D subsurface geological models allows them to be used in many different applications ranging from resource exploration (Gong et al., 2004; Paulen et al., 2006; Kaufmann and Martin 2008) and delineation of groundwater source protection areas (Ross et al., 2005; Burt, 2007; Zwiers et al., 2008), to the reconstruction of past geologic events and processes (MacCormack et al., 2005; Logan et al., 2006). Although 3D subsurface models are now routinely used in both geological and hydrogeological applications, the accuracy and reliability of the 3D subsurface models being generated is often questionable (Thorleifson and Berg, 2002; Keefer and Rittenhouse, 2005; Venteris, 2007). A 'reliable' 3D subsurface model is considered here to be a representation of subsurface conditions that most closely conforms to the known stratigraphy and geological history of the region, provides consistent results when repeatedly run, is compatible with information entered for individual data points, and is supported by data from 'proxy' sources. The reliability of 3D subsurface models is particularly questionable in areas where data are sparse,

unevenly distributed and/or come from sources where there is little to no control on the quality or accuracy of the input data.

The increased demand for 3D models to be created in short time frames has created a dependency on large, readily available digital databases such as the Ontario Water Well Database (OWD, a digital database recording sediment types encountered during drilling of individual water wells in the province) for input data. A major issue with relying on water well data as the primary (or only) data source is that large digital databases commonly contain data of variable quality. The geologic data collected by well drillers can lack consistency in terms of the classification of sediment types and wells are often wrongly located by position or elevation (Logan et al., 2006; Russell et al., 2007; Dumedah and Schuurman, 2008). Typically, this lack of positional and descriptive accuracy is a result of the driller's being focused on finding water rather than being concerned with precisely describing the characteristics of subsurface sediments and the elevation of unit contacts.

A serious concern with the 'unedited' use of large digital databases, such as the OWD, as the primary source of data for 3D subsurface modelling is the variable quality of the input data, which severely reduces the reliability of model outputs (Goodchild and Clark, 2002; Burt, 2004; Dey et al., 2005; Logan et al., 2006; Carter and Castillo, 2006; Venteris, 2007). Most 3D modelers are beginning to acknowledge that their datasets are composed of variable quality data (Thorleifson and Berg, 2002; Bajc et al., 2004; Logan et al., 2006; Kaufmann and Martin, 2008) but many others do not. Unfortunately, despite recognition of the problem of variable data quality in the modelling process, little is being

done to address and rectify this issue (Logan et al., 2006; Keefer and Rittenhouse, 2005; Burt 2007). According to Wang et al. (1995), the need for controls on data quality will become increasingly important as liability issues associated with actions taken based on the results of model outputs increase. As more datasets become available in digital format, there is more opportunity for unreliable data to be distributed along the various information highways that provide information for subsurface modelling and analysis. Manipulation and amalgamation of databases increases the likelihood that metadata will become separated from the data rendering the model user unsure as to the quality and nature of the data the model is based upon (Devillers et al. 2002). It has been estimated by Strong et al. (1997) that the impact of unconstrained use of low quality data could cost both society and the economy *billions* of dollars in lawsuits and poor decision-making based on inaccurate information contained in model outputs.

The variability of data quality, particularly within large digital databases, presents a major problem when trying to create accurate and reliable 3D models. Most modelling programs take the data point values at face-value and do not consider that some may be more reliable than others and should therefore be given more weight (influence) in the calculation of the node values used to create modelled units. Ideally, datasets used for 3D subsurface modelling should be composed of high quality data points (obtained from sources with a high degree of reliability such as outcrop descriptions or borehole logs) that are evenly distributed and span the entire study area, but this does not generally occur in practice (Issaks and Srivastava, 1989; Houlding, 1994). Typically, in regional studies, high quality data are clustered together around local study sites and are sparse across the

larger study area. In order to create an effective regional scale model it may therefore be necessary to include variable quality data from other sources to enhance the spatial data coverage. Unfortunately, the inclusion of significant numbers of low quality data points within an overall dataset may override the influence of high quality data and negatively affect both the accuracy and reliability of the model output (Weir 2002).

This paper presents a methodology for 'quality weighting' input data used in 3D subsurface modelling that allows high quality data to have a greater influence on the model output than less reliable (low quality) data. Subsurface data from the McMaster University campus, Hamilton, Ontario (Figure 2.1) and surrounding area are utilized here to test this new methodology. The McMaster campus area was selected because of the availability of both high and low quality subsurface data, and proxy data against which model outputs can be compared. For this study, the 3D geometry of a coarse sand and gravel unit lying approximately 10m below the ground surface was modelled as it forms a significant local aquifer and has been the focus of other hydrogeological and contaminant migration studies (Conestoga Rovers and Associates 1996). The study area covers 0.62 square kilometres and contains 113 boreholes that penetrate the sandy gravel aquifer, of which 44 are considered to be high quality records and 69 are low quality records (Figure 2.2, see section 2.2). In addition to the availability of both high and low quality borehole data from the McMaster campus area, investigations of groundwater contamination in the surrounding area provide data on the location and direction of groundwater flow pathways that may be used to identify permeable units in the subsurface. These proxy

Figure 2.1: A) & B) Maps showing the location of McMaster Campus in Southern Ontario. Photos courtesy of Google Earth and Hamilton Maps.

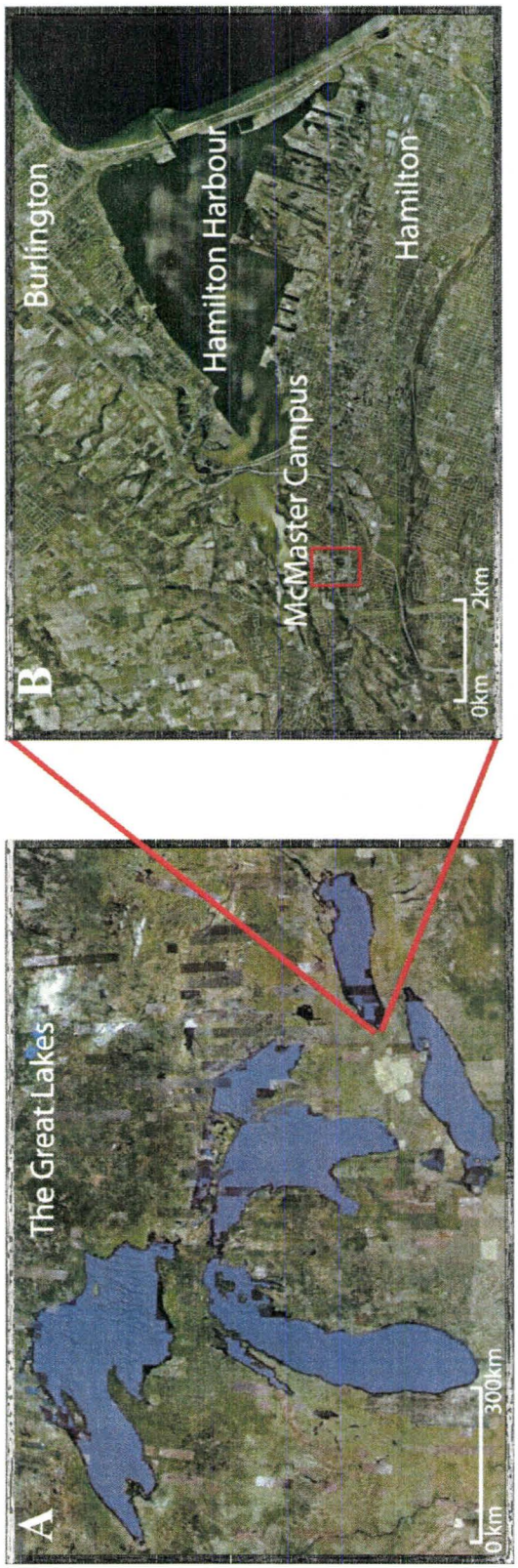

B
Burlington
Hamilton Harbour
McMaster Campus
Hamilton
0km
2km
A
The Great Lakes
0km
300km

Figure 2.2: Georeferened airphoto of the McMaster campus showing the location of the borehole data classified according to the quality of the data. High quality data points are shown as circles, low quality data points by squares, and erroneous data points (outliers) are shown as stars.


340m
0m

data are used here to validate model outputs and test the effectiveness of the 'quality weighting' methodology proposed here.

2.2 Sources of Data and Data Classification

3D modelling programs used in Quaternary geological and hydrogeological applications require input data on subsurface sediment types and the elevation of bounding contacts between different sediment types as well as borehole location data in order to accurately model physical properties through space. These data can come from a variety of sources including the OWD, foundation reports available from agencies such as the Ontario Ministry of Transportation, the borehole database compiled by the Ontario Geologic Survey (OGS), the Hamilton Wentworth Urban Geology Database (HWUGD) compiled by the Geological Survey of Canada (GSC), soil surveys conducted by local and municipal agencies, and individual construction and engineering reports.

The quality of subsurface data available from each of these sources is extremely variable and depends to a large extent on the initial objective of data collection. Data considered to be the most reliable, and highest quality for 3D subsurface modelling purposes come from site specific soil, engineering, or construction reports for which a detailed understanding of the subsurface sediment characteristics and the subsurface elevation of unit contacts were a primary goal of data collection. Less reliable, lower quality data typically come from large digital databases such as the OWD for which the primary goal of the initial data collection was to locate water sources, and some of the

records were created by drillers with little expertise in the area of sediment description (Logan et al., 2006; Venteris, 2007). This can lead to inconsistent reporting of sediment types, which were of secondary importance in the data collection process, and to subsequent inaccuracies in the calculation of subsurface unit elevations and thicknesses. Inaccuracies in sedimentary unit thicknesses recorded in water well databases are described by Logan et al. (2006) and can be substantial.

Unfortunately, as the demand for 3D subsurface geological models has been steadily increasing over the past few years, so too has the dependency on large, readily available digital databases, such as the OWD, for input data in order to produce models in shorter time frames. These databases are often utilized for 3D subsurface modelling because they are easily accessible, available in digital format, and also provide good coverage in rural areas which are generally lacking in other sources of data. However, the inclusion of inaccurate data can seriously 'dilute' the influence of any available high quality data, negatively affecting both the accuracy and reliability of the model output.

In addition, the requirement to create 3D models quickly, and often for large geographic areas, has resulted in the development of many 3D modelling programs that function essentially as 'black boxes' requiring very little operator control. Hence, deficiencies in data quality or coverage are seldom acknowledged or compensated for and the quality of the model output is often compromised. In many studies the only data quality control measures implemented involve finding and eliminating anomalous data points (outliers), such as those with very obvious unrealistic surface elevations or incorrect geographic coordinates. This is often done by visually examining two

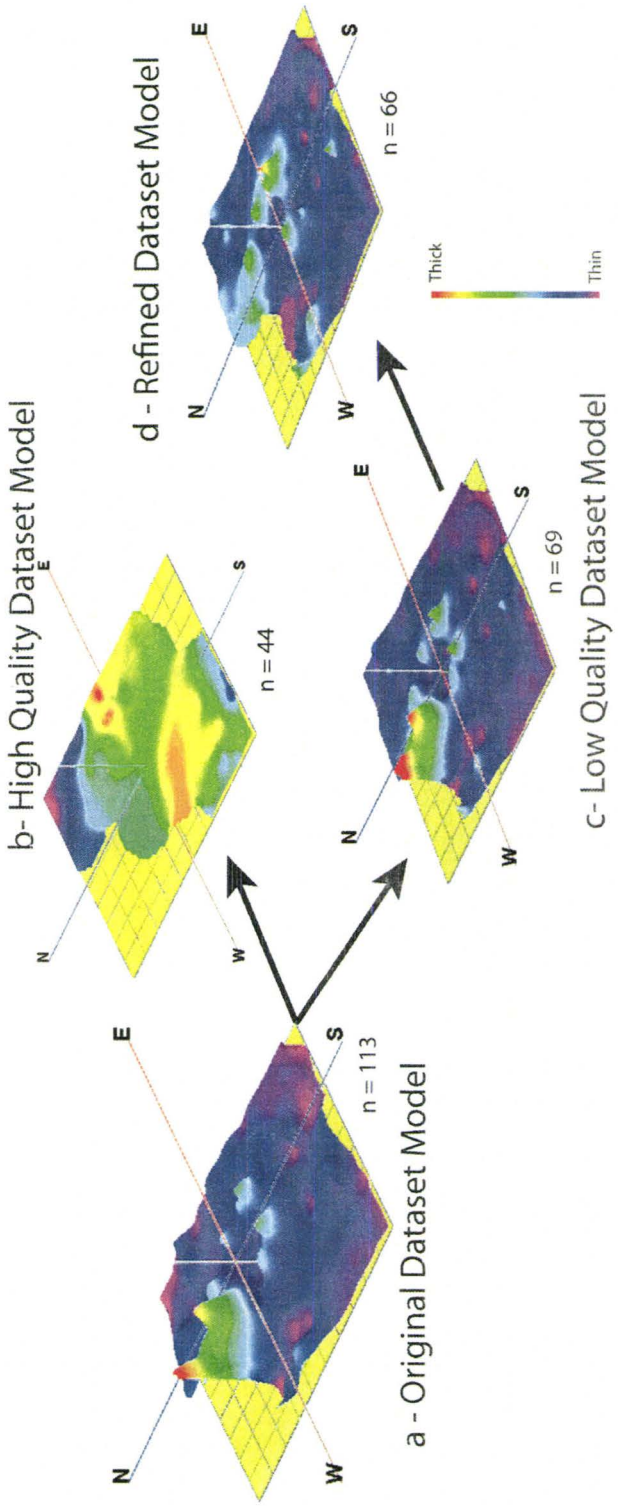
dimensional cross-sections generated from the data and then manually deleting the borehole records that appear to be 'outliers' (Macfarlane and Schneider, 2007; Venteris, 2007). The problem with this process is that it is unlikely to eliminate all erroneous data points, which are then incorporated into the model. This is of particular concern when modelling large areas with sparse data coverage as it can be difficult to locate and gather sufficient data to allow identification of potential outliers. Also, certain studies, such as those conducted for the mining industry, are faced with the added complexity that it may be the so-called 'outliers' that are the points of interest. There is no set procedure for determining the presence of outlier data (Costa, 2003), which can be identified in various ways depending on the focus of the study and the modelling procedure utilized. Discriminating outliers that represent true values from those that are erroneous data points can be difficult and requires careful data screening prior to modelling in order to identify data points that are inconsistent with others in the vicinity (Barnett and Lewis, 1994; Venteris, 2007).

In the McMaster University campus study area 113 borehole records identify the underlying sand and gravel aquifer. All of the available data were complied into a single database (herein referred to as the Original Dataset). These data were then classified according to the perceived quality of the borehole records, and subdivided into two separate databases containing either high or low quality data (herein termed the High Quality and Low Quality datasets respectively). A similar classification of input data into various categories prior to modelling was carried out in a study conducted by Burt and Bajc (2007) in which they identified high quality data (continuous cored holes, outcrop

logs, and engineering test holes), medium quality data (mud rotary and questionable consultants logs), and low quality data (water well records). Of the 113 borehole records available from the McMaster campus, 44 are considered to be high quality records and 69 are low quality records (Figure 2.2). The high quality borehole records were obtained from an environmental investigation and assessment study and geotechnical engineering reports that contain detailed descriptions of subsurface sediments and the elevation of contacts between units. The 69 low quality borehole records came from two large digital databases (the OWD and the Hamilton Wentworth Urban Geology Database – HWUGD) that contain only minimal information about sediment characteristics and may include inaccurate documentation of borehole locations and the elevation of unit contacts.

In order to evaluate the effects of data quality on 3D model output, each of the three datasets (Original, High Quality, and Low Quality) were used to separately model the sand and gravel unit using inverse distance weighting in ROCKWORKS 2006, although any interpolation algorithm could be used (Figure 2.3). Initial model outputs showed that the Low Quality Dataset included some very obvious outliers that identified the sand and gravel unit to have a thickness approximately 7 times greater than that recorded by surrounding data points. This extreme variation in thickness is incompatible with the geological context of the unit and inconsistent with surrounding data points, therefore these erroneous points were removed (Venteris, 2007). The removal of these 'outliers' created a modified dataset that will be referred to as the Refined Dataset (Figure 2.3). This fourth dataset was included in the analysis because in some studies, tests are done to identify and remove the most obvious outliers as they have been known to have

Figure 2.3: The data were separated into 4 datasets based on quality and then used to model the thickness of the sand and gravel aquifer using ROCKWORKS 2006. The dataset containing all the available data (the Original Dataset; a) was split into two separate datasets; one containing only high quality data (b) and the other containing only low quality data (c). The outliers were removed from the Low Quality Dataset to create a Refined Dataset (d).


a - Original Dataset Model
n = 113
b- High Quality Dataset Model
n = 44
c- Low Quality Dataset Model
n = 69
d - Refined Dataset Model
n = 66
Thick
Thin
N
E
S
W

significant impact on the analysis and interpolation results (Barnett and Lewis, 1994; Costa, 2003; Venteris, 2007). In order to test the improvement in the model output resulting from the use of a Quality Weighted approach over current methods, it was important to consider models generated with this Refined Dataset.

2.3 Data Modelling

Low quality data can have a large negative impact on the output model due to the process by which 3D modelling programs interpolate subsurface units from spatially scattered point data (Lee et al. 1992). Most modelling programs store available borehole information as a series of data points which are used by a selected mathematical process (the algorithm) to calculate node values that will form the grid (Figure 2.4). A node is an estimated value calculated by the gridding algorithm at each grid-line intersection along the grid surface, and its value is based on proximal (nearby) point data. The node values are then used by the 3D software to create grids that represent estimated bounding surfaces which are essentially visual representations of the combined node values. Current modelling algorithms assign 'weights' to the data point values based on their relative distance from a grid node, and do not take into consideration the quality/reliability of the value (Figure 2.5). Therefore, when there are data points of varying quality within the search radius of a particular grid node, the closest data point will have the most influence on the estimated value of that grid node regardless of its quality or reliability (Figure 2.5). This can be a problem if the closest data point is of low

Figure 2.4: Diagram to show how data points located in space (A) are overlain by a grid (B) populated by grid nodes which are values calculated by the selected interpolation algorithm (C).

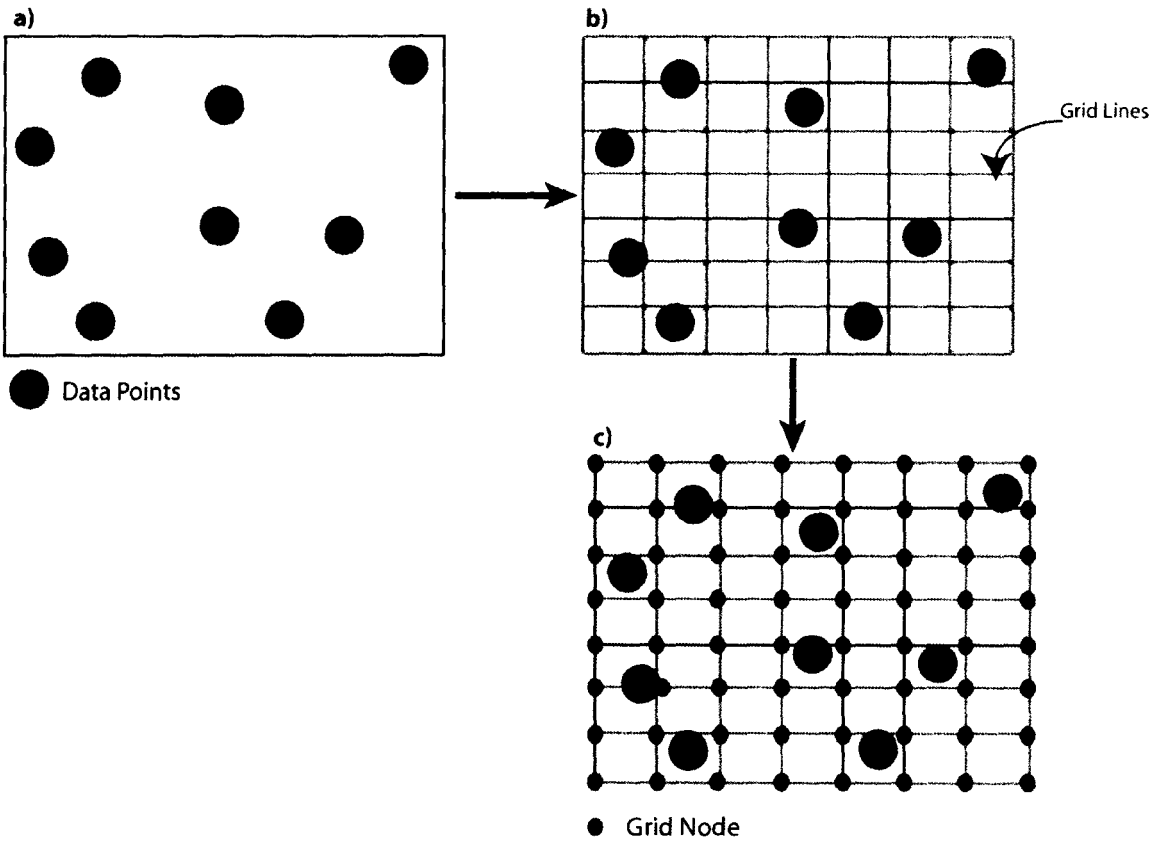
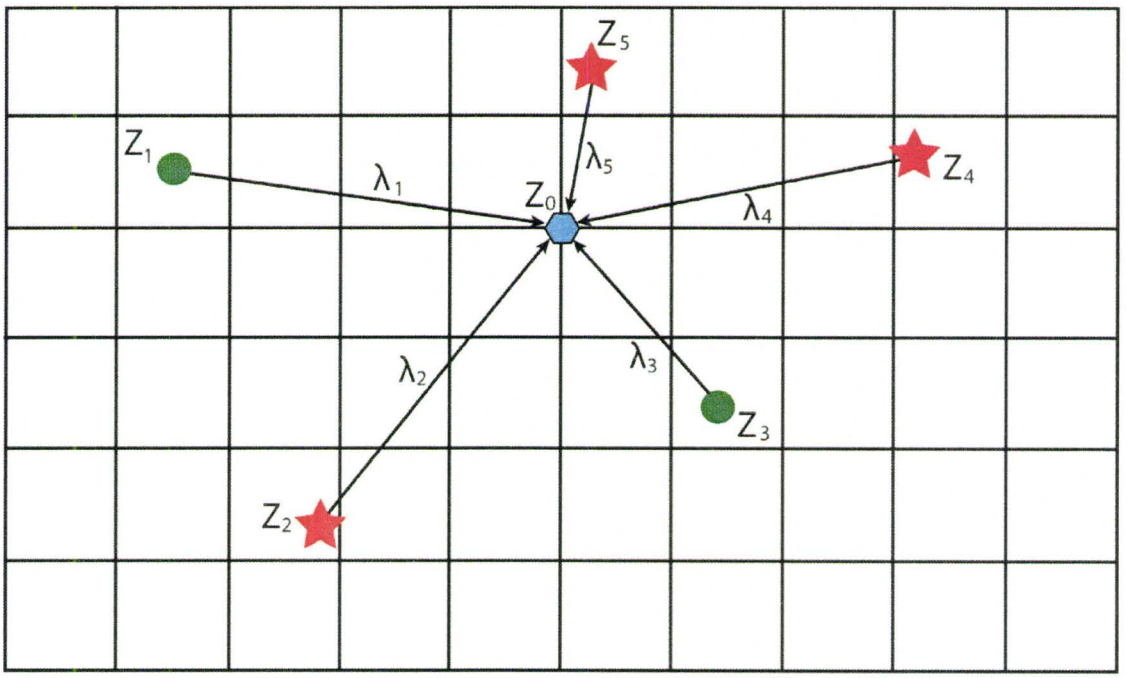

a)
b)
Grid Lines
Data Points
c)
Grid Node

Figure 2.5: Diagram to show how the weights are determined for gridding algorithms. Typical algorithm weights are based on the distance of the data points (circles & stars) from the node of interest (hexagon).



Z_0 = Interpolated Node Value (⬡)
Z_n = Data Points (measured observations)
λ_n = Weights Assigned to Data Point Values
★ = Low Quality Data
● = High Quality Data

quality (less reliable) because it will have more influence on the estimated value for the surrounding grid nodes, which may result in an inaccurate prediction. Ideally, high quality data points within the search radius should have the greatest influence on the node values thereby increasing the reliability of the predictions and subsequent model.

2.3.1 Creating a differential 'Quality Weighting' mechanism

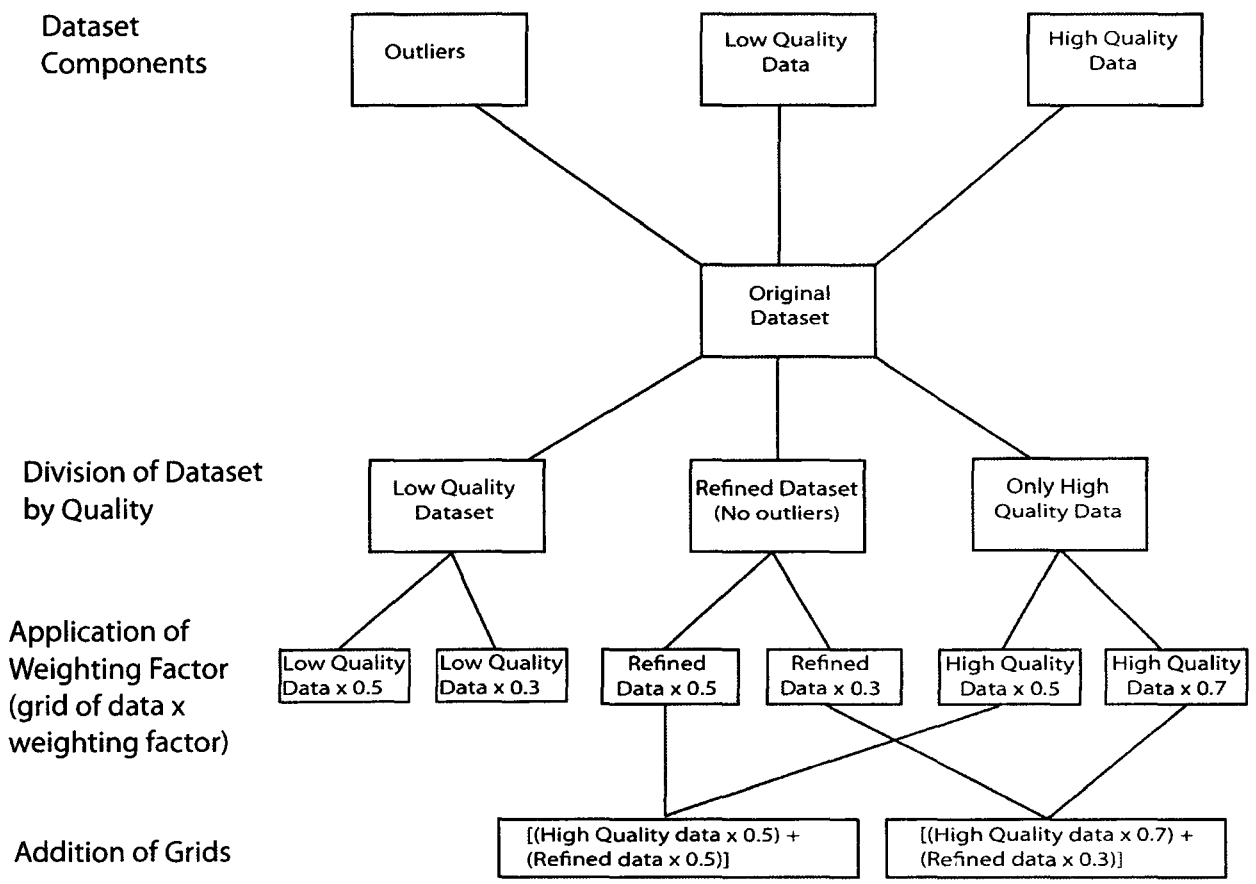
In order to differentially weight the data of high and low quality and modify their influence on model creation, the data points from each of the four McMaster campus datasets (Original, High Quality, Low Quality, and Refined Datasets) were used independently to calculate grid node values which could be modelled and visualized (Figure 2.6). Separate grid models predicting the thickness of the sandy gravel unit were then created using each of the four datasets. These individual grid models were all created with a 1x1 grid cell size so they could be mathematically recombined with one another using a grid math process. This allows a relative 'weighting' (w_n) of the data points to be imposed on the individual grids (Grid A_n) combined to create the final model (Grid B).

$$(\text{Grid } A_1 \times w_1) + (\text{Grid } A_2 \times w_2) = \text{Grid B } [A_1(w_1) + A_2(w_2)]$$

$$\text{Where } w_1 + w_2 + \ldots\ldots + w_n = 1$$

By performing this process, it was possible to assign a higher weighting factor to the higher quality data giving it more 'influence' in the output results of the model. The impact of this relative weighting process on the model output was further explored by

Figure 2.6: Flow chart showing how the grids created by the high and low quality datasets were then multiplied by a 'weighting factor' to either enhance or decrease the influence of the respective data on the final output model. The weighted grids were then mathematically recombined with one another using a grid math process. Assigning a larger relative weighting factor to the grid created by the high quality data allows it to have a greater influence on the final model output.


Dataset Components
Outliers
Low Quality Data
High Quality Data
Original Dataset
Division of Dataset by Quality
Low Quality Dataset
Refined Dataset (No outliers)
Only High Quality Data
Application of Weighting Factor (grid of data x weighting factor)
Low Quality Data x 0.5
Low Quality Data x 0.3
Refined Data x 0.5
Refined Data x 0.3
High Quality Data x 0.5
High Quality Data x 0.7
Addition of Grids
[(High Quality data x 0.5) + (Refined data x 0.5)]
[(High Quality data x 0.7) + (Refined data x 0.3)]

factoring each of the grid models produced from the datasets by a certain % value to either enhance or reduce the influence of those data in the final model. For example, if two modelled grids (e.g. Grid A_1 and A_2) are each factored by 0.5 and then recombined; both grids have equal influence (50% grid A_1 and 50% grid A_2) on the resultant combination grid.

$$(\text{Grid } A_1 \times 0.5) + (\text{Grid } A_2 \times 0.5) = \text{Grid B } [A_1(0.5) + A_2(0.5)]$$

However, if Grid A_1 is factored by 0.7 and Grid A_2 is factored by 0.3 before they are combined, then Grid A_1 will have much greater impact on the interpolation results than Grid A_2.

$$(\text{Grid } A_1 \times 0.7) + (\text{Grid } A_2 \times 0.3) = \text{Grid B } [A_1(0.7) + A_2(0.3)]$$

This methodology allows the user to select certain grids to have a greater or lesser influence on the final model output. There are no set guidelines for choosing the relative grid weights as these need to be determined by the user on the basis of their understanding of the geological complexity of the area, their confidence in the data, the spatial distribution of data points, and the purpose of their study. The complexity of the subsurface geology can have a considerable effect on how certain datasets are weighted. If the subsurface units are organized in a 'layer cake' fashion with little spatial variability across the study area, then the variation in the data values would be minimal, and points that are inaccurately located would have little effect on the final model. In this situation, differential weighting of the data may have minimal impact, and it would be reasonable to assign similar weights to all of the data. However if the subsurface geology is complex

with significant thickness variation within and between individual units, then it is necessary to use as much data as possible in order to accurately define subsurface unit geometries. In this case, it is more difficult to identify outliers and points that are misplaced, both of which could have a large negative impact on the accuracy of the final model output (Costa, 2003). In complex environments there is greater opportunity for less reliable data sources to introduce undetected errors into the model. Hence, when expert knowledge indicates a complex geological framework in the study area, it may be best to assign a greater weight to the higher quality and more reliable data, while utilizing the lower quality data to help constrain the model in areas where high quality data points are sparse. Using expert knowledge to determine data quality has been used in several previous studies (Logan et al., 2006; Burt and Bajc, 2007; Venteris, 2007).

The spatial distribution of data across the study area can also have an effect on how datasets are differentially weighted in the modelling process. If high quality data are clustered in one region of the study area, it may be not appropriate to give a very high weighting to these data as this may unnecessarily distort the model in favour of the clustered data values which may not be representative of the whole study area. Conversely, if high quality data are well dispersed across the study area, the model may benefit from assigning them a relatively higher weighting factor in order to ensure that the final model most closely conforms to the high quality data points in those locations.

Finally, assigning relative weights to datasets can also be influenced by the purpose of the study and the mode of data collection. Primary data, collected for the purpose of the current study, are considered to be of high quality as the user is familiar

with the methods used for data collection, and is able to enforce quality control mechanisms. The use of secondary data collected for a different purpose may not reliably record the required features and can introduce error into the model. However, these secondary data can be extremely important in providing a broad spread of data points to enhance the limited regional coverage provided by high quality data. Assigning these lower quality data a weighting factor that allows them to influence the model output but limits their impact is appropriate. It is possible for the same data to be considered different quality to different users (Devillers and Jeansoulin, 2006).

Taking the above factors into consideration, the Quality Weighted methodology allows the user to assign relative weightings to two or more data sets, allocating the highest % weighting to the category desired to have most influence on the model output, and a lesser % weighting to the other categories. When assigning weights to the data, it is important to consider the geological complexity, confidence in the data, the spatial distribution of data points, and the purpose of the study. The weights can be assigned to datasets split into either High and Low quality, or can be applied to datasets classified into three or more categories (e.g., Burt and Bajc, 2007). In these cases, the user would allocate the highest % weighting to the category desired to have most influence on the model output, and a lesser % weighting to the other categories. For example, a 50%-30%-20% or even a 60%-30%-10% weighting could be applied as long as the relative weights add to 1.

For this study of the McMaster campus and surrounding area, expert knowledge of the subsurface geology was obtained from previously published studies that suggest the

presence of an ancient shoreline beach deposit approximately 10 meters beneath the McMaster campus (Karrow, 1963; Conestoga-Rovers and Associates, 1996). The High Quality Dataset indicated the thickness of this sand and gravel unit to be between 0.19m and 3.07m where as the Low Quality Dataset showed thickness values between 0.03 and 27.12m (Table 2.1). The upper thickness values are unreasonable for this type of shoreline deposit and some values included in the Low Quality databset are therefore considered to be unreliable. However, the inclusion of low quality data in the production of the model is deemed necessary as the high quality data are clustered along the northern and eastern sections of the study area and missing or sparse in other areas (Figure 2.2). In order to produce a model based on good spatial data coverage, it was therefore necessary to allow the more regionally extensive, but lower quality data some influence over the production of the final model. It was decided to apply a 70% and 30% weighting to the high and low quality data respectively to create a model that was most strongly aligned with the high quality data but constrained by the lower quality data in the areas where the high quality data were absent.

2.4 Testing the Method: Model Outputs

In order to test the Quality Weighted methodology proposed here, the output from a Quality Weighted model is compared to a series of un-weighted models to see whether this process is able to improve the accuracy of the final output. The comparison can be done visually by examining output images and by creating maps to identify the

Table 2.1: Actual (observed) and interpolated grid thickness node values with corresponding volumes and standard deviations for the sandy gravel aquifer unit for both the weighted and unweighted datasets.

Dataset	Interpolated Minimum	Interpolated Maximum	Volume	Standard Deviation	Actual Minimum	Actual Maximum
Original Dataset	0.31	15.82	6,398,493	1.97	0.03	27.12
High Quality Dataset	0.19	3.07	3,576,689	0.71	0.15	3.6
Low Quality Dataset	0.04	16.15	6,400,121	2.34	0.03	27.12
Refined Dataset	0.04	11.92	5,327,766	1.35	0.03	12.4
High(0.7) + Low(0.3)	0.74	6.07	4,503,571	0.78	-	-
High(0.5) + Low(0.5)	0.89	8.95	5,121,492	1.21	-	-
High(0.7) + Refined (0.3)	0.73	3.72	4,180,955	0.58	-	-
High(0.5) + Refined (0.5)	0.89	4.79	4,583,799	0.83	-	-

differences between output grids, and quantitatively by comparing the volume estimates created for subsurface units by each model.

2.4.1 Visual Comparison of Model Outputs

Visual comparisons were made between model outputs generated using the Quality Weighted methodology and those generated from the individual High Quality, Low Quality, Refined, and Original Datasets (Figure 2.3). The High Quality Dataset produces a model showing the subsurface sandy gravel unit to have a relatively consistent thickness across the study area (thickness ranges between 0.19 and 3.07 m; Table 2.1) and a gently undulating surface topography (Figure 2.3B). The thickness of this unit, modelled using both the Original Dataset and the Low Quality Dataset are much more variable (thickness ranges between 0.03m and 27.12m; Table 2.1) with an irregular surface topography controlled to a large extent by the presence of several erroneous data points (outliers) in the central north-west region of the study area (Figure 2.3A, C). The unit modelled by the Refined Dataset does not have the extreme values present in the Low Quality Dataset but still shows considerable thickness variation (between 0.03 and 12.4m, Table 2.1). Much of this variation in unit thickness may be due to erroneous data points that are still included in this dataset (Table 2.1, Figure 2.3D).

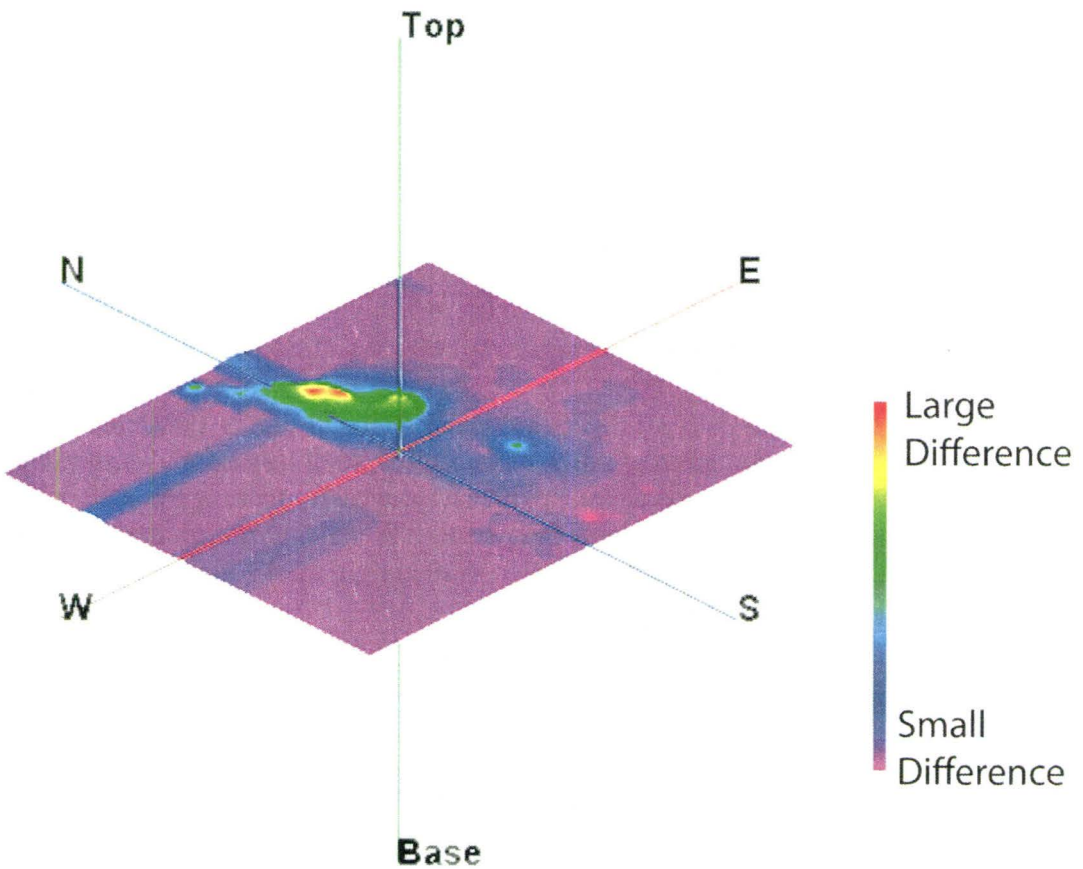
2.4.2 Grid Math

A grid math process involving subtraction of one grid from another was utilized to visualize and evaluate the effects of differentially weighting the high and low quality data on the output models. This process involved subtracting the weighted grids from the un-

weighted grids and the results are shown as areas of similarity and difference on a series of maps presented in Figure 2.7.

Identifying the differences between grid models created with the Low Quality Dataset and the Refined Dataset shows that the only significant difference between the two grids lies in areas adjacent to erroneous data points (outliers; Figure 2.9). The dark shaded areas (Figure 2.7) identify regions of the study area impacted the most strongly by the extreme outliers. The lighter sections of the map represent areas where the removal of the outliers had little or no effect. This same process was used to compare the differences between the Quality Weighted grids and the un-weighted grids (Figures 7, 8, 9). The Quality Weighted grid that combined [High (0.7) + Refined (0.3)] data was compared to the grid composed only of high quality data in order to identify the impact of including lower quality data that is constrained in its degree of influence by the weighting process. The most significant differences between the two maps occur along the north-west perimeter of the study area where the high quality grid lacks data points (Figure 2.8) and the Quality Weighted grid was able to use the lower quality data points to constrain the extremities of the grid surface (Figure 2.8). However, in the areas where high quality data were available, there is little difference between the [High (0.7) + Refined (0.3)] Quality Weighted grid and the grid composed of only of High Quality data points. This suggests that the combined Quality Weighted grid methodology was able to limit the effects of the lower quality data in areas where high quality data exist, while allowing low quality data to influence the grid in areas where high quality data are sparse.

Figure 2.7: Map showing the difference in thickness of the sand and gravel unit between the model generated with Low Quality Dataset and Refined Dataset. The greatest difference in thickness occurs in the area of the outliers which were removed from the Refined Dataset. Areas where the two grids are very similar appear as purples and blues, the green areas of the grid indicate where there are small differences, whereas areas of reds and yellows highlight the areas where the greatest differences occur.


Top
N
E
W
S
Base
Large Difference
Small Difference

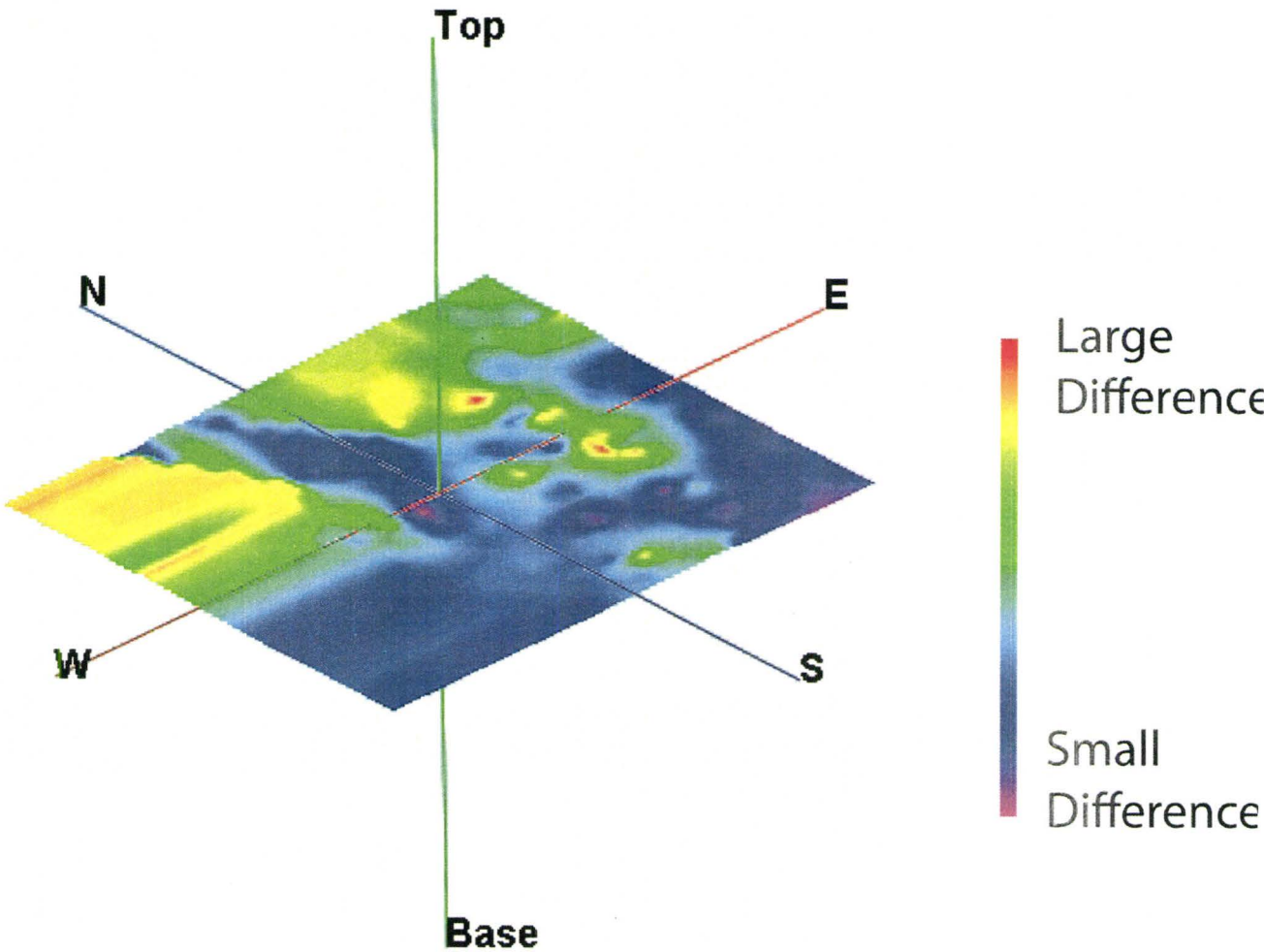
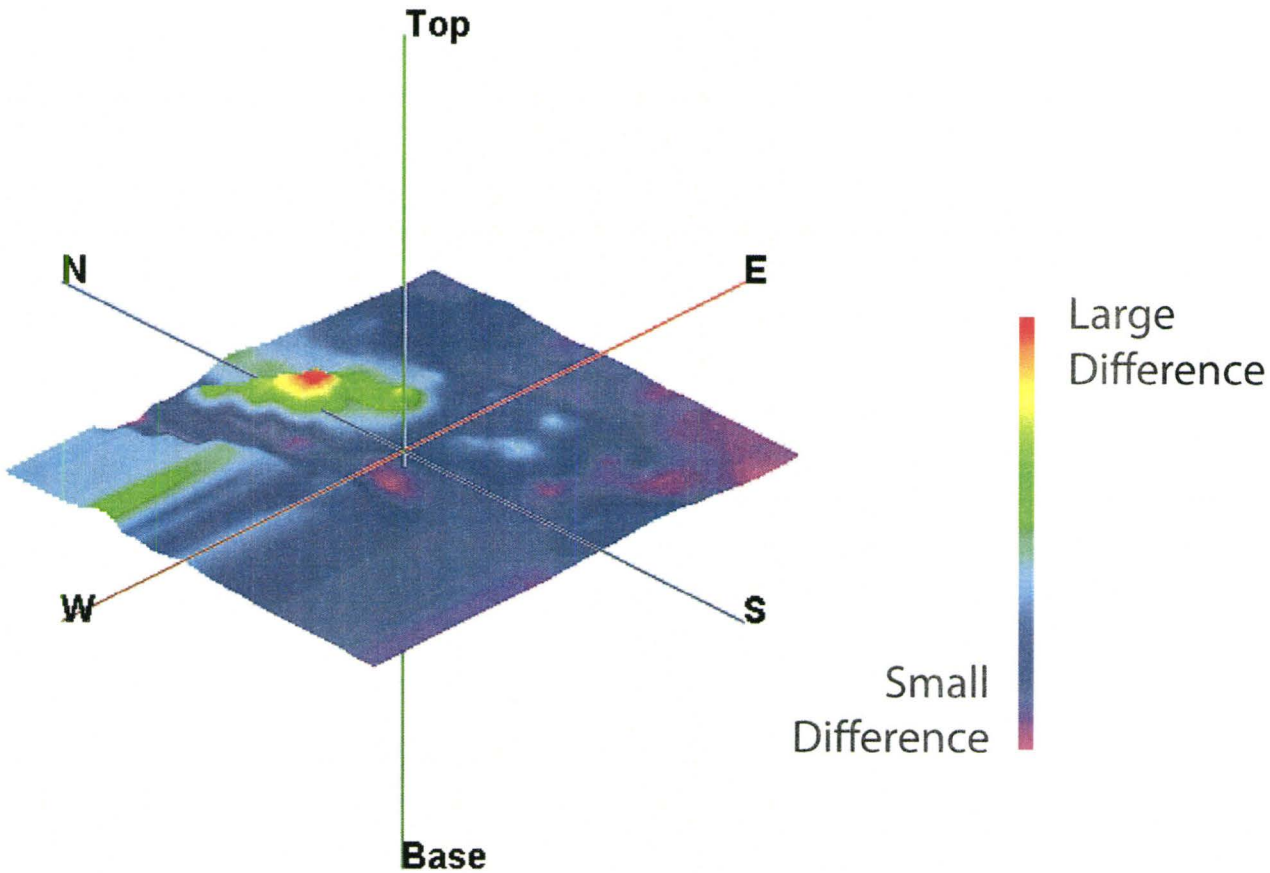

Top
N
E
W
S
Base
Large Difference
Small Difference

Figure 2.9: Map of the Original Dataset model – High (0.7) + Low (0.3) model showing how the Quality Weighting method has reduced the impact of the extreme outliers. The greatest difference in unit thickness occurs in the area of the outliers (which are present in both grids) however their influence has been greatly reduced using the Quality Weighted method.


Top
N
E
W
S
Base
Large Difference
Small Difference

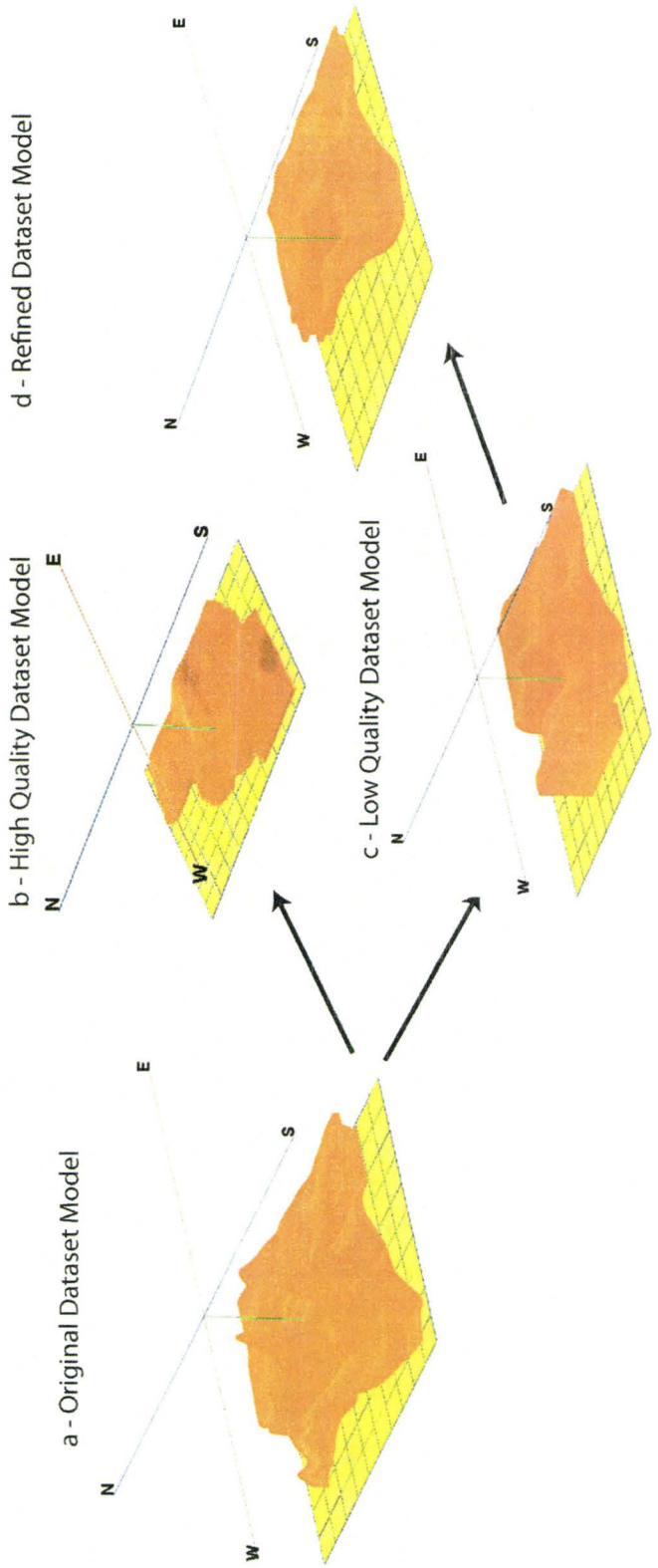
Comparing the Original Dataset with the Quality Weighted Dataset [High (0.7) + Low (0.3)] shows that the greatest differences occur in the area of the outliers which are present in both datasets but that the influence of these erroneous points has been greatly reduced in the Quality Weighted model output (Figure 2.9). Therefore it is evident that the weighting factors are allowing the higher quality data to influence even the most extreme values of the outliers in the Quality Weighted grids which resulted in such a large difference between the two grids in the northern section of the study area (Figure 2.9).

2.4.3 Volumetrics

Another method of assessing the differences between the models created from different quality datasets is to quantify the variation in the projected volumes calculated for the sandy gravel aquifer unit beneath the McMaster campus area.

Subsurface volume estimates of the sandy gravel unit were obtained by creating voxel models using ROCKWORKS 2006. Voxel models use the X, Y, and Z data to create a solid model which can then be used to calculate the number of cubic units (volume) contained within a specified geological layer. Once voxel models were created from each of the datasets (High Quality, Low Quality, Refined, and Original Datasets; Figure 2.10), it was then possible to compare the volume of the sandy gravel unit predicted by each of the interpolated models. Datasets created using the Quality Weighted method were also used to produce voxel models in the following combinations;

Figure 2.10: Voxel models of the sand and gravel aquifer unit produced by the a) Original, b) High Quality, c) Low Quality, and d) Refined Datasets.


a - Original Dataset Model
b - High Quality Dataset Model
c - Low Quality Dataset Model
d - Refined Dataset Model
N
E
S
W

[High (0.7) + Low (0.3)], [High (0.5) + Low (0.5)], [High (0.7) + Refined (0.3)], and [High (0.5) + Refined (0.5)].

The estimated volumes for the sandy gravel unit predicted by the interpolated 3D voxel models show a considerable amount of variation (Table 2.1). The most notable difference is the volume prediction based on the model for the Original Dataset which is 44% greater than that derived from the High Quality Dataset alone (Table 2.1). A portion of the increased volume may be the result of the High Quality Dataset not being as spatially extensive as the Original Dataset. However, when the model generated from the Original Dataset was compared to the [High (0.7) + Refined (0.3)] Quality Weighted model, which covers the same spatial area, there was still a 35% difference in unit volume estimate (Table 2.1). These results show the large amount of variation and uncertainty that can be introduced into the model prediction of unit volumes through the use of variable quality data. Such uncertainty can have significant impact on the reliability of the output model, and may lead to wrongly informed decision-making in key industries such as mining, environmental remediation or groundwater exploration.

2.4.4 Impact of the Quality Weighting method on Predicted Grid Node Values

A further test of the effectiveness of the Quality Weighted methodology is to compare interpolated thickness values with actual (observed) values to confirm that the process of mathematically recombining the grids allows the High Quality Dataset to have greater influence over the model output. In order to do this the interpolated maximum thickness values for the nodes (herein referred to as maximum node values) created for

each of the models can be compared with actual maximum thickness values determined from the most reliable data sources (i.e. High Quality Dataset). The maximum node values calculated from the Low Quality Dataset (16.15m; Table 2.1) and the Original Dataset (15.82m; Table 2.1) are considerably higher than the actual maximum thickness recorded in the High Quality Dataset (3.6m; Table 2.1). This is most likely due to the influence of erroneous data points (outliers) in the Original and Low Quality Datasets causing an overestimation of unit thickness. In contrast, the High Quality Dataset produced estimated node values of 3.07m, very close to the actual value of 3.6m (Table 2.1). The Quality Weighted [High (0.5) + Low (0.5)] model produced maximum node estimates of 8.95m, but when the High Quality Dataset was given a higher weighting, as in the [High (0.7) + Low (0.3)] weighted model, the interpolated maximum node value was reduced to 6.07m (Table 2.1). Results from the [High (0.5) + Refined (0.5)] weighted model show a reduction in the maximum node value due to the removal of outliers (4.79m; Table 2.1) and show closer agreement to actual values when the weighting is adjusted to [High (0.7) + Refined (0.3)] producing a node value of 3.72m (Table 2.1). This clearly demonstrates the impact of mathematically increasing the influence of high quality data on creating model outputs that more closely conform to actual values.

2.4.5 Impact on the Standard Deviation of the Output Models

The Quality Weighting method was also effective in reducing the standard deviation of the model values (Table 2.1) which implies a greater degree of statistical confidence in the results obtained using this methodology. The standard deviation was

highest in the Low Quality data model (2.34) and was lowest in the [High (0.7) + Refined (0.3)] data model (0.58; Table 2.1). Therefore, statistically the most reliable model is the one produced using the [High (0.7) + Refined (0.3)] data weighting.

The volume estimation, node value calculations and standard deviation results produced by the [High (0.7) + Refined (0.3)] model are more similar to the high quality data output than the [High (0.5) + Low (0.5)] model output. The values in Table 2.1 show that by comparing the grid statistics for the models produced by each dataset, it is evident that the grid math process utilized was able to influence the weight of the data and allowed the high quality data to have more influence over the final output.

2.5 Validation of the Quality Weighting Method

It is extremely difficult to confidently validate the accuracy of 3D subsurface geologic models without having to drill or excavate the entire study area which is typically not feasible. In this study, one of the most effective ways to quantify the validity of the Quality Weighted method was to calculate the Root Mean Square Prediction Error (RMSPE). The model with the smallest RMSPE value is considered to be the best and most accurate (Johnston et al. 2001).

In this study it was assumed that the values from the High Quality Dataset are the most accurate and reliable, and the RMSPE was calculated by comparing the interpolated model values to the high quality data points. In order to establish which model produced node values that most closely match input values from the High Quality Dataset,

comparisons were made between the High Quality Dataset and the [High (0.7) + Refined (0.3)] and Original Dataset models. The validation results were calculated using the following equation;

$$RMSPE = \sqrt{\frac{\sum_{i=1}^{n}\left(\hat{Z}\,(s_i) - z(s_i)\right)^2}{n}}$$

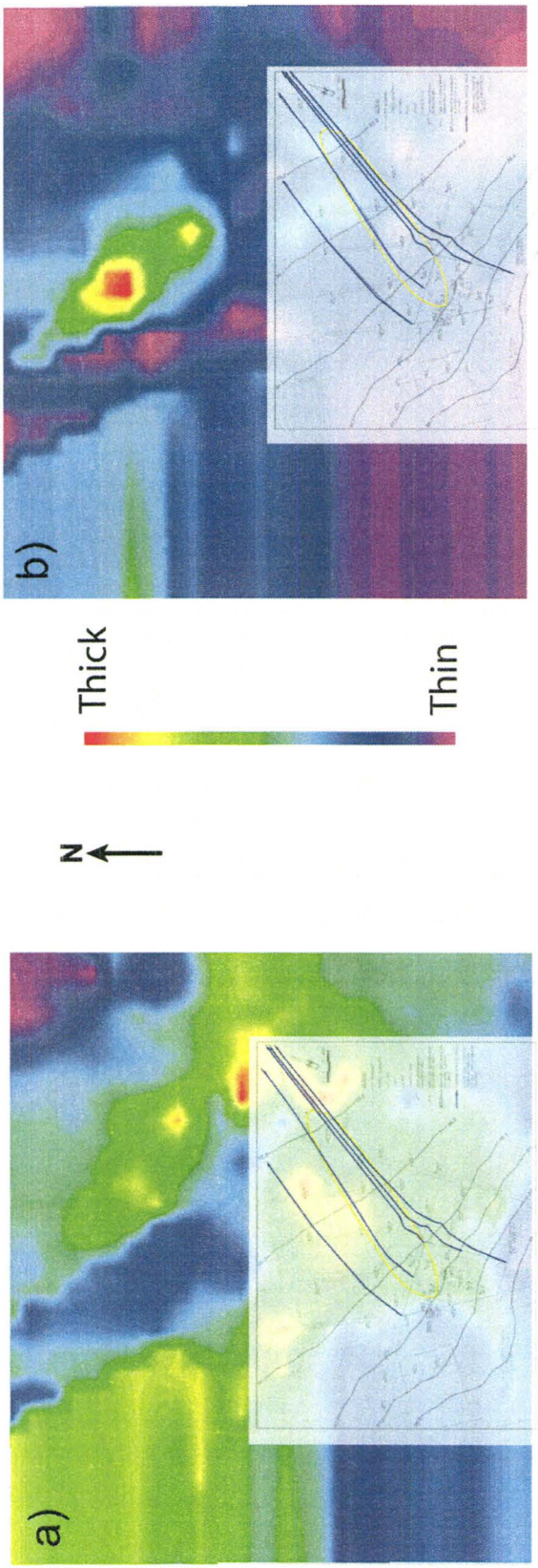
Where $\hat{Z}\,(s_i)$ is the interpolated value at the point (s_i), $z(s_i)$ is the original (observed) value from the input dataset at that same location, and n is the number of points within the input dataset. The mean values were squared in order to ensure that any deviation (either positive or negative) from $z(s_i)$ would be identified. Models producing interpolated values most similar to the measured values from the High Quality Dataset will produce the lowest RMSPE value, and are considered to be the most accurate. The RMSPE value produced by interpolation of the Original Dataset was 0.58, whereas the value calculated for the [High (0.7) + Refined (0.3)] Quality Weighted model was 0.28. This indicates that the interpolations made using the Quality Weighting method produced a model that more closely conforms to measured values from the High Quality Dataset than the model generated by a non-weighted method.

2.5.1 Comparison of Model Output with Proxy Data

Another method of validating the accuracy of 3D model outputs is to compare with proxy data that provides information about subsurface unit thickness and geometry. In order to test that the Quality Weighted methodology was in fact producing a more accurate and realistic representation of the position and form of the sandy gravel unit than

the output from the model created using the Original Dataset in an un-weighted form, the output from the Quality Weighted [High (0.7) + Low (0.3)] model was compared to the location of groundwater and contaminant migration pathways in the study area. These pathways were determined independently by Conestoga Rovers and Associates (1996) using groundwater flow, hydraulic head and water chemistry data during an investigation of groundwater contamination in the region of the McMaster campus. Considering that groundwater (and contaminants) preferentially flow through areas with the greatest proportion of coarse grained sediment which would have the greatest conductivity (Fetter, 2001; Schwartz and Zhang, 2003), then the contaminant plume delineated by Conestoga Rovers and Associates (1996) should map in the same position as the greatest thickness of the sandy gravel unit represented by the 3D model. Comparison of various output models with the location of the contaminant plume mapped by Conestoga Rovers and Associates (1996) on the basis of water quality data shows that the unit thickness model generated from the Quality Weighted [High (0.7) + Refined (0.3)] model more closely matches the position of the mapped contaminant plume (Figure 2.11a) than the model generated from the un-weighted Original Dataset (Figure 2.11b). This comparison of model outputs with independently generated proxy data suggests that there is an improvement in the accuracy of subsurface model outputs when the high quality data are given more influence in the creation of interpolated units using a quality weighting methodology.

Figure 2.11: The thickest portions of the subsurface aquifer identified on the isopach map generated from the Quality Weighted [High (0.7) + Refined (0.3)] model (a) more closely correlates with the mapped contaminant plume pathways (transparent overlay) determined independently by Conestoga Rovers and Associates (1996) than the model created by the un-weighted Original Dataset (b).


b)
Thick
Thin
N
a)

2.6 Conclusion

The focus of this study was to determine the effects of data quality on the generation of accurate 3D subsurface models and to develop a methodology that most effectively utilized data of varying quality in the modelling process. The study of the McMaster University campus area shows that significantly different 3D model outputs can be generated from data of variable quality, in this case illustrated by models generated from High Quality, Low Quality, Refined, and Original Datasets. The concept of 'quality weighting' input data proposed here employs a grid math process to impose a relative 'weighting' factor on High and Low Quality input datasets in order to better utilize all types of data while enhancing the influence of the high quality data and the reliability of the output model. The proposed Quality Weighting method is also able to constrain the negative impact of the lower quality data on the model output but utilizes these data to constrain the model in areas where high quality data are unavailable. This weighting process allows all data points to be used in the modelling process, yet is able to increase the influence of the high quality data over the lower quality data. Comparison of model outputs created for the McMaster University campus area indicates that the Quality Weighted model outputs more closely conform to the available high quality data points and proxy data than un-weighted model outputs.

It is no longer acceptable to simply include a disclaimer that a dataset used in any type of 3D modelling study contains data of variable quality and not differentially utilize these data in the interpolation of the model. If the user is capable of identifying variable

quality data within their dataset, then they should make use of a differential weighting mechanism, such as the Quality Weighted methodology proposed here, to increase the accuracy and reliability of their model output.

Acknowledgments

We would like to thank Dr. Jeff Harris and Dr. Antonio Paez for their helpful comments and suggestions pertaining to this research. The subsurface data was graciously provided by McMaster University. We would also like to thank NSERC for their assistance in providing support by means of a PGS D scholarship to Kelsey MacCormack and a Discovery Grant to Dr. Carolyn Eyles.

Reference List

Bajc, A. F., Endres, A. L., Hunter, J. A., Pullen, S. E., & Shirota, J. (2004). Three-Dimensional Mapping of Quaternary Deposits in the Waterloo Region, Southwestern Ontario. *Illinois State Geological Survey (IGSG) Open File Series 2004-2008,* 12-15.

Barnett, V. & Lewis, T. (1994). *Outliers in Statistical Data.* (3rd ed.) New York: John Wiley & Sons.

Burt, A. (2004). Three-dimensional mapping of Quaternary (surficial) deposits in the Barrie area, central Ontario. In Summary Field Work and Other Activities 2004. *Ontario Geological Survey,* 35-1-35-5.

Burt, A. (2007). Three-dimensional geological modelling of thick Quaternary deposits in the Barrie-Oro area, central Ontario: new modelling techniques. In Summary of field Work and Other Activities 2007. *Ontario Geological Survey, Open File Report 6145:* 35-1-35-5.

Burt, A. & Bajc, A. F. (2007). New products and advancements in 3-D modelling protocols based on studies in thick drift areas in Ontario, Canada. *Three Dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4,* 9-13.

Carter, T. R. & Castillo, A. C. (2006). Three-dimensional mapping of Paleozoic bedrock formations in the subsurface of southwestern Ontario: A GIS application of the Ontario petroleum well database. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 435-450). St. John's: Geological Association of Canada.

Conestoga-Rovers & Associates (1996). *Remedial Action Plan, Henkel Canada Limited, Hamilton, Ontario.*

Costa, J. F. (2003). Reducing the impact of outliers in ore reserves estimation. *Mathematical Geology, 35,* 323-345.

Devillers, R., Gervais, M., Bedard, Y., & Jeansoulin, R. (2002). Spatial Data Quality: from metadata to quality indicators and contextual end-user manual. In *2002 OEEPE/ISPRIS Joint Workshop on Spatial Data Quality Management* (pp. 45-55).

Devillers, R. & Jeansoulin, R. (2006). Spatial Data Quality: Concepts. In *Fundamentals of Spatial Data Quality.* (pp. 1-312). London: Wiley.

Dey, W. S., Davis, A. M., Abert, C. C., Curry, B. B., & Seiving, J. C. (2005). Three-dimensional geologic mapping of groundwater resources in Kane County, Illinois. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Geological Survey of Canada, Open File 5048,* 21-24.

Dumedah, G. & Schuurman, N. (2008). Minimizing the effects of inaccurate sediment description in borehole data using rough sets and transition probability. *Journal of Geographical Systems, 40,* 291-315.

EarthFX (2004). *Viewlog Borehole Management System.* Toronto: EarthFX.

Fetter, C. W. (2001). *Applied Hydrogeology.* (4 ed.) Upper Saddle River, NJ: Prentice Hall.

Gong, J., Cheng, P., & Wang, Y. (2004). Three-dimensional modelling and application in geological exploration engineering. *Computers & Geosciences, 30,* 391-404.

Goodchild, M. F. & Clarke, K. C. (2002). Data Quality in Massive Data sets. In J.Abello, P. M. Pardalos, & M. G. C. Resende (Eds.), *Handbook of Massive Data Sets* (pp. 643-659). Norwell, MA: Kluwer Academic Publishers.

Houlding, S. W. (1994). *3D Geoscience Modelling.* Hong Kong: Springer-Verlag Berlin Heidelberg.

Isaaks, E. H. & Srivistava, R. M. (1989). *An Introduction to Applied Geostatistics.* New York: Oxford University Press.

Jackson, I. (2004). Communicating the Vision? *Three Dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Series 2004-8,* 32-34.

Jackson, I. (2007). So where do we go from here? *Three-dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4,* 19-22.

Karrow, P. F. (1963). *Pleistocene Geology of the Hamilton - Galt Area* (Rep. No. 16). Ontario Department of Mines.

Kaufmann, O. & Martin, T. (2008). 3D geological modeling from boreholes, cross-sections and geological maps, application over former natural gas storage in coal mines. *Computers & Geosciences, 34,* 278-290.

Keefer, D. A. & Rittenhouse, S. (2005). Estimating the uncertainty of 3D geologic maps. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Geological Survey of Canada, Open File 5048,* 31-35.

Lee, J., Snyder, P. K., & Fisher, P. F. (1992). Modeling the effect of data errors on feature extraction from digital elevation models. *Photogrammetric Engineering & Remote Sensing, 58,* 1461-1467.

Logan, C., Russel, H. A. J., Sharpe D.R., & Kenny, F. M. (2006). The role of GIS and expert knowledge in 3-D modelling, Oak Ridges Moraine, southern Ontario. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 519-542). St. John's: Geological Association of Canada.

MacCormack, K. E., MacLachlan, J. C., & Eyles, C. H. (2005). Viewing the subsurface in three dimensions: Initial results of modeling the Quaternary sedimentary infill of the Dundas Valley, Hamilton, Ontario. *Geosphere, 1,* 23-31.

Macfarlane, A. P. & Schneider, N. (2007). Practical saturated thickness: A more realistic measure of groundwater availability in heterogeneous aquifers. *Three Dimensional Geologic Mappign for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4: 9-13,* 81-84.

Parks, K., Andriashek, L., & Atkinson, N. (2005). Lowering barriers to public communication with 3D groundwater mapping at Alberta Geological Survey: Examples from Canada's Oil Sands Area. *Three-Dimensional Geological Mapping for Groundwater Applications: Workshop Extended Abstracts, Geological Survey of Canada Open File 5048,* 57-60.

Paulen, R. C., McClenaghan, M. B., & Harris, J. R. (2006). Bedrock topography and drift thickness models from the Timmins area, northeastern Ontario: An application of GIS to the Timmins overburden drillhole database. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 413-434). St. John's: Geological Association of Canada.

RockWare (2006). Rockworks v. 2006: An updated computer program for spatially analyzing data and visualizing 3-dimensional subsurface models [Computer software]. Denver.

Ross, M., Parent, M., & Lefebvre, R. (2005). 3D geologic framework models for regional hydrogeology and land-use management: a case study from a Quaternary basin of southwestern Quebec, Canada. *Hydrogeology Journal, 13,* 690-707.

Russel, H. A. J., Sharpe D.R., & Cummings, D. I. (2007). A framework for buried-valley aquifers in Southern Ontario. In *OttawaGeo2007* (pp. 386-393).

Schwartz, F. W. & Zhang, H. (2003). *Fundamentals of Ground Water.* New York: Wiley.

Strong, D. M., Lee, Y. W., & Wang, R. Y. (1997). Data Quality in Context. *Communications of the ACM, 40,* 103-110.

Thorleifson, L. H. & Berg, R. C. (2002). Introduction - The need for high-quality three-dimensional geological information for groundwater and other environmental applications. *Geological Survey of Canada, Open File 1449.*

Venteris, E. R. (2007). 3-D modeling of glacial stratigraphy using public water well data, geologic interpretation, and geostatistics. *Three-dimensional Geological Mapping for Groundwater Applications: Workshop Extended Abstracts, Minnesota Geological Survey Open-File Report 07-4,* 81-84.

Wang, R. Y., Storey, V. C., & Firth, C. P. (1995). A framework for analysis of data quality research. *IEEE Transactions on Knowledge and Data Engineering, 7,* 623-639.

Weir, M. (2002). Monte Carlo simulation of long-term spatial error propagation in forestry databases. In S.Wenzhong (Ed.), *Spatial Data Quality* (pp. 1-340). Florida: CRC Press LLC.

Zwiers, W. G., Rainsford, D. R. B., & Bajc, A. F. (2008). Project Unit 06-026: investigation of the Dundas Buried Bedrock Valley. *Summary of Field Work and Other Activities 2008, Ontario Geological Survey, Open File Report 6226,* 33-1-33-7.

CHAPTER 3

EVALUATING THE IMPACT OF DATA QUANTITY, DISTRIBUTION, AND ALGORITHM SELECTION ON THE ACCURACY OF 3D SUBSURFACE MODELS USING SYNTHETIC GRID MODELS OF VARYING COMPLEXITY

Abstract

Testing the accuracy of 3D modelling algorithms used for geological applications is extremely difficult as model results cannot be easily validated without the implementation of costly drilling programs or excavations. This paper presents a new approach to evaluate the effectiveness of common interpolation algorithms used in 3D subsurface modelling, that utilizes four synthetic grids to represent subsurface environments of varying geologic complexity. The four grids are modelled with two different algorithms commonly used for geological applications (Inverse Distance Weighting; IDW and Ordinary Kriging; OK), using data extracted from the synthetic grids in different spatial distribution patterns (regular, random, clustered, and sparse), and with different numbers of data points (100, 256, 676 and 1600). Utilizing synthetic grids for this evaluation allows quantitative statistical assessment of the accuracy (Root Mean Square Error [RMSE] and Bias Error [BE]) of the two interpolation algorithms being tested.

The results showed that generally, the OK algorithm produced more accurate models of the four grids than IDW, regardless of the number or distribution of data points. Algorithm selection appears to have the most impact on model accuracy when relatively simple grids are modelled using relatively few data points. Using a greater number of data points for interpolation typically improved model output, although using large numbers of data points was found to negatively impact the accuracy of relatively simple models. This suggests that optimum amounts of data are required for accurate and cost-effective interpolation of units of varying complexity. The most accurate models were created by regularly and randomly distributed data points, followed by sparse and clustered data respectively. These results imply that in certain geological situations relatively small numbers of randomly distributed sparse data points can generate more accurate 3D models than larger amounts of data that are clustered together.

3.1 Introduction

Three-dimensional (3D) geo-cellular models are becoming increasingly useful for geoscientific applications in many fields of study such as resource exploration (Gong et al., 2004; Paulen et al., 2006; Kaufmann and Martin, 2008), delineation of groundwater source protection areas (Ross et al., 2005; Burt, 2007; Zwiers et al., 2008), and for the reconstruction of past geologic events and processes (MacCormack et al., 2005; Logan et al., 2006). Such models are valuable to both private industry and government agencies as they readily communicate complex concepts to both specialists and the general public (Shi et al., 2002; Kessler et al., 2005; Parks et al., 2005; RockWare, 2006; Jackson, 2007;

Zwiers et al., 2008). However, the increased use of 3D models for a broad range of applications has raised concerns about the accuracy and reliability of model outputs and the relationship between output quality, input data and the type of interpolation algorithm employed in the modelling process (Weber and Englund, 1992; Weber and Englund, 1994; Zimmerman et al., 1999; Jones et al., 2003).

This paper will explore the performance of the two most commonly used and assessed interpolation algorithms, Ordinary Kriging (OK) and Inverse Distance Weighting (IDW; Tabios and Salas, 1985; Weber and Englund, 1992; Weber and Englund, 1994; Brus et al., 1996; Walker and Loftis, 1997; Nalder and Wein, 1998; Zimmerman et al., 1999; Schloeder et al., 2001; Jones et al., 2003; Kravchenko, 2003; Dille et al., 2003; Lapen and Hayhoe; 2003), on the modelling of four synthetic grids that represent subsurface geologic environments of variable complexity. The advantage of using synthetic datasets to conduct this evaluation is that the point values for each surface being modelled are known at every location, which allows quantitative analysis of the variability between actual and interpolated values. In order to evaluate the influence of input data point distribution on the accuracy of the interpolations made, the synthetic grids were sampled using four different sampling patterns (clustered, random, regular, and sparse). These sampling patterns were selected to represent the types of data distribution that may be encountered in various geoscientific applications. The number of data points used for interpolation was also varied (100, 256, 676, and 1600 points were modelled independently) in order to identify the optimum number of data points required to create a reasonably accurate model in situations of varying subsurface complexity.

This information was used to conduct a cost-benefit analysis to identify the point at which the inclusion of more data (cost) did not produce sufficient enhancement of model accuracy (benefit).

The objective of this paper is to evaluate the effectiveness of common interpolation algorithms used in 3D subsurface modelling using synthetic models of varying geologic complexity, with different input data density and spatial distribution patterns. This evaluation will provide valuable information that can be used to guide selection of the most appropriate algorithm for interpolating subsurface units, and ultimately will lead to more effective and efficient means of modelling subsurface environments.

3.2 Methods

Comparing the effectiveness of interpolation algorithms has been previously conducted using digital elevation models (DEM; Weber and Englund, 1992; Weber and Englund, 1994), contaminant plume data (Jones et al., 2003), soil data (Brus et al., 1996; Walker and Loftis, 1997; Schloeder et al., 2001; Kravchenko, 2003; Paulen et al., 2006), weed seedling density (Dille et al., 2002), and climatological data (Tabios and Salas, 1985; Nalder and Wein, 1998; Lapen and Hayhoe, 2003; Moffat et al., 2007). A notable limitation of many of these studies is that the comparison of interpolated values is made with an 'original' model and/or surface that itself has been derived through interpolation. In such cases, it is likely that the 'original' (interpolated) surface deviates from the real

surface, and thus goodness-of-fit measures will not represent the true performance of the interpolation method. There is some inherent error propagation within the process of using sampled points from an interpolated surface to interpolate any subsequent surfaces, and this can seriously limit the degree to which algorithm accuracy can be determined (Heuvelink, 1998; Zimmerman et al., 1999; Burrough, 2001). Zimmerman et al., (1999) attempted to resolve the issue of error propagation on interpolated surfaces by utilizing mathematical equations to generate synthetic surfaces, from which points could be sampled and re-interpolated. This work allowed quantitative comparison of the interpolated grid with the original mathematical surface and concluded that spatial interpolation accuracy should only be estimated using synthetic surfaces, for which values are known for all locations (Zimmerman et al., 1999). However, the limitation of using mathematically-generated synthetic surfaces to test the effectiveness of algorithms used in 3D subsurface modelling is that these surfaces do not closely resemble the form of realistic geological units or boundaries that would be encountered in subsurface investigations. Hence, the synthetic grids used in the present study were created specifically to represent the type and form of units or surfaces that may be encountered in geological situations.

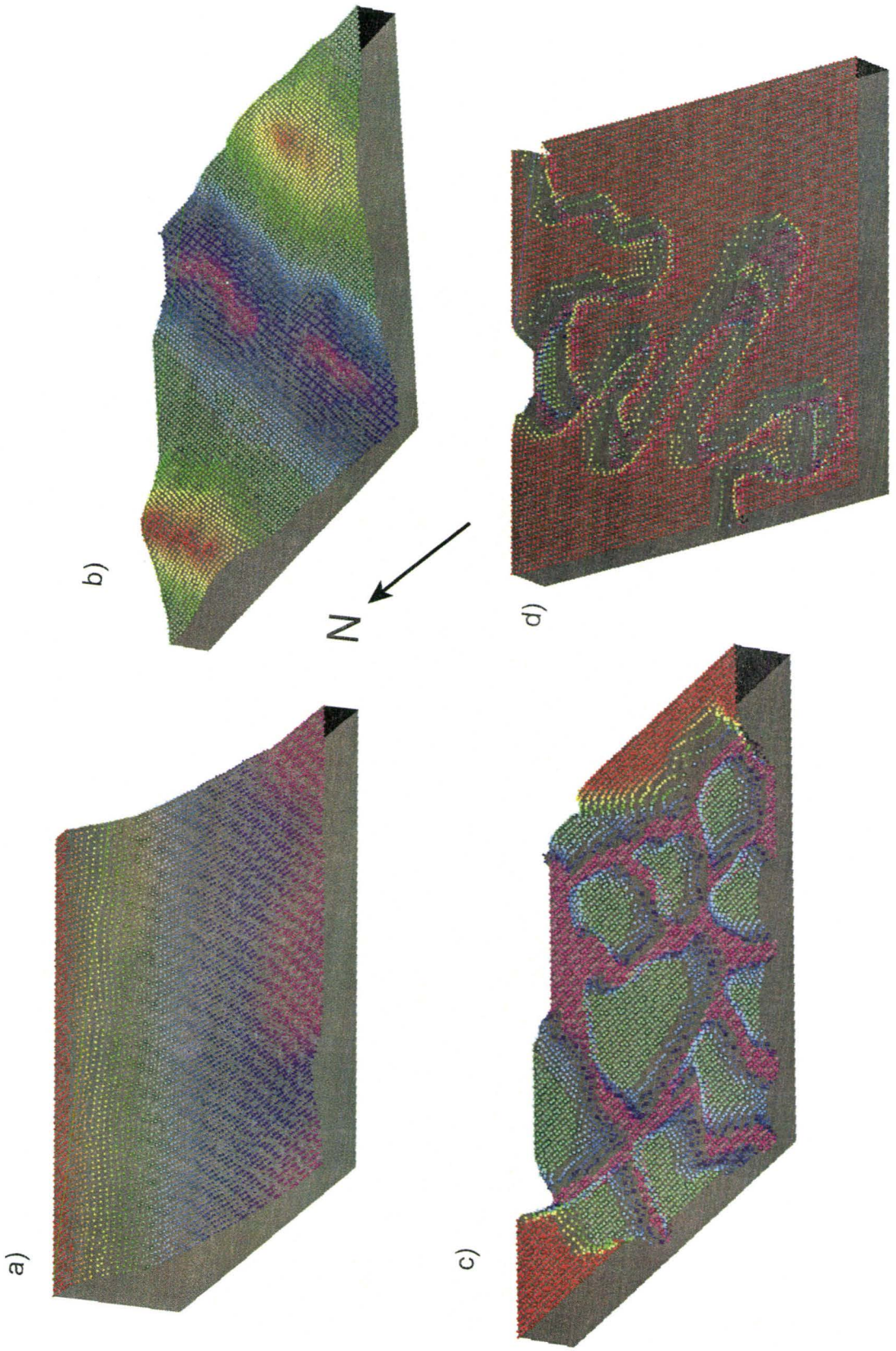
3.2.1 Synthetic Surface Development

Four synthetic grids were created to represent realistic geological surfaces of varying complexity (Figure 3.1). The first synthetic grid takes the form of a simple, gently sloping unidirectional surface with lateral continuity in the direction perpendicular to the slope (grid 1; Figure 3.1a). This surface could represent a gently dipping bedrock

valley wall or one element of a regional-scale basin system. The second synthetic grid surface is slightly more complex, and consists of a linear trough between areas of relatively high elevation (grid 2; Figure 3.1b). This may be used to represent a simple valley form, or several elements of a regional scale basin system. The third synthetic grid surface consists of a series of interconnected troughs separated by irregularly spaced linear 'highs' trending in one direction (grid 3; Figure 3.1c). This surface could represent the irregular topography characteristic of an eroded bedrock surface, a braided river system, or a smaller scale setting with more localized variability. The fourth grid is characterised by a sinuous trough cut into a flat surface (grid 4; Figure 3.1d) and may be used to represent an incised meandering river system or a local scale setting with features showing high directional variability. Each of the four synthetic surfaces represents a geologic setting of differing complexity and challenge for the modelling process.

The four synthetic grids were created using ROCKWORKS 2006 software. This software was selected as it allows the user to alter and manually manipulate grids using the 'Grid Edit' function. Four grids, each with identical 80x80 grid dimensions, and each with a grid spacing of 1 arbitrary unit (6400 grid cells for each surface) were created. The choice of this grid size and spacing allowed adequate detail to be included for each surface while not being computationally exhausting. Once the grid size was set, a blank grid was opened using the grid editing function. Each of the 6400 grid cells was then assigned a thickness value between 1 and 9 to create the topographic surfaces on each of the four synthetic grid models. The range of thickness values was selected as it provided

Figure 3.1: Synthetic grids created to represent realistic geologic environments from which the data points for modeling were extracted. a) Grid 1 forms a gently sloping surface that may represent one element of a basin system or gently dipping bedrock valley wall, b) Grid 2 consists of two linear 'highs' separated by a central trough and represents a simple valley form, c) Grid 3 shows a series of interconnecting troughs separated by linear 'highs' and may represent an eroded bedrock surface or a braided river system, and d) Grid 4 consists of a flat surface incised by a highly sinuous channel and represents an incised meandering river system.


b)
N
d)
a)
c)

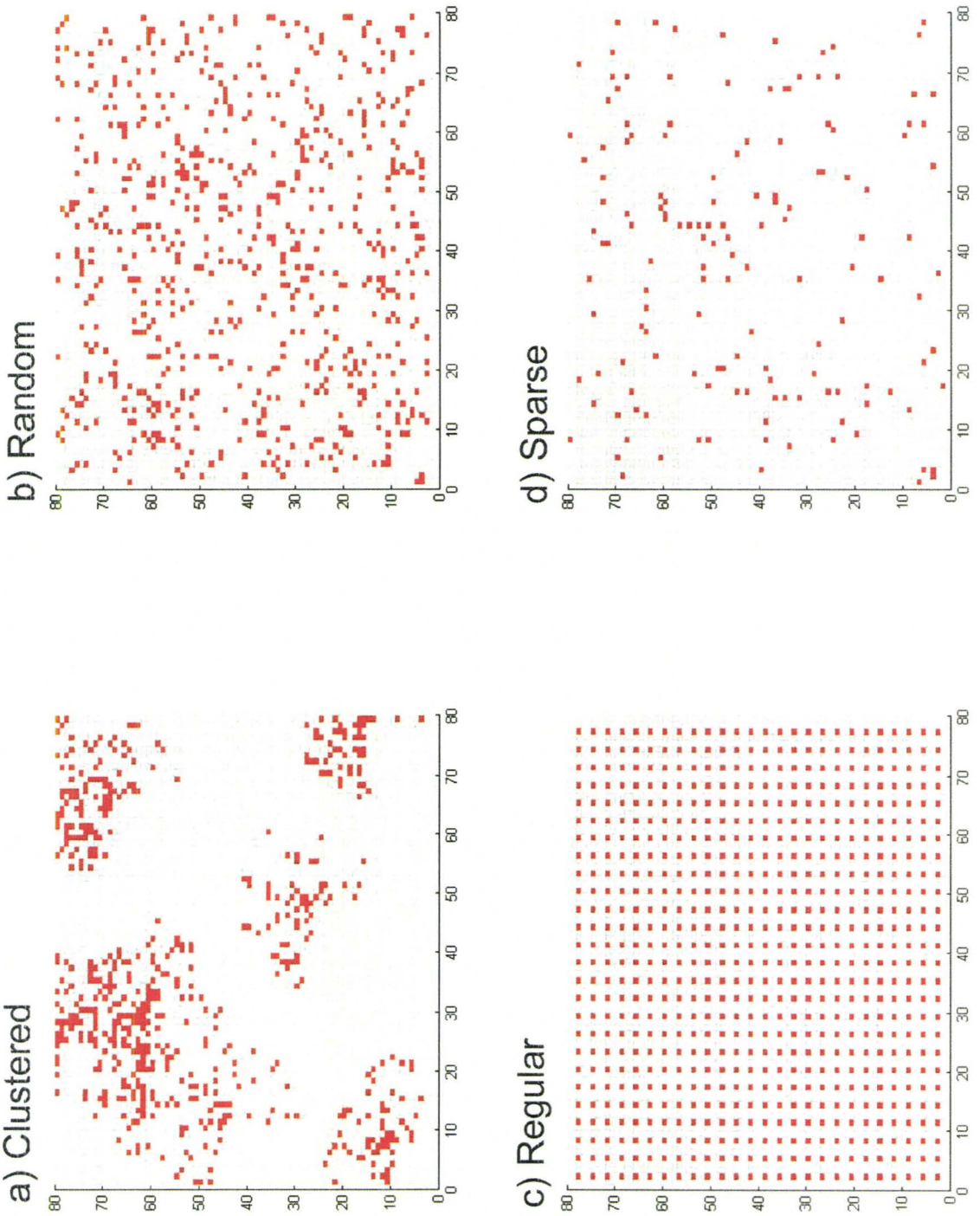
sufficient topographic variability to realistically represent each geological setting while not resulting in excessive variability between data points.

Once each grid was created, a smoothing filter was applied to smooth the surface and to ensure a realistic transition in values between neighbouring grid cells. A 7x7 smoothing filter (i.e. the value of every cell was averaged by the value of all the neighbouring cells within a surrounding 7 cell by 7 cell box) was applied to grid 1 (Figure 3.1a) to create a softer, more gradual slope. Grids 2, 3, and 4 (Figure 3.1b, 3.1c, 3.1d) were smoothed using a 3x3 filter (the smallest available) which utilized a much smaller bounding box. This smaller filter size was used on grids 2, 3, and 4 to maintain the required topographic variability.

3.2.2 Extracting Sample Data from each Model

To simulate the range of sampling patterns that may be applied in real-world subsurface modelling situations, a variety of data subsets were created for each synthetic surface by varying both the quantity of data points as well as their distribution. Four separate datasets containing 100, 256, 676 or 1600 data points (representing 1.6, 4, 10.5 and 25% surface coverage, respectively) were extracted from each of the synthetic surfaces in four common sampling distribution patterns: a) clustered, b) random c) regular, and d) sparse (Figure 3.2; Krajewski and Gibbs, 1996; Zimmerman et al., 1999; Davis 2002). Subsurface geologic studies rarely disclose the percentage of the study area covered by data points, but they typically provide a map to show their distribution. Many studies incorporate data from numerous sources to maximize the amount of data used for

Figure 3.2: Data points were extracted from the synthetic grids in 4 spatial distribution patterns a) clustered, b) random, c) regular, and d) sparse. Sample distribution patterns for the 676 point dataset are shown.


a) Clustered
b) Random
c) Regular
d) Sparse
0
10
20
30
40
50
60
70
80

model generation (Logan et al., 2006; Paulen et al., 2006) and this often results in a clustered distribution of data points across the study area.

In order to test the impact of data density and data distribution on model accuracy, a total of 16 different density x distribution treatments were applied using custom-made MATLAB functions designed to select a specified number of data points in a desired distribution. The use of MATLAB scripts for this process eliminated the introduction of user bias into the selection of points (Bond et al., 2007). To avoid basing the results on any one set of point extractions, a Monte Carlo approach was used to perform the extraction process 10 times for each of the random, clustered and sparse distributions. The regular point distribution did not require these multiple simulations as the extracted points would be the same in all 10 iterations. This approach allowed the variability associated with each of the density x distribution treatments to be quantified, and ensured that the results represented the average for each sampling treatment, rather than a non-representative chance outcome.

Clustered sampling distributions (Figure 3.2a), were created by establishing a total of 10 data clusters of sampling points on the simulated surface of interest, regardless of the number of sample points used. The location of each cluster centre on the surface was randomly assigned, and the desired number of sample points was portioned equally among each cluster. The location of sample points within each cluster was generated by randomly assigning a direction and radial distance (between 1 and 15 units) from the cluster centre. Any location assignment that resulted in sample placement beyond the

range of the grid or in a repeated sample cell was discarded, and replaced with a subsequent random assignment.

Random sample distributions (Figure 3.2b) were created by repeating computer-generated random assignment of x and y grid locations without replacement, for the desired quantity of data points on each synthetic surface. Regular sample distributions (Figure 3.2c), were produced by imposing a square-grid of equally-spaced sample points on each of the simulated surfaces. The spacing between sample points was universally adjusted to accommodate the specified number of data points; this ensured maximum spatial coverage of the grid surface, while preserving the equal spacing and distribution (number of rows and columns) of sample point locations.

Sparse sampling distributions (Figure 3.2d) were a challenge to create, as there is currently no consensus on the definition of sparse data, despite the fact that datasets are often referred to as 'sparse' in the literature (Wu et al., 2005; de Kemp, 2006; Bond et al., 2007). It is suggested here that a dataset can be considered to be 'sparse' when the user feels that they have insufficient data to interpolate their model to the desired level of accuracy. The sparse data distribution was simulated by down-sampling the randomly assigned datasets, creating datasets of 40, 75, 150 and 400 points from the 100, 256, 676 and 1600 point datasets respectively. The 256, 676, and 1600 random datasets were down-sampled to 22-29% of the originally selected data points to create the sparse distribution dataset and the 100 point dataset was down-sampled to 40% of the original dataset in order to contain sufficient data points to produce the variogram necessary for interpolation by the kriging algorithm.

3.2.3 Grid Interpolation and Comparison

Each of the 1280 sample data subsets generated were re-imported into ROCKWORKS 2006 and interpolated using the Inverse Distance Weighting (IDW) and Ordinary Kriging (OK) algorithms in order to evaluate their performance in recreating the original surfaces. ROCKWORKS 2006 offers numerous options to provide the user some influence over the interpolation process, such as selecting the number of neighbours included for interpolation, changing search radius size, and identifying the type of variogram to be used. In order to keep the modelling process consistent and to minimize the impact of external variables, the subset data were all interpolated in a similar manner in this study. For IDW the data subsets were interpolated using a search radius cut-off of 15% and a minimum number of 8 data points. The OK algorithm was also applied consistently to all the data subsets using default settings that employ a spherical variogram, a minimum of 8 data points, and a maximum search radius of 15%.

IDW is a deterministic interpolation technique that estimates a surface from measured points based on the similarity to surrounding measured data points. The IDW method is built upon the assumption that things close to one another are more similar than those further apart (Issaks and Srivastava, 1989, Krajewski and Gibbs, 1996; Davis, 2002). Therefore, the weights of the surrounding measured data points are assigned based on the assumption that the data points closest to the prediction location will have a greater influence on the predicted value than those further away. IDW is a local interpolator which is typically the best choice for interpreting local anomalies because it

uses only the proximal data points to produce estimates (Krajewski and Gibbs, 1996; Johnston et al., 2001).

The general formula used for the IDW algorithm is defined by the following equation;

$$\hat{Z}(s_0) = \sum_{i=1}^{N} \lambda_i Z(s_i)$$

Where: $\hat{Z}(s_0)$ = the value of the attribute that the algorithm is trying to predict at the locations_0.

N = the number of the measured data points in the neighborhood surrounding s_0 that will be used to calculate the predicted value.

λ_i = the weights that are assigned to each data point.

$Z(s_i)$ = the observed/measured value at locations_i.

IDW performs best either when the measured data points are uniformly or densely distributed, or when the user is interested in preserving local anomalies within the dataset. However, IDW typically struggles when interpolating from datasets which are predominantly clustered or have areas of sparse data coverage (Krajewski and Gibbs, 1996). When IDW is used to interpolate clustered data, the measured values have been shown to greatly bias the surrounding predicted values (Weber and Englund, 1994;

Paulen et al., 2006), thus impacting the model accuracy. IDW is also known to have trouble interpolating data containing local anomalous values (high variability over relatively small distances) which are often accentuated creating artificial peaks or troughs (resulting in *bulls-eyes*) on the interpolated surface (Krajewski and Gibbs, 1996; Johnston et al., 2001; Paulen et al., Harris, 2006).

The second algorithm evaluated in this study is Ordinary Kriging (OK), which is referred to as a geostatistical interpolator because it utilizes both statistical and mathematical methods to predict attribute values. OK assumes an unknown constant mean or trend, and random residual errors (Issaks and Srivastava, 1989; Davis, 2002). The equation for ordinary kriging in its most basic form is;

$$Z_{(s)} = \mu + \varepsilon_{(s)}$$

Where; $Z_{(s)}$ is the variable of interest

μ is the deterministic trend

$\varepsilon_{(s)}$ are the autocorrelated errors

All kriging methods are built upon the concept of autocorrelation, which is the statistical relationship between spatially random variables. Autocorrelation is incorporated into the algorithm through the use of a semivariogram, which measures the strength of the statistical correlation as a function of the distance between the data points used to determine the kriging weights (Issaks and Srivastava, 1989; Krajewski and Gibbs, 1996). Kriging is similar to IDW in that both algorithms apply weights to the

surrounding measured values in order to calculate predicted values at specified locations. However, kriging not only considers the distance of the data points from the prediction location, it also uses the semivariogram to incorporate the spatial autocorrelation of the data points into the prediction calculation. OK was selected for this analysis because it is a robust estimator that is not overly sensitive to either the variogram selected or user specified controls on the algorithm (Weber and Englund, 1994). OK is also an exact interpolator, meaning that the estimated Z values exactly equal the data point values at their locations. It is also capable of dealing with clustered datasets because the weights are assigned not only on the distance to, but also on the spatial arrangement of the measured/observed data points. Therefore, a group of clustered data points would be assigned a similar weight to those of neighbouring individual scattered data points, a process that avoids producing estimates that are skewed by the clustered data point values. Finally, the kriging weights must result in a mean square error equal to zero to minimize the errors, thereby increasing the accuracy of the prediction (Issaks and Srivastava, 1989).

One of the disadvantages of using OK as an interpolator is that it can often be utilized as a 'black box' tool by users who do not fully understand how the predictions were calculated or if they are realistic (Goodchild and Haining, 2004). This may compromise the valid application of model outputs. The kriging algorithm is also very computationally intensive and can require a substantial amount of time for the estimates to be generated, especially with large and complex datasets. In addition, if there is a large amount of spatial variability within the dataset, it may not be possible to fit a reliable

variogram, which would result in poor estimates with large associated errors (Weber and Englund, 1994).

Overall, OK is often the best choice for interpolating datasets that contain clustered or irregularly distributed data points (Zimmerman et al., 1999; Weber and Englund, 1994). However, kriging should be used with caution when using small datasets or when large scale anomalies are present, as these affect the fit of the variogram model, which in turn affects the accuracy of the predicted model values.

In order to determine the effect of sampling density, point distribution, grid complexity, and algorithm selection on output accuracy, the interpolated models were compared to the original synthetic grids using custom MATLAB functions. These functions were created to provide a quantitative comparison of each interpolated grid with the original synthetic grid. The differences between the interpolated and original grids were quantitatively assessed using a number of statistical metrics including the Root Mean Square Error (RMSE), relative RMSE (rRMSE), Mean Average Error (MAE), and Correlation Coefficient (r2). These comparison statistics produced a substantial amount of data for all 1280 grids which could not all be shown nor discussed within this paper; consequently, RMSE and BE were chosen to describe the results. The RMSE was determined to be the best overall comparative statistic as it provides an un-biased indication of how similar the interpolated values are to the original values from the synthetic grids (Zimmerman et al., 1999; Jones et al., 2003). A smaller RMSE value indicates that the interpolated values for the model are more similar to the original synthetic values and infers that the model is more accurate (Zimmerman et al., 1999;

Davis, 2002; Dille et al., 2003; Jones et al., 2003; Mueller et al., 2004). The RMSE values calculated for each of the models are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. Bias errors (BE) are also included in the analysis as they provide important information about whether the interpolated grids were either under or over-estimating the original synthetic values using the various sampling treatments (Elith et al., 2002; Mueller et al., 2004; Hengl et al., 2004). These metrics are represented by:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}\left(\hat{Z}\,(s_i) - z(s_i)\right)^2}{n}}$$

$$BE = \frac{\sum_{i=1}^{n}(\hat{Z}(s_i) - z(s_i))}{n}$$

Where $\hat{Z}\,(s_i)$ is the interpolated value at the point (s_i), and $z(s_i)$ is the observed (true) value from the synthetic dataset at that same location, and n is the number of points within the input dataset.

3.3 Results and Discussion

Average RMSE values were calculated for each of the 10 simulations generated for each synthetic grid as a summary statistic to show how the values change in response to the grid complexity (represented by the four synthetic surfaces), different numbers of data points, variable data point distributions, and the use of selected interpolation algorithms (Figure 3.3). The interpolated models of grid 2 were visualized in Figure 3.3

to illustrate differences between the model outputs under each sampling and algorithm treatment.

3.3.1 Number of Data Points

Data were extracted into separate datasets of 100, 256, 676, and 1600 data points. To assess the effectiveness of utilizing various numbers of data points to accurately model the 4 synthetic surfaces, RMSE values were calculated and graphed for each point number dataset and for all 4 spatial distribution patterns (Figures 3.4, 3.5). The results showed that RMSE values for grids 1 and 2 were consistently the highest when only 100 points were used and decreased slightly with the addition of data (Figures 3.4, 3.5). RMSE values increased substantially for all point number datasets when modelling grids 3 and 4, particularly when few data points were used (Figure 3.4).

The RMSE results were also graphed separately for each grid to show how the values changed with increasing numbers of data points for each data distribution pattern, and for each algorithm (Figure 3.5). Results for all 4 synthetic grids show a consistent drop in RMSE with the addition of more data points. However, the increased number of data points used for interpolation had relatively low impact when modelling relatively simple surfaces (e.g. grids 1 and 2; Figure 3.5 a, b) as shown by the small difference in RMSE results with the addition of data. The number of data points became a more significant factor when modelling more complex surfaces such as those represented by grids 3 and 4 (Figure 3.5 c, d).

Figure 3.3: Flow diagram showing how the four synthetic grids (a.) were sampled to create the individual data subsets, which were then interpolated and modelled. Each synthetic grid (a.) was created with 6400 data points which were then sampled using 100, 676, and 1600 points in clustered, random, regular and sparse distribution patterns (b.). Visualizations of grid 2 were modelled using either IDW or OK with various amounts of data, in a variety of distributions (clustered, random, regular, and sparse) are also shown (c.).

Grid 1
Grid 2
Grid 3
Grid 4
a. Create Synthetic Datasets / Models (6400 points)
b. Matlab Script Developed to Extract Data Points in Various Patterns
Clustered
Random
Regular
Sparse
100 Point Extraction Set
256 Point Extraction Set
676 Point Extraction Set
1600 Point Extraction Set
c. Interpolate Extracted Points Using Inverse Distance Weighting and Ordinary Kriging
Inverse Distance Weighting
Ordinary Kriging
Grid 2 IDW Clustered Point Pattern
Grid 2 IDW Random Point Pattern
Grid 2 IDW Regular Point Pattern
Grid 2 IDW Sparse Point Pattern
Grid 2 Kriging Clustered Point Pattern
Grid 2 Kriging Random Point Pattern
Grid 2 Kriging Regular Point Pattern
Grid 2 Kriging Sparse Point Pattern
100 Points
676 Points
1600 Points

Figure 3.4: Graphs showing the Root Square Mean Error (RMSE) associated with models constructed for the four grids using each sampling distribution. The RMSE values were analyzed for models interpolated using a) 100, b) 256, c) 676, and d) 1600 data points. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.

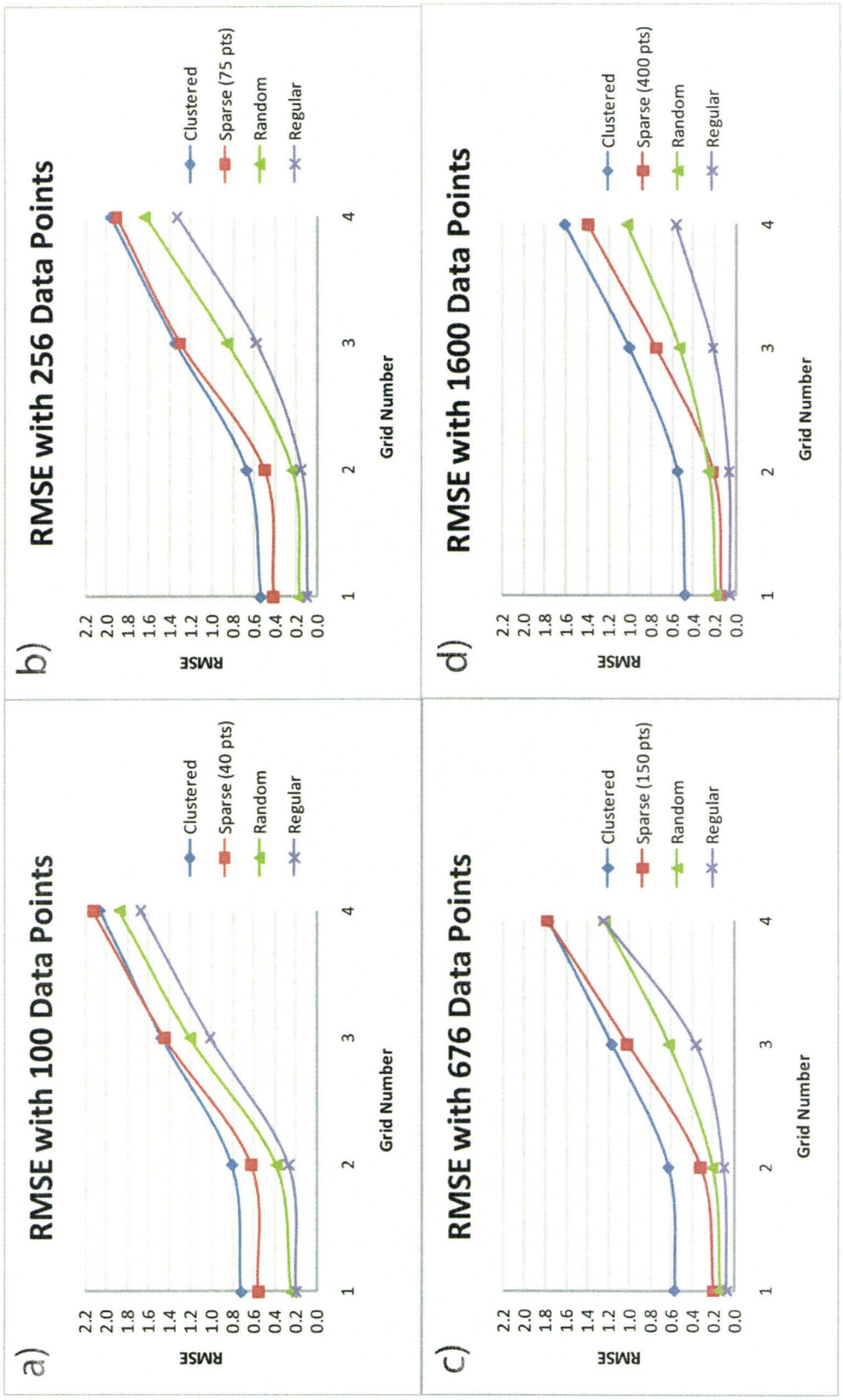
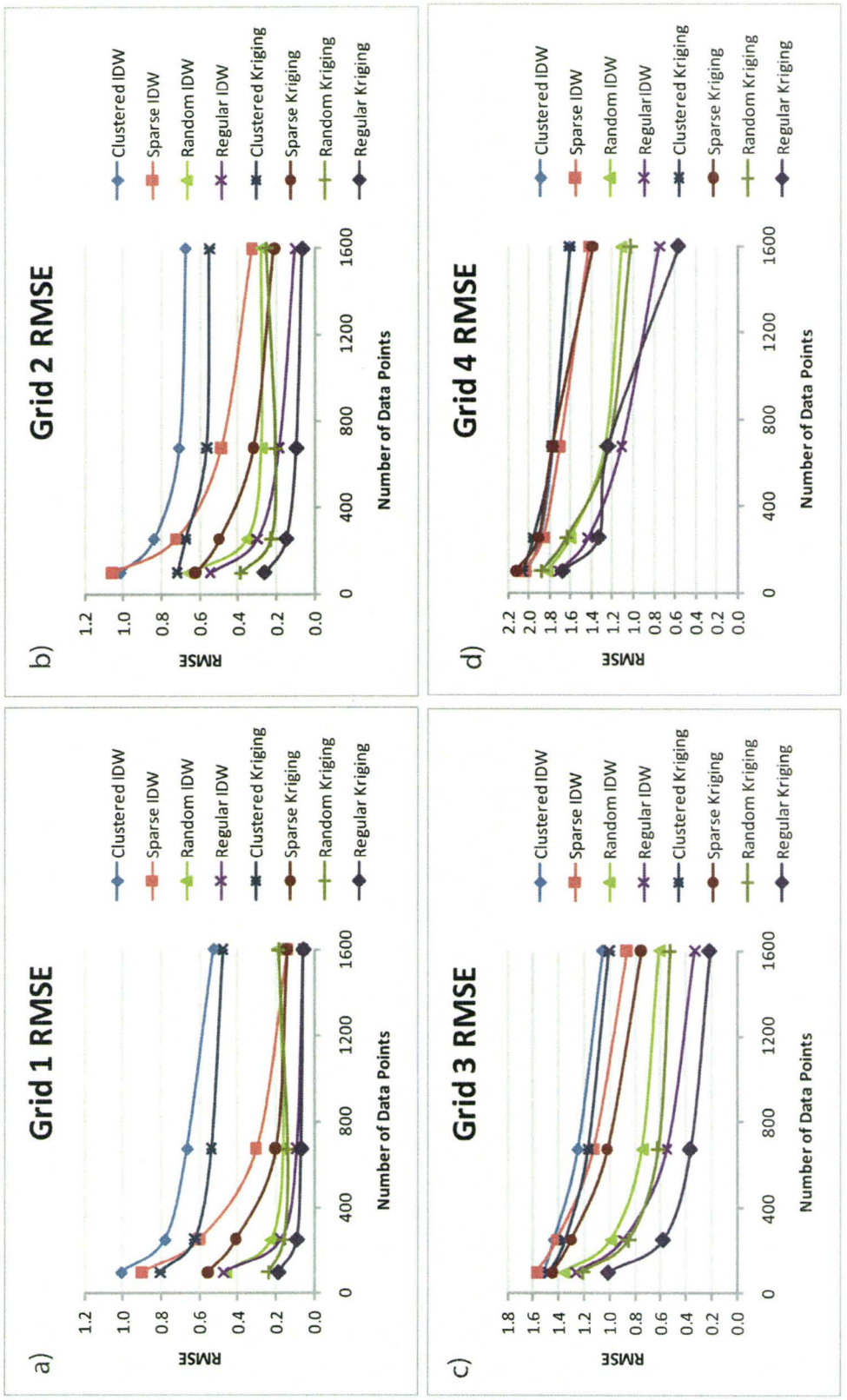

a)
RMSE with 100 Data Points
RMSE
Grid Number
Clustered
Sparse (40 pts)
Random
Regular
b)
RMSE with 256 Data Points
RMSE
Grid Number
Clustered
Sparse (75 pts)
Random
Regular
c)
RMSE with 676 Data Points
RMSE
Grid Number
Clustered
Sparse (150 pts)
Random
Regular
d)
RMSE with 1600 Data Points
RMSE
Grid Number
Clustered
Sparse (400 pts)
Random
Regular

Figure 3.5: Graphs showing how the RMSE values calculated for the four synthetic grids (a) grid 1, b) grid 2, c) grid 3, and d) grid 4) vary according to data distribution pattern (clustered, random, regular, and sparse), number of data points and algorithm used for interpolation (OK and IDW). RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids. Note change of scale for grids 3 and 4.


a)
Grid 1 RMSE
b)
Grid 2 RMSE
c)
Grid 3 RMSE
d)
Grid 4 RMSE
RMSE
Number of Data Points
Clustered IDW
Sparse IDW
Random IDW
Regular IDW
Clustered Kriging
Sparse Kriging
Random Kriging
Regular Kriging

The results shown in Figure 3.5 also indicate that the rate of RMSE decrease, used here as an indicator of increase in model accuracy, appears to drop substantially as more data points are added. This trend of diminishing returns was explored further by plotting the RMSE results for a greater selection of point number datasets (40, 75, 100, 150, 256, 400, 676, and 1600 points) containing randomly distributed data for each of the 4 synthetic grids (Figure 3.6). Initially, when few data points are available, the RMSE values decrease rapidly with the addition of data points, but the rate of decline reduces beyond 676 points for grid 4, 400 points for grid 3, 256 points for grid 2, and after 100 points for grid 1 (Figure 3.6). These cut-off values indicate the points at which there is only a slight drop in RMSE for the increasing number of data points used in the modelling process. These results will be discussed further below.

3.3.1.1 Discussion of the impact of data quantity on the interpolation accuracy

The results presented above suggest that for the relatively simple models with low variability (e.g. grids 1 and 2), using too much data for interpolation can cause the algorithms to over-predict the natural variability of the model and may reduce the overall accuracy of the model output. These results also indicate that this issue is particularly problematic when the OK algorithm is used. OK appears to be more susceptible to the negative effects of increased numbers of data points when modelling simple grids than IDW as the increase in OK RMSE values was greater than those for IDW when 1600 points were used compared to 676 points (Table 3.1; Figure 3.6). The increases in RMSE were also greater for Grid 1 than for Grid 2 regardless of the algorithm utilized to

Figure 3.6: Graphs showing decline of RMSE values as the number of randomly distributed data points available for interpolation increases using either the a) IDW, or b) OK algorithms. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.

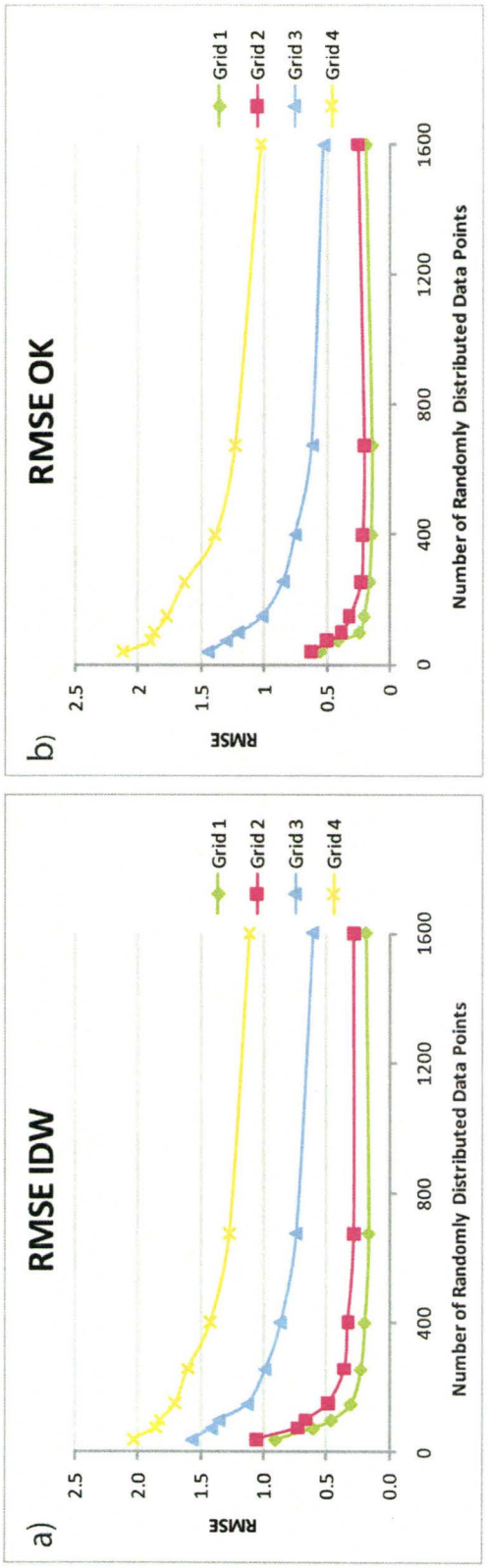

a)
RMSE IDW
RMSE
Number of Randomly Distributed Data Points
Grid 1
Grid 2
Grid 3
Grid 4
b)
RMSE OK
RMSE
Number of Randomly Distributed Data Points
Grid 1
Grid 2
Grid 3
Grid 4

Table 3.1: RMSE results for randomly distributed data points used to model the 4 synthetic grids with IDW and OK, using various quantities of data points. The cells highlighted in green indicate the point at which the rate of RMSE declined in relation to the inclusion of additional data points. The cells highlighted in orange identify the point at which RMSE values began to increase with the inclusion of additional data points.

	Inverse Distance Weighting				Ordinary Kriging			
# Points	Grid 1	Grid 2	Grid 3	Grid 4	Grid 1	Grid 2	Grid 3	Grid 4
40	0.901088	1.0594877	1.5669001	2.0379808	0.555573	0.6241006	1.4473919	2.1222325
75	0.602675	0.7244089	1.413174	1.8597298	0.412312	0.5003979	1.3022464	1.9064596
100	0.459834	0.6634433	1.3542082	1.8247403	0.239153	0.3859805	1.206956	1.8784484
150	0.305061	0.4881621	1.1290641	1.7027243	0.203138	0.3213554	1.0196441	1.7758394
256	0.22691	0.3543596	0.9900332	1.60565	0.159447	0.2294842	0.8518109	1.6351889
400	0.19628	0.3276552	0.8682869	1.427056	0.143118	0.2146624	0.7565951	1.3908847
676	0.164746	0.2795117	0.7456308	1.2759103	0.138121	0.2062527	0.6224012	1.2328671
1600	0.187382	0.2804597	0.6121876	1.1150159	0.188697	0.2546518	0.5300647	1.0266279

interpolate 1600 data points (Table 3.1; Figure 3.6). Using large amounts of data for interpolation thus appears to have a stronger negative impact on the modelling of the relatively simple surface represented by Grid 1 than on the slightly more complex Grid 2.

3.3.1.2 Cost Benefit Analysis

The results presented here provide information that may be used to guide selection of the optimal number and distribution of data points required to model a subsurface unit. Depending on the complexity of the subsurface unit being modelled, increasing the number of data points for interpolation beyond a certain point provides minimal increase to the model accuracy (as demonstrated by a decline in RMSE – see above). Since there is generally a cost associated with collecting additional data points, it may be possible to conduct a cost-benefit analysis to determine whether the cost of obtaining more data would provide significant benefit to the model accuracy. In general, the model accuracy for all grids increased as the number of randomly distributed data points increased, but there appears to be a cut-off point beyond which the inclusion of additional data points may have little to no impact on increasing the accuracy of the model. For example, when grid 1 was modelled with OK using 256 and 676 data points the RMSE remained at 0.14 for both model runs (Figure 3.6b; Table 3.1). This shows that the addition of 420 data points (676 – 256 = 420) provided no enhancement of the model accuracy.

These results can also be used as a guideline for how many data points (or % data coverage) are required to interpolate different types of subsurface environment of varying geological complexity. When relatively simple surfaces (e.g. grid 1) are predicted in the

subsurface, random data coverage of between 1.6% and 2.3% (100-150 data points in this study), should be sufficient to create an accurate model. In this situation, the inclusion of additional data will have minor impact on model accuracy and may even have negative effects, particularly if OK algorithms are used. In more complex geological environments (e.g. grids 2, 3 and 4), increasing the number of data points can increase model accuracy to a certain point, after which the gains are minimal. Increasing the data coverage beyond a 4% random coverage for grid 2 (256 data points, Table 3.1), 6.3 % for grid 3 (400 data points, Table 3.1), and 10.6% for grid 4 (676 data points, Table 3.1) has minimal impact on model accuracy.

3.3.2 Data Point Distribution

The distribution of data points across a study area can have profound impact on the accuracy of the model output (Schloeder et al., 2001; Kravchenko, 2003; Ross et al., 2005). To evaluate the impact of data distribution on model accuracy, the RMSE results for each of the output models were graphed according to sampling distribution and interpolation algorithm (Figure 3.5). The regular sampling distribution consistently produced models with the lowest RMSE for all four synthetic grids, regardless of the number of sampling points, and algorithm used (Figure 3.5). Randomly distributed data produced the second lowest RMSE results in most situations. Clustered and sparsely distributed data generally both produced relatively high RMSE values. Sparse data distributions did not perform well when modelling the more complex geological situations with very limited numbers of data points (e.g. Grid 4; Figure 3.5d) but produced reasonably accurate models (lower RMSE; Figure 3.5 a,b) when modelling

grids 1and 2 with the 1600 point dataset. The clustered data produced RMSE results similar to the sparse datasets when few data points were available, but consistently produced the least accurate models of all distributions when more data were used in the modelling process (Figure 3.5). The modelled results for the four synthetic grids show that when more than 150 sparse data points were used, the randomly-distributed sparse data produced an output that was consistently more accurate than that generated by more data points in a clustered distribution (Figure 3.5).

3.3.2.1 Discussion of Data point distribution

The distribution of data points used in the modelling process appears to be an important factor affecting interpolation accuracy. The most accurate models were created by regularly and randomly distributed data points, with less accurate models resulting from clustered and sparsely distributed data. Even though the sparse datasets contained only a fraction (approximately 1/3) of the data points contained within the clustered datasets, they most often produced a more accurate model. This was particularly evident for the more simple grids 1 and 2 (Figure 3.5 a,b). These results suggest that in certain geological situations it is better to have fewer data points that are randomly distributed (e.g. sparse distribution) than more data that are clustered together. The poor performance of the clustered data may be due to their concentration in isolated regions of the study area, leaving large regions with no data coverage (Figure 3.2). This causes the algorithm to interpolate over large areas with little or no information to constrain the predictions. Another reason for the poor performance of clustered data is that data clusters can fall in areas of high surface variability (e.g. Figure 3.1, parts of grids 2, 3 and

4) which may cause the algorithm to over-predict the amount of natural variability present across the whole model. Conversely, if a cluster containing a high number of data points falls in an area with little variation (e.g. Figure 3.1, smooth areas of grids 3 and 4), an under-prediction of the variability may occur.

It is interesting to note that when the 1600 point dataset was used to interpolate grids 1 and 2 using OK, the sparse dataset produced lower RMSE results than both the clustered and random datasets (Figure 3.5a,b). This is surprising given that both the sparse and random datasets consist of randomly distributed data, and only differ in the number of data points they contain. The RMSE results also show that when modelling grids 1 and 2, a sparse dataset consisting of 400 randomly distributed points produced a slightly more accurate model than 1600 randomly distributed data points (Figure 3.5a,b). This may be due to the model over-estimating actual subsurface variability when large numbers of data points were used for interpolation (see section 3.1.1).

3.3.2.2 Which is more important; the number of data points or their distribution?

The results presented here demonstrate that inputting more data points into a model does not necessarily produce a more accurate model, and that the distribution of data points across the study area may be a more significant factor in determining model accuracy. In the case of regularly distributed data, additional data input does appear to produce more accurate results (Figure 3.5). For randomly distributed data, additional points are beneficial in situations where the subsurface unit being modelled is relatively complex (Figure 3.5). However, the vast majority of 3D subsurface models are

interpolated using either clustered or sparsely distributed data (Paulen et al., 2006; Bond et al., 2007; Keefer, 2007), and the results presented here suggest that, in most situations, randomly-distributed sparse data will produce more accurate results than larger quantities of clustered data. Only when the surface to be modelled is complex (e.g. grid 4) can the larger amounts of clustered data (100) out-perform randomly-distributed sparse data (40; Figure 3.5d). In summary, when modelling in relatively simple geological environments, the distribution of data points appears to be more important than the number of data points used in the modelling process in controlling model accuracy. However, when modelling more complex geological environments, the number of data points becomes more important than their spatial distribution.

3.3.3 Algorithm Comparison

In order to evaluate the effect of the modelling algorithm on model accuracy, comparisons were made between the output of models using ordinary kriging (OK) and inverse distance weighting (IDW), the two most commonly used subsurface geologic modelling algorithms (Englund 1990; Weber and Englund, 1992; Brus et al., 1996; Zimmerman et al., 1999; Schloeder et al., 2001; Jones et al., 2003; Dille et al., 2003).

Graphs of RMSE results were produced to determine if the number of data points used for interpolation had an impact on the accuracy of the models produced by each algorithm (Figure 3.6). For this analysis, a randomly distributed data set was used to isolate the effects of grid complexity and data quantity on the ability of each algorithm to produce accurate interpolations. The results show that both algorithms were able to

model grid 1 most accurately (lowest RMSE) and the predictions for grid 4, the most complex surface, were the least accurate (highest RMSE values; Figure 3.6). The results also show that there is a greater difference in the RMSE produced by the two algorithms when fewer data points are used to interpolate relatively simple surfaces, than when more data are available, or when the algorithms interpolate more complex surfaces (Figure 3.6). For example, when both algorithms were used to model grid 1 using 40 data points, IDW produced a RMSE of 0.90 and OK produced a RMSE of 0.56 (Table 3.1). When 40 data points were used to model grid 2, IDW produced an RMSE of 1.06 whereas the RMSE for OK was only 0.62 (Table 3.1). However when modelling the more complex grids, there was little difference between RMSE results produced by IDW and OK (Table 3.1). For grid 4, RMSE results for IDW progressively reduced with the inclusion of additional data points and out-performed OK until more than 400 data points were included, at which point OK was able to produce more accurate models (Table 3.1). For grids 1, 2 and 3, OK produced lower RMSE results regardless of the number of data points available for interpolation; however, this difference diminished as the number of data points increased (Table 3.1).

Graphs of RMSE results were also used to analyze whether the performance of either the OK or IDW algorithm was affected by the spatial distribution of data. The regularly distributed data produced the smallest RMSE, followed by random, sparse, and clustered datasets when both the OK and IDW algorithms were used (Figure 3.5). For grids 1 and 2, there was a greater difference between the RMSE results for all data distributions when fewer data points were available (Figure 3.5 a,b). As the number of

data points increased to 1600, the difference in RMSE results between IDW and OK for grids 1 and 2 decreased for all distribution patterns (Figure 3.5 a,b). For grids 3 and 4, there was minor difference between IDW and OK for all spatial distribution patterns (Figure 3.5 c,d).

The RMSE results for each algorithm were also graphed based on the distribution and quantity of data on 4 separate graphs of grid complexity (Figure 3.5). These graphs show that when modelling simple geological environments (grids 1 and 2) utilizing less than 256 points OK was able to produce grids with much lower RMSE values than IDW (Figure 3. 5 a,b). When more than 256 points were used for interpolation the results for OK and IDW were more similar (Figure 3.5 a,b). However, for models representing more complex geological environments (grid 4) IDW was able to produce more accurate results when less than 400 data points were available (Figure 3.5 c,d).

3.3.3.1 Discussion on the Effect of Algorithm Selection

The results presented above show that the OK algorithm most commonly produced more accurate model results than IDW, regardless of the number and distribution of data points used for interpolation, or the complexity of the grids being modelled, with the exception of when complex grids were modelled with relatively few data points (Figure 3.5; Table 3.1). It is, however, important to examine circumstances in which the two algorithms performed with the greatest similarity or difference. The results presented in Figure 3.5 show that there is a greater difference in the performance of the IDW and OK algorithms when fewer data points are available for interpolation, and that

in such situations OK most often produces the more accurate model (lower RMSE). OK is able to produce more accurate models (with lower RMSE values) than IDW due to differences in how the two algorithms utilize the data points to interpolate each model. OK is able to produce lower RMSE results due to the inclusion of variograms which incorporate the degree of spatial autocorrelation between neighbouring data points and include that information as a spatial weighting factor during the interpolation process. This approach has shown to be a benefit when modelling less complex surfaces with fewer data points, as this provides OK with additional information about the relationship of the data that IDW does not consider. However, a minimum of 20-50 data points are required to make use of a variogram for interpolation purposes (Webster and Oliver, 1992; Krajewski and Gibbs, 1996). Therefore, if very low numbers of data points are available, the benefit of variogram analysis is reduced and as a result, IDW is able to produce more accurate models based purely on distance relationships. When fewer data points are available for modelling more complex surfaces (i.e. grid 4), IDW is able to produce models with lower RMSE probably because there are insufficient data available for the OK algorithm to produce a good variogram considering the highly variable nature of the grid. When an effective variogram cannot be produced by the data, OK results are negatively affected (Issaks and Srivastava, 1989; Krajewski and Gibbs 1996). The results of this study also show that when more than 256 points (representing a 4% or greater coverage of the study area) are utilized, the RMSE for OK and IDW are similar for all four synthetic grids (Figure 3.5). This suggests that 256 (or more) randomly distributed

data points provide sufficient coverage of the study area to minimize the benefit of the variogram analysis used by OK.

Both the OK and IDW algorithms performed most effectively with regularly distributed data and less well with random, sparse, and clustered datasets in order (Figure 3.5). Differences in the accuracy with which each of the algorithms modelled data of variable spatial distribution does not appear to be very significant, particularly when more complex surface are modelled with large numbers of data points (Figure 3.5). However, OK does create slightly more accurate models than IDW when clustered data are utilized.

Overall, these results show that algorithm selection has the greatest impact when interpolating more complex models with limited amounts of data. In these instances, the IDW algorithm appears to produce the most accurate results, although OK produces the most accurate models in all other situations.

3.3.4 Bias Error Analysis

All models are predictions of reality and will therefore be subject to a certain amount of error. Ultimately, the errors within model predictions should be minimized and be as close to zero as possible. However, it is important to understand whether the error inherent in any model is producing under-or over-estimations of actual values. Bias error measures the amount of deviation of the interpolated model values from the actual (original) values. If the bias error is negative, then the predicted values are less than the actual values, and if they are positive then the predicted values are greater than the actual values. Bias errors were calculated for all interpolation results in this study to determine

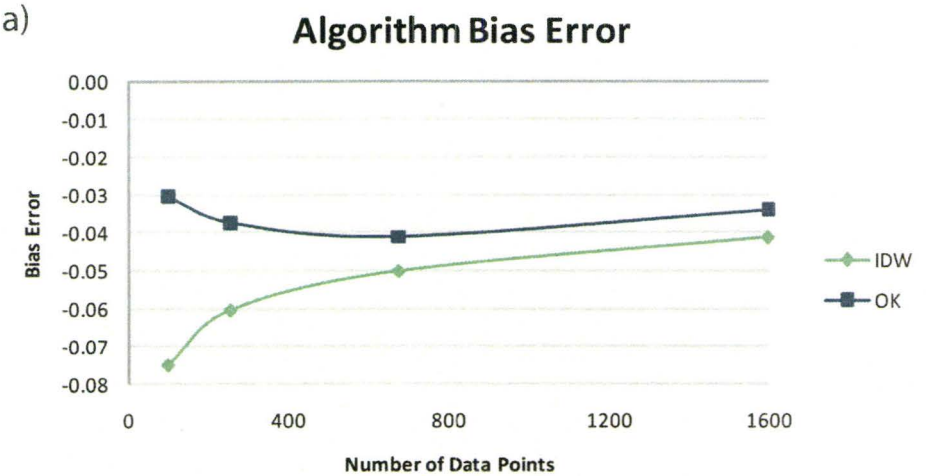
whether over- or under-estimations were occurring during the interpolation process and to identify situations in which these estimation errors were most likely to occur. The results from all simulations conducted for each sampling treatment were averaged together to provide an estimate of the bias errors that would typically occur for that particular sampling treatment (Figure 3.7).

Bias errors produced from all 10 Monte Carlo simulations were averaged for all interpolated models taking into account the number and distribution of data points, the grid complexity, and the algorithm used to interpolate the data (Appendix 3.1). The results showed that negative bias errors occurred for approximately 83% of the models produced using 100 points, 63% of those created with 256 points, 88% of those produced with 676 points, and 79% of those with 1600 points. This indicates that the interpolated models were most commonly producing under-estimations of the actual values. When the bias errors were combined for each of the models created using the same number of data points (e.g. 100, 256, 676, and 1600 data points), the values were -1.26, -1.17, -1.05, and -0.97 respectively, and show that overall, bias errors decreased as the number of data points used for interpolation increased (Figure 3.7a).

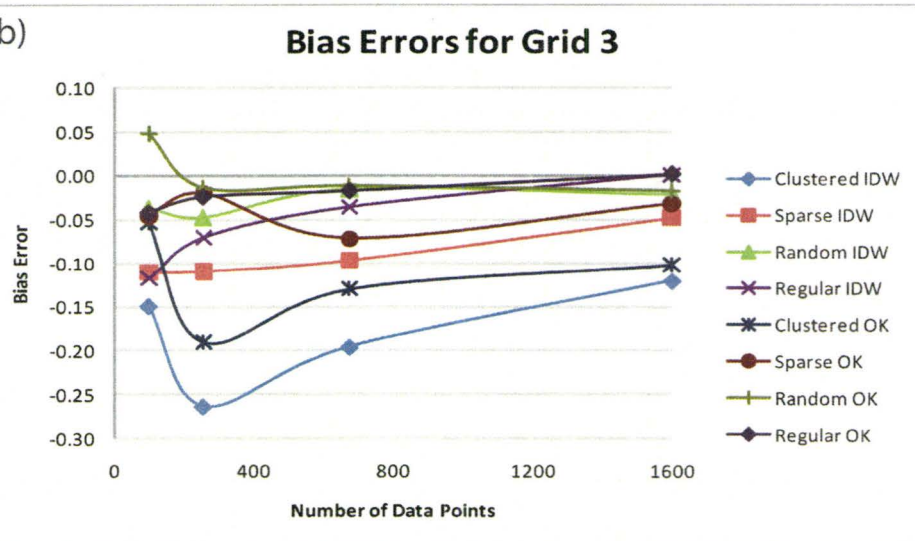
In order to determine the extent to which bias errors varied with respect to the number of data points used in modelling, algorithm selection, and data distribution patterns the errors were graphed (Figure 3.7b, c). Grid 3 was selected for this purpose as it is reasonably complex and represents a grid that may be commonly encountered in

Figure 3.7: Bias Error Analysis a) graph showing the decrease in the range of average bias errors calculated for the IDW and OK algorithms as the number of data points included in the modelling process increases. Note that the average errors are all negative and suggest that the models represent under-estimations of actual values. b) Bias errors for models of grid 3 using different numbers of data points, data distribution patterns and algorithm. c) Bias errors for models of grids 1 - 4 using 256 data points modelled with IDW and OK in clustered, random, regular and sparse distributions. Note: Bias error values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.

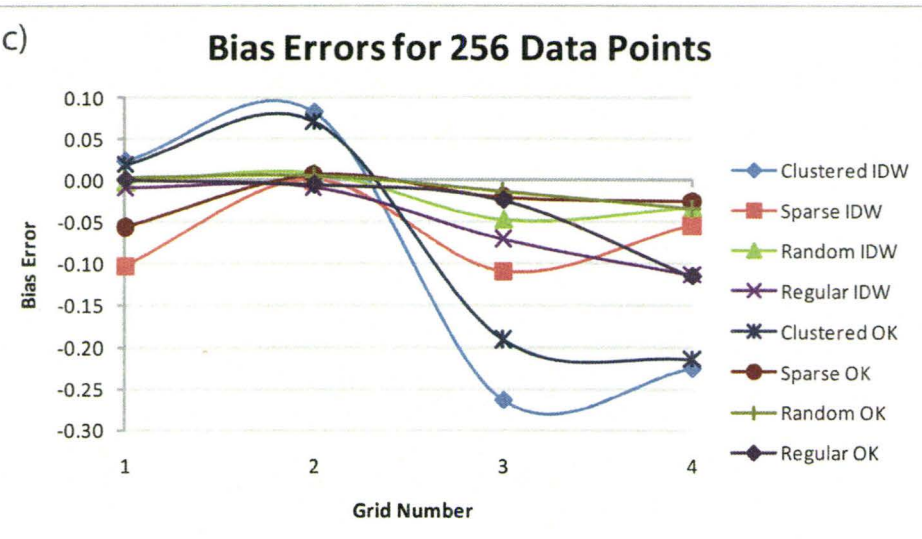
a)


Algorithm Bias Error
Bias Error
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
-0.06
-0.07
-0.08
0
400
800
1200
1600
Number of Data Points
IDW
OK

b)


Bias Errors for Grid 3
Bias Error
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
0
400
800
1200
1600
Number of Data Points
Clustered IDW
Sparse IDW
Random IDW
Regular IDW
Clustered OK
Sparse OK
Random OK
Regular OK

c)


Bias Errors for 256 Data Points
Bias Error
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
1
2
3
4
Grid Number
Clustered IDW
Sparse IDW
Random IDW
Regular IDW
Clustered OK
Sparse OK
Random OK
Regular OK

subsurface geological investigations. A wide range of bias errors was produced when 256 or fewer points were used for interpolation but this range became smaller with increasing numbers of data points (Figure 3.7b). Comparison of the bias errors produced by the IDW and OK algorithms revealed that the greatest range in values occurred when few data points were used with the IDW algorithm (Figure 3.7a). Bias error became less negative as the number of data points used for interpolation with the IDW algorithm increased; in contrast, bias error became slightly more negative with increasing data availability when the OK algorithm was used (Figure 3.7a).

Analysis of the impact of data distribution on bias error indicates that random and regularly distributed data consistently report the lowest bias errors, regardless of how many data points were included in the model (Figure 3.7b). The clustered datasets produced negative (under-estimation) bias errors, which were affected by both the algorithm used and the number of data points (Figure 3.7b). Overall, OK was able to produce models with bias errors closer to zero than IDW when modelling all data distributions (Figure 3.7b).

As a final stage of bias error analysis, the bias errors produced from models of each of the synthetic grids (grids 1 – 4), using different data point distributions (regular, random, clustered, sparse) and a constant number of data points (256; Figure 3.7c) were analysed. The bias errors identified for grid 1, representing a relatively simple geological setting, are close to zero for all data point distributions, with only slightly positive and negative values (Figure 3.7c). Bias errors for grid 2 are near zero or slightly positive (over-estimations; Figure 3.7c), whereas the bias errors for grids 3 and 4 are all larger and

in the negative range (under-estimations; Figure 3.7c). This analysis also showed that clustered data typically produced the greatest bias errors (either positive or negative; Figure 3.7c).

3.3.4.1 Discussion of Bias Error Analysis

It is important to quantify and understand the nature of bias errors associated with the generation of 3D subsurface models, as this information could have important implications for decisions made for geological applications of the model results. Knowing what sampling conditions are most likely to cause either over- or under-estimation of actual values is vital information when assessing the accuracy and reliability of model outputs.

The bias errors calculated for all interpolations were predominantly negative (Figure 3.7a) indicating that the interpolated models were most commonly producing under-estimations of the actual values. However, the number of data points utilized for interpolation had an impact upon the bias errors, as a decrease in error was noted as the number of data points increased (Figure 3.7b). This indicates that although the interpolated models all tended to represent under-estimations, those produced with the largest number of data points typically deviated from the actual (synthetic) values less than those produced with fewer data points.

Analysis of the relationship between bias errors and grid complexity revealed that as the grids became more complex, the range of bias errors also increased in magnitude and moved into the negative range (Figure 3.7c). This suggests that the more complex

the grid being modelled, the greater the tendency for interpolated values to be under-estimated. Data distribution patterns also influence error bias, with clustered data distributions consistently producing models with the greatest positive and negative bias errors (Figure 3.7b). Overall, regular and random point distributions produced models with minimal bias errors (Figure 3.7b).

Finally, the gridding algorithm selected for interpolation had a significant impact on how the data were used to interpolate a model. The bias errors produced by interpolations made with both the OK and IDW algorithms were predominantly negative indicating that both algorithms generally produced under-estimations of actual values (Figure 3.7a). However, models interpolated with OK consistently produced values closer to zero than those with IDW, which implies that models produced with the OK algorithm are typically less biased than those generated with IDW (Figure 3.7b). These results were supported by the analysis of bias errors generated from models of the four synthetic grids produced using 256 data points that showed OK produced lower bias errors than IDW for all grid types and data distribution patterns (Figure 3.7c). Overall, this analysis shows that there is a considerable tendency for IDW and to a lesser extent OK, to produce under-estimates of actual unit values when modelling complex grids.

3.5 Conclusions

Three-dimensional (3D) geo-cellular models are increasingly used for decision making and geoscientific applications in many fields of study. This increased use of 3D

models for a broad range of applications has raised concerns about the accuracy and reliability of model outputs and the relationship between output quality, input data and the type of interpolation algorithm employed in the modelling process (Weber and Englund, 1992; Weber and Englund, 1994; Zimmerman et al., 1999; Jones et al., 2003). Unfortunately, no studies to date have quantitatively assessed the impact of these variables on the modelling of geologically realistic synthetic surfaces. This paper presents a new method for evaluating the effectiveness of common interpolation algorithms used in 3D subsurface modelling, by testing their ability to accurately model four synthetic grids of varying geologic complexity with various numbers of data points (100, 256, 676 or 1600) in varying spatial distribution patterns (regular, random, clustered, and sparse). The results of quantitative statistical tests evaluating the impact of these variables on model output and uncertainty can be summarized as follows:

- ***Number of Data Points***: The inclusion of additional data points in the modelling process produced a drop in RMSE in the majority of model treatments. The number of data points used for interpolation had the greatest influence on model accuracy when modelling the relatively complex grids. The accuracy of models of the relatively simple grids was less impacted by the addition of data points, and some models were negatively influenced when higher numbers of data points were included. This finding is supported by bias error analysis that showed an overall decrease in bias errors as the number of data points utilized for interpolation increased. Although the interpolated models all tended to represent under-estimations of the original grid values,

those produced with the largest number of data points typically deviated less from the actual values than those produced with fewer data points. These results also suggest optimum numbers of data points (data coverage) are required for accurate and cost-effective interpolation of units of varying complexity. For example, increasing the data coverage beyond a 4% random coverage for grid 2, 6.3 % for grid 3, and 10.6% for grid 4 produced minimal improvements in model accuracy.

- ***Data Point Distribution***: The spatial distribution of data points input into the model is an extremely important factor affecting interpolation accuracy. The most accurate models were created by regularly and randomly distributed data points, followed by sparse and clustered data respectively. The results presented here suggest that in certain geological situations more accurate models will be created using relatively few data points that are randomly distributed (e.g. sparse distribution) than using more data with a clustered distribution. To produce an accurate model of relatively simple geological environments, the distribution of data points was found to be a more influential variable than the number of data points. In contrast, when modelling more complex geological environments, the number of data points had a greater influence on model accuracy than the spatial distribution of data.
- ***Algorithm Selection***: Overall, the OK algorithm produced more accurate representations of the modelled grids than IDW, regardless of the distribution of data points used for interpolation, or the complexity of the grids being

modelled. This conclusion is supported by the results of bias error analysis that show OK producing lower bias errors than IDW for the majority of data distributions and grid complexities. IDW produced slightly more accurate models than OK in situations where complex grids (e.g. grid 4) were modelled with relatively low numbers of data points. However, the difference in RMSE values between OK and IDW decrease as the model complexity and number of data points used for modelling increases. This implies that algorithm selection has the greatest impact on model accuracy when interpolating relatively simple grids with limited data.

When modelling spatial data there is always a high level of uncertainty, especially in subsurface environments where the unit(s) of interest are defined by data only available in select locations. Consequently, it is extremely difficult to validate the output of 3D subsurface models and to identify the many factors that may impact their reliability and accuracy. Despite this uncertainty, 3D models are becoming increasingly popular for visualizing complex geological environments and decisions are often made based on these model predictions. Thus, it is important to ensure that the models are as accurate as possible and that potential sources of uncertainty are identified and minimized. The results of this study can be used to guide the selection of modelling parameters used in 3D subsurface investigations and will allow the more effective and efficient creation of accurate and reliable 3D models.

Reference List

Bond, C. E., Gibbs, A. D., Shipton, Z. K., & Jones, S. (2007). What do you think this is? "Conceptual uncertainty" in geoscience interpretation. *GSA Today, 17,* 4-10.

Brus, D. J., De Gruijter, J. J., Marsman, B. A., Visschers, R., Bregt, K. A., Breeuwsma, A. et al. (1996). The performance of spatial interpolation methods and choropleth maps to estimate properties at points: a soil survey case study. *Environmetrics, 7,* 1-16.

Burrough, P. A. (2001). GIS and geostatistics: Essential partners for spatial analysis. *Environmental and Ecological Statistics, 8,* 361-377.

Burt, A. (2007). Three-dimensional geological modelling of thick Quaternary deposits in the Barrie-Oro area, central Ontario: new modelling techniques. In Summary of field Work and Other Activities 2007. *Ontario Geological Survey, Open File Report 6145:* 35-1-35-5.

Davis, J. C. (2002). *Statistics and data analysis and geology.* John Wiley and Sons.

de Kemp, E. A. (2006). 3-D interpretive mapping: An extension of GIS technologies for the geoscientist. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 591-612). St. John's: Geological Association of Canada.

Dille, J. A., Milner, M., Groeteke, J. J., Moretensen, D. A., & Williams, M. M. (2003). How good is your weed map? A comparison of spatial interpolators. *BioOne, 51,* 44-55.

Elith, J., Burgman, M. A., & Regan, H. M. (2002). Mapping epistemic uncertainties and vague concepts in predictions of species distribution. *Ecological Modelling, 157,* 313-329.

Englund, E. J. (1990). A variance of Geostatisticians. *Mathematical Geology, 22,* 417-455.

Gong, J., Cheng, P., & Wang, Y. (2004). Three-dimensional modeling and application in geological exploration engineering. *Computers & Geosciences, 30,* 391-404.

Goodchild, M. F. & Haining, R. P. (2004). GIS and spatial data analysis: converging perspectives. *Papers in Regional Science, 83,* 363-385.

Hengl, T., Heuvelink, G. B. M., & Stein, A. (2004). A generic framework for spatial prediction of soil variables based on regression-kriging. *Geoderma, 120,* 75-93.

Heuvelink, G. B. M. (1998). *Error Propagation in Environmental Modelling with GIS.* London: Taylor Francis.

Isaaks, E. H. & Srivistava, R. M. (1989). *An Introduction to Applied Geostatistics.* New York: Oxford University Press.

Jackson, I. (2007). So where do we go from here? *Three-dimensional Geologic mapping for Groundwater Applications, Minnesota Geological Survey Open File Report 07-4,* 19-22.

Johnston, K., Ver Hoef, J. M., Krivoruchko, K., & Lucas, N. (2001). *Using ArcGIS Geostatistical Analyst.* USA: ESRI.

Jones, N. L., Davis, R. J., & Sabbah, W. (2003). A comparison of Three-dimensional interpolation techniques for plume characterization. *Groundwater, 41,* 411-419.

Kaufmann, O. & Martin, T. (2008). 3D geological modeling from boreholes, cross-sections and geological maps, application over former natural gas storage in coal mines. *Computers & Geosciences, 34,* 278-290.

Keefer, D. A. & Rittenhouse, S. (2005). Estimating the uncertainty of 3D geologic maps. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Geological Survey of Canada, Open File 5048,* 31-35.

Kessler, H., Lelliott, M., Bridge, D., Ford, F., Sibusch, H. G., Mathers, S. et al. (2005). 3D geosciences models and their delivery to customers. *Three-dimensional Geologic Mapping for Groundwater Applications.Geological Survey of Canada, Open File 5048,* 39-42.

Krajewski, S. A. & Gibbs, B. L. (1996). *Understanding Contouring.* Colorado: Gibbs Associates.

Kravchenko, A. N. (2003). Influence of spatial structure on accuracy of interpolation methods. *Soil Science Society of America Journal, 67,* 1564-1571.

Lapen, D. R. & Hayhoe, H. N. (2003). Spatial analysis of seasonal and annual temperature and precipitation normals in southern Ontario, Canada. *Journal of Great Lakes Research, 29,* 529-544.

Logan, C., Russel, H. A. J., Sharpe D.R., & Kenny, F. M. (2006). The role of GIS and expert knowledge in 3-D modelling, Oak Ridges Moraine, southern Ontario. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 519-542). St. John's: Geological Association of Canada.

MacCormack, K. E., MacLachlan, J. C., & Eyles, C. H. (2005). Viewing the subsurface in three dimensions: Initial results of modeling the Quaternary sedimentary infill of the Dundas Valley, Hamilton, Ontario. *Geosphere, 1,* 23-31.

Moffat, A. M., Papale, D., Reichstein, M., Hollinger, D. Y., Richardson, A. D., Barr, A. G. et al. (2007). Comprehensive comparison of gap-filling techniques for eddy covariance net carbon fluxes. *Agricultural and Forest Meteorology, 147,* 209-232.

Mueller, T. G., Pusuluri, P. B., Mathias, K. K., Cornelius, P. L., Barnhisel, R. I., & Shearer, S. A. (2004). Map quality for ordinary kriging and inverse distance weighted interpolation. *Soil Science Society of America Journal, 68,* 2042-2047.

Nalder, I. A. & Wein, R. W. (1998). Spatial interpolation of climatic Normals: test of a new method in the Canadian boreal forest. *Agricultural and Forest Meteorology, 92,* 211-225.

Parks, K., Andriashek, L., & Atkinson, N. (2005). Lowering barriers to public communication with 3D groundwater mapping at Alberta Geological Survey: Examples from Canada's Oil Sands Area. *Three-Dimensional Geological Mapping for Groundwater Applications: Workshop Extended Abstracts, Geological Survey of Canada Open File 5048,* 57-60.

Paulen, R. C., McClenaghan, M. B., & Harris, J. R. (2006). Bedrock topography and drift thickness models from the Timmins area, northeastern Ontario: An application of GIS to the Timmins overburden drillhole database. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 413-434). St. John's: Geological Association of Canada.

RockWare (2006). Rockworks v. 2006: An updated computer program for spatially analyzing data and visualizing 3-dimensional subsurface models [Computer software]. Denver.

Ross, M., Parent, M., & Lefebvre, R. (2005). 3D geologic framework models for regional hydrogeology and land-use management: a case study from a Quaternary basin of southwestern Quebec, Canada. *Hydrogeology Journal, 13,* 690-707.

Schloeder, C. A., Zimmerman, N. E., & Jacobs, M. J. (2001). Comparison of methods for interpolating soil properties using limited data. *Soil Science Society of America Journal, 66,* 479.

Shi, W., Goodchild, M. F., & Fisher, P. F. (2002). *Spatial Data Quality.* USA: CRC Press LLC.

Tabios, G. Q. & Salas, J. D. (1985). A comparative-analysis of techniques for spatial interpolation of precipitation. *Water Resources Bulletin, 21,* 365-380.

Walker, D. D. & Loftis, J. C. (1997). Alternative spatial estimators for ground-water and soil measurements. *Groundwater, 35,* 593-599.

Weber, D. & Englund, E. J. (1992). Evaluation and comparison of spatial interpolators. *Mathematical Geology, 24,* 381-391.

Weber, D. & Englund, E. J. (1994). Evaluation and comparison of spatial interpolators II. *Mathematical Geology, 26,* 589-603.

Webster, R. & Oliver, M. A. (1992). Sample adequately to estimate variograms of soil properties. *Journal of Soil Science, 43,* 177-192.

Wu, Q., Xu, H., & Zou, X. (2005). An effective method for 3D geological modeling with multi-source data integration. *Computers and Geosciences, 31,* 35-43.

Zimmerman, D., Pavlik, C., Ruggles, A., & Armstrong, M. P. (1999). An experimental comparison of Ordinary and Universal Kriging and inverse distance weighting. *Mathematical Geology, 31,* 375-390.

Zwiers, W. G., Rainsford, D. R. B., & Bajc, A. F. (2008). Project Unit 06-026: investigation of the Dundas Buried Bedrock Valley. *Summary of Field Work and Other Activities 2008, Ontario Geological Survey, Open File Report 6226,* 33-1-33-7.

APPENDIX 3.1: GRID COMPARISON DATA

Number of Data Points	Grid Complexity	Data Distribution	Algorithm	Root Mean Square Error (RMSE)										Relative Root Mean Square Error (rRMSE)										Mean Average Error (MAE)										Bias Error (BE)										Correlation Coefficient (r2)									
100	Grid 1	Cluster	IDW	1.4430	1.4271	1.3342	0.9644	1.1003	0.7137	0.6766	0.7333	0.8914	0.8158	0.3279	0.3243	0.3032	0.2192	0.2500	0.1622	0.1538	0.1666	0.2026	0.1854	0.8129	0.7537	0.7474	0.5775	0.6150	0.4625	0.4333	0.5297	0.6379	0.5744	-0.2532	-0.4820	-0.4078	0.1979	-0.1629	0.2889	0.0143	0.0677	0.1198	0.1974	0.6758	0.6829	0.7228	0.8552	0.8115	0.9207	0.9287	0.9163	0.8763	0.8964
100	Grid 1	Cluster	OK	1.3043	1.2127	1.0198	0.8210	0.9532	0.4950	0.4725	0.6033	0.5251	0.6434	0.2964	0.2756	0.2318	0.1866	0.2166	0.1125	0.1074	0.1371	0.1193	0.1462	0.6904	0.5637	0.5088	0.4683	0.4932	0.3056	0.3003	0.3942	0.3606	0.4111	-0.2677	-0.4134	-0.3231	0.1468	-0.1815	0.1889	0.0681	0.0625	0.1009	0.1715	0.7351	0.7710	0.8380	0.8950	0.8585	0.9618	0.9652	0.9433	0.9571	0.9355
100	Grid 1	Sparse	IDW	1.0282	1.0094	0.8497	0.9858	0.7399	0.8145	0.7295	0.9940	0.9691	0.8907	0.2336	0.2294	0.1931	0.2240	0.1681	0.1851	0.1658	0.2259	0.2202	0.2024	0.5912	0.5787	0.5686	0.6173	0.4853	0.5127	0.4978	0.5820	0.5995	0.5409	-0.2517	-0.3033	0.1716	-0.0729	-0.0306	-0.1884	0.0412	-0.1962	-0.0111	-0.1390	0.8354	0.8413	0.8876	0.8487	0.9147	0.8967	0.9171	0.8462	0.8538	0.8765
100	Grid 1	Sparse	OK	0.7458	0.5435	0.5149	0.7401	0.4076	0.3962	0.4561	0.5996	0.5870	0.5650	0.1695	0.1235	0.1170	0.1682	0.0926	0.0900	0.1036	0.1362	0.1334	0.1284	0.3966	0.3052	0.3112	0.3948	0.2736	0.2672	0.2937	0.3472	0.3590	0.3592	-0.1578	-0.1321	0.1324	-0.1635	0.0193	-0.0330	0.0022	-0.0770	0.0471	-0.0425	0.9134	0.9540	0.9587	0.9147	0.9741	0.9756	0.9676	0.9440	0.9463	0.9503
100	Grid 1	Random	IDW	0.4313	0.5291	0.5068	0.4426	0.5138	0.4077	0.3516	0.4184	0.5822	0.4148	0.0980	0.1202	0.1152	0.1006	0.1168	0.0926	0.0799	0.0951	0.1323	0.0943	0.2955	0.3203	0.3117	0.2885	0.3231	0.2667	0.2401	0.2733	0.3346	0.2710	0.0393	-0.0405	-0.0695	0.0154	-0.0500	-0.0066	-0.0075	0.0086	-0.1180	-0.0516	0.9710	0.9564	0.9600	0.9695	0.9589	0.9741	0.9807	0.9727	0.9472	0.9732
100	Grid 1	Random	OK	0.2023	0.2647	0.2636	0.2683	0.2453	0.2526	0.1606	0.1943	0.3364	0.2035	0.0460	0.0601	0.0599	0.0610	0.0557	0.0574	0.0365	0.0441	0.0764	0.0462	0.1278	0.1663	0.1572	0.1720	0.1477	0.1671	0.1033	0.1273	0.1985	0.1287	0.0322	-0.0031	-0.0122	0.0138	-0.0071	-0.0014	0.0113	0.0156	-0.0309	0.0049	0.9936	0.9891	0.9892	0.9888	0.9906	0.9901	0.9960	0.9941	0.9824	0.9936
100	Grid 1	Regular	IDW	0.4747	0.4747	0.4747	0.4747	0.4747	0.4747	0.4747	0.4747	0.4747	0.4747	0.1079	0.1079	0.1079	0.1079	0.1079	0.1079	0.1079	0.1079	0.1079	0.1079	0.2733	0.2733	0.2733	0.2733	0.2733	0.2733	0.2733	0.2733	0.2733	0.2733	-0.0899	-0.0899	-0.0899	-0.0899	-0.0899	-0.0899	-0.0899	-0.0899	-0.0899	-0.0899	0.9649	0.9649	0.9649	0.9649	0.9649	0.9649	0.9649	0.9649	0.9649	0.9649
100	Grid 1	Regular	OK	0.1893	0.1893	0.1893	0.1893	0.1893	0.1893	0.1893	0.1893	0.1893	0.1893	0.0430	0.0430	0.0430	0.0430	0.0430	0.0430	0.0430	0.0430	0.0430	0.0430	0.1067	0.1067	0.1067	0.1067	0.1067	0.1067	0.1067	0.1067	0.1067	0.1067	-0.0227	-0.0227	-0.0227	-0.0227	-0.0227	-0.0227	-0.0227	-0.0227	-0.0227	-0.0227	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944
100	Grid 2	Cluster	IDW	1.4249	0.9571	0.8738	0.9317	0.8982	0.9849	0.9178	1.1117	1.0318	1.0542	0.2807	0.1885	0.1721	0.1835	0.1769	0.1940	0.1808	0.2190	0.2032	0.2077	0.9983	0.7343	0.6601	0.6964	0.6787	0.7242	0.6700	0.8078	0.7827	0.8206	-0.6925	0.3015	0.3320	0.0157	0.1403	-0.2441	0.1222	-0.3563	0.0410	0.2187	0.5097	0.7788	0.8156	0.7904	0.8052	0.7657	0.7966	0.7016	0.7429	0.7316
100	Grid 2	Cluster	OK	1.2306	0.5601	0.7183	0.6163	0.5807	0.6640	0.5723	0.8180	0.6630	0.7546	0.2424	0.1103	0.1415	0.1214	0.1144	0.1308	0.1127	0.1611	0.1306	0.1486	0.7271	0.4167	0.4563	0.4315	0.3992	0.4464	0.3767	0.4939	0.4677	0.5230	-0.5006	0.1525	0.2487	0.0421	0.0946	-0.0636	0.1018	-0.1082	-0.1206	0.1378	0.6343	0.9242	0.8754	0.9083	0.9186	0.8935	0.9209	0.8384	0.8938	0.8625
100	Grid 2	Sparse	IDW	1.0069	1.0313	0.9413	1.0938	1.1754	0.9162	0.9472	1.1626	1.2486	1.0716	0.1983	0.2031	0.1854	0.2154	0.2315	0.1805	0.1866	0.2290	0.2459	0.2111	0.7759	0.8426	0.7561	0.8735	0.8870	0.7384	0.7410	0.9290	0.9623	0.8307	0.0049	-0.2248	-0.0723	-0.3950	0.0277	-0.0927	-0.2583	0.2745	-0.0720	-0.2387	0.7552	0.7432	0.7860	0.7111	0.6664	0.7973	0.7833	0.6736	0.6235	0.7227
100	Grid 2	Sparse	OK	0.6262	0.5885	0.5539	0.5442	0.7072	0.6170	0.6306	0.6890	0.6673	0.6173	0.1233	0.1159	0.1091	0.1072	0.1393	0.1215	0.1242	0.1357	0.1314	0.1216	0.4096	0.4386	0.3871	0.3984	0.4754	0.4108	0.4518	0.5117	0.4978	0.4462	-0.0437	0.0554	0.0428	-0.0462	-0.0049	0.0590	-0.1236	0.0858	-0.0477	-0.1346	0.9053	0.9164	0.9259	0.9285	0.8792	0.9081	0.9040	0.8854	0.8925	0.9080
100	Grid 2	Random	IDW	0.7101	0.6097	0.6610	0.6453	0.6554	0.7438	0.5887	0.6474	0.6594	0.7136	0.1399	0.1201	0.1302	0.1271	0.1291	0.1465	0.1160	0.1275	0.1299	0.1405	0.5038	0.4627	0.5026	0.5019	0.4902	0.5623	0.4559	0.4800	0.4877	0.5365	-0.0568	-0.0565	0.1028	-0.0189	0.0605	-0.2231	-0.0423	-0.2123	-0.1462	0.0927	0.8782	0.9102	0.8945	0.8995	0.8963	0.8664	0.9163	0.8988	0.8950	0.8770
100	Grid 2	Random	OK	0.3634	0.3565	0.3860	0.3520	0.3951	0.4709	0.3107	0.3711	0.4143	0.4397	0.0716	0.0702	0.0760	0.0693	0.0778	0.0928	0.0612	0.0731	0.0816	0.0866	0.2381	0.2465	0.2774	0.2521	0.2594	0.3062	0.2237	0.2478	0.2978	0.3018	-0.0058	-0.0443	0.0944	-0.0081	0.0471	-0.0837	-0.0208	-0.0731	-0.0622	0.0564	0.9681	0.9693	0.9640	0.9701	0.9623	0.9465	0.9767	0.9667	0.9586	0.9533
100	Grid 2	Regular	IDW	0.5454	0.5454	0.5454	0.5454	0.5454	0.5454	0.5454	0.5454	0.5454	0.5454	0.1074	0.1074	0.1074	0.1074	0.1074	0.1074	0.1074	0.1074	0.1074	0.1074	0.4086	0.4086	0.4086	0.4086	0.4086	0.4086	0.4086	0.4086	0.4086	0.4086	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	0.9282	0.9282	0.9282	0.9282	0.9282	0.9282	0.9282	0.9282	0.9282	0.9282
100	Grid 2	Regular	OK	0.2647	0.2647	0.2647	0.2647	0.2647	0.2647	0.2647	0.2647	0.2647	0.2647	0.0521	0.0521	0.0521	0.0521	0.0521	0.0521	0.0521	0.0521	0.0521	0.0521	0.1877	0.1877	0.1877	0.1877	0.1877	0.1877	0.1877	0.1877	0.1877	0.1877	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.9831	0.9831	0.9831	0.9831	0.9831	0.9831	0.9831	0.9831	0.9831	0.9831
100	Grid 3	Cluster	IDW	1.6948	1.5081	1.5783	1.4157	1.2872	1.6172	1.8122	1.5251	1.2959	1.3685	0.4600	0.4093	0.4284	0.3842	0.3494	0.4389	0.4919	0.4139	0.3517	0.3714	1.3263	1.2022	1.2476	1.1173	1.0497	1.2058	1.3563	1.1937	1.0573	1.0372	-0.4822	-0.0818	0.1002	0.0240	-0.0193	-0.4245	-0.3249	-0.2627	-0.2926	0.2711	0.1746	0.3464	0.2841	0.4241	0.5238	0.2485	0.0563	0.3316	0.5174	0.4619
100	Grid 3	Cluster	OK	1.7006	1.3953	1.5286	1.4157	1.2383	1.4990	1.8958	1.3375	1.3680	1.3590	0.4616	0.3787	0.4149	0.3842	0.3361	0.4069	0.5145	0.3630	0.3713	0.3688	1.3197	1.0504	1.1751	1.1173	0.9673	1.0747	1.3485	1.0130	0.9936	0.9658	-0.4688	-0.1026	0.2334	0.0240	-0.0523	-0.1866	-0.4154	-0.0246	0.1760	0.2865	0.1690	0.4405	0.3286	0.4241	0.5593	0.3543	-0.0328	0.4859	0.4622	0.4693
100	Grid 3	Sparse	IDW	1.5314	1.6062	1.4475	1.5631	1.5511	1.5856	1.5244	1.5651	1.7605	1.5343	0.4156	0.4359	0.3929	0.4242	0.4210	0.4303	0.4137	0.4248	0.4778	0.4164	1.2615	1.3035	1.2119	1.2662	1.2605	1.3170	1.2647	1.3099	1.3841	1.2827	0.1162	-0.4106	-0.0457	0.2143	0.2608	-0.2978	-0.1353	-0.5509	-0.1517	-0.1052	0.3261	0.2587	0.3979	0.2979	0.3086	0.2775	0.3322	0.2961	0.1094	0.3235
100	Grid 3	Sparse	OK	1.4348	1.4110	1.4214	1.5279	1.4253	1.4676	1.3153	1.4028	1.6233	1.4445	0.3894	0.3830	0.3858	0.4147	0.3868	0.3983	0.3570	0.3807	0.4406	0.3921	1.1470	1.1020	1.0996	1.1627	1.1107	1.1546	1.0622	1.1636	1.2430	1.1978	0.0335	-0.2315	0.0276	0.4035	0.2619	-0.2827	0.0804	-0.5454	-0.2363	0.0390	0.4084	0.4279	0.4194	0.3292	0.4162	0.3811	0.5028	0.4345	0.2428	0.4004
100	Grid 3	Random	OK	1.3247	1.2313	1.5783	1.1401	1.4610	1.5218	1.2698	1.4046	1.2959	1.3146	0.3595	0.3342	0.4284	0.3094	0.3965	0.4130	0.3446	0.3812	0.3517	0.3568	1.0337	0.9659	1.2476	0.8509	1.1737	1.2125	0.9915	1.1386	1.0573	1.0403	-0.0527	0.0859	0.1002	0.1601	-0.2145	-0.0177	0.0580	-0.1693	-0.2926	-0.0080	0.4957	0.5644	0.2841	0.6265	0.3866	0.3345	0.5367	0.4330	0.5174	0.5034
100	Grid 3	Random	OK	1.1198	1.1065	1.5286	1.1401	1.1709	1.2214	1.2319	1.1232	1.2959	1.1312	0.3039	0.3003	0.4149	0.3094	0.3178	0.3315	0.3344	0.3049	0.3517	0.3070	0.8059	0.8241	1.1751	0.8509	0.9177	0.8985	0.9492	0.8546	1.0573	0.8369	0.0587	0.1583	0.2334	0.1601	-0.1058	0.1277	0.0420	-0.0393	-0.2926	0.1403	0.6396	0.6481	0.3286	0.6265	0.6060	0.5713	0.5639	0.6375	0.5174	0.6323
100	Grid 3	Regular	IDW	1.2603	1.2603	1.2603	1.2603	1.2603	1.2603	1.2603	1.2603	1.2603	1.2603	0.3421	0.3421	0.3421	0.3421	0.3421	0.3421	0.3421	0.3421	0.3421	0.3421	1.0404	1.0404	1.0404	1.0404	1.0404	1.0404	1.0404	1.0404	1.0404	1.0404	-0.1175	-0.1175	-0.1175	-0.1175	-0.1175	-0.1175	-0.1175	-0.1175	-0.1175	-0.1175	0.5436	0.5436	0.5436	0.5436	0.5436	0.5436	0.5436	0.5436	0.5436	0.5436
100	Grid 3	Regular	OK	1.0123	1.0123	1.0123	1.0123	1.0123	1.0123	1.0123	1.0123	1.0123	1.0123	0.2748	0.2748	0.2748	0.2748	0.2748	0.2748	0.2748	0.2748	0.2748	0.2748	0.7610	0.7610	0.7610	0.7610	0.7610	0.7610	0.7610	0.7610	0.7610	0.7610	-0.0415	-0.0415	-0.0415	-0.0415	-0.0415	-0.0415	-0.0415	-0.0415	-0.0415	-0.0415	0.7055	0.7055	0.7055	0.7055	0.7055	0.7055	0.7055	0.7055	0.7055	0.7055
100	Grid 4	Cluster	IDW	1.9864	1.9755	2.0872	1.9484	1.9310	2.2505	1.9530	2.0268	2.0208	2.0171	0.3232	0.3214	0.3396	0.3170	0.3142	0.3662	0.3178	0.3298	0.3288	0.3282	1.4497	1.2828	1.5302	1.4257	1.3834	1.9027	1.2784	1.6294	1.3933	1.2529	-0.1857	0.2975	-0.6406	-0.4103	-0.2175	-0.9426	0.0752	-0.6358	-0.1947	0.3120	0.1063	0.1161	0.0133	0.1402	0.1555	-0.1472	0.1361	0.0696	0.0751	0.0784
100	Grid 4	Cluster	OK	1.9938	2.0504	2.1693	2.0082	1.9310	2.3862	2.0423	2.0423	1.9293	2.0474	0.3244	0.3336	0.3530	0.3268	0.3142	0.3882	0.3323	0.3323	0.3139	0.3331	1.4452	1.2880	1.5244	1.4390	1.3834	2.0151	1.3564	1.6424	1.1835	1.2021	-0.1746	0.3746	-0.5611	-0.3844	-0.2375	-0.9938	0.0143	-0.6104	0.1725	0.3333	0.0996	0.0478	-0.0659	0.0866	0.1555	-0.2896	0.0553	0.0553	0.1569	0.0506
100	Grid 4	Sparse	IDW	2.2238	1.9861	2.1313	2.0413	2.1653	1.9990	1.9649	1.9518	2.0144	1.9018	0.3618	0.3232	0.3468	0.3321	0.3523	0.3253	0.3197	0.3176	0.3278	0.3094	1.3481	1.3088	1.6829	1.5221	1.7149	1.6250	1.4214	1.3723	1.2935	1.5130	0.6022	0.3454	-0.6157	0.0052	-0.6960	-0.5402	0.0543	0.1292	0.4368	-0.3855	-0.1201	0.1065	-0.0289	0.0562	-0.0619	0.0949	0.1255	0.1372	0.0809	0.1808
100	Grid 4	Sparse	OK	2.3063	2.0433	2.1444	2.1417	2.3716	1.9851	2.0757	2.0509	1.9837	2.1196	0.3753	0.3325	0.3489	0.3485	0.3859	0.3230	0.3377	0.3337	0.3228	0.3449	1.3053	1.3642	1.6302	1.5999	1.9090	1.3984	1.3412	1.4413	1.2170	1.7082	0.7255	0.3833	-0.5777	0.0075	-0.7907	-0.4081	0.0050	0.1348	0.4749	-0.5005	-0.2047	0.0543	-0.0415	-0.0389	-0.2739	0.1074	0.0241	0.0473	0.1088	-0.0176
100	Grid 4	Random	IDW	1.7947	1.7809	1.8540	1.8134	1.8378	1.9236	1.8459	1.8005	1.7661	1.8305	0.2920	0.2898	0.3017	0.2951	0.2990	0.3130	0.3003	0.2930	0.2874	0.2978	1.2227	1.1631	1.2137	1.2745	1.2027	1.2923	1.2108	1.3174	1.1928	1.1413	-0.0097	0.1878	0.0993	-0.0678	0.1138	0.1095	0.0455	-0.2531	0.0478	0.2850	0.2705	0.2817	0.2214	0.2552	0.2350	0.1619	0.2282	0.2657	0.2935	0.2410
100	Grid 4	Random	OK	1.9172	1.7137	1.8302	1.7820	1.8940	2.0423	1.9330	1.9387	1.8627	1.8708	0.3119	0.2788	0.2978	0.2899	0.3082	0.3323	0.3145	0.3154	0.3031	0.3044	1.3007	1.0400	1.0707	1.1250	1.2420	1.3912	1.1995	1.4264	1.2671	1.1795	0.0134	0.1336	0.2175	0.0206	0.1205	0.0978	-0.0645	-0.2830	0.0260	0.2767	0.1675	0.3349	0.2413	0.2808	0.1875	0.0553	0.1537	0.1487	0.2142	0.2072
100	Grid 4	Regular	IDW	1.7054	1.7054	1.7054	1.7054	1.7054	1.7054	1.7054	1.7054	1.7054	1.7054	0.2775	0.2775	0.2775	0.2775	0.2775	0.2775	0.2775	0.2775	0.2775	0.2775	1.1714	1.1714	1.1714	1.1714	1.1714	1.1714	1.1714	1.1714	1.1714	1.1714	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.0053	0.3413	0.3413	0.3413	0.3413	0.3413	0.3413	0.3413	0.3413	0.3413	0.3413
100	Grid 4	Regular	OK	1.6743	1.6743	1.6743	1.6743	1.6743	1.6743	1.6743	1.6743	1.6743	1.6743	0.2724	0.2724	0.2724	0.2724	0.2724	0.2724	0.2724	0.2724	0.2724	0.2724	1.0637	1.0637	1.0637	1.0637	1.0637	1.0637	1.0637	1.0637	1.0637	1.0637	-0.0013	-0.0013	-0.0013	-0.0013	-0.0913	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	0.3651	0.3651	0.3651	0.3651	0.3651	0.3651	0.3651	0.3651	0.3651	0.3651

Number of Data Points	Grid Complexity	Data Distribution	Algorithm	Root Mean Square Error (RMSE)										Relative Root Mean Square Error (rRMSE)										Mean Average Error (MAE)										Bias Error (BE)										Correlation Coefficient (r2)									
256	Grid 1	Cluster	IDW	0.5469	0.4487	0.6069	0.4336	0.5487	0.6929	0.8031	0.7932	0.8065	0.9788	0.1243	0.1020	0.1379	0.0985	0.1247	0.1574	0.1825	0.1802	0.1833	0.2224	0.3342	0.2743	0.3789	0.3010	0.3759	0.4367	0.4212	0.3788	0.4877	0.5395	0.1028	0.1783	0.0618	0.1637	0.1077	0.1302	-0.2055	-0.1755	-0.0230	-0.1099	0.9534	0.9686	0.9426	0.9707	0.9531	0.9252	0.8996	0.9020	0.8987	0.8508
256	Grid 1	Cluster	OK	0.4074	0.4487	0.4939	0.3261	0.4566	0.5512	0.7266	0.6206	0.6016	0.7491	0.0926	0.1020	0.1122	0.0741	0.1038	0.1252	0.1651	0.1410	0.1367	0.1702	0.2405	0.2743	0.2908	0.2105	0.2850	0.3142	0.3436	0.2899	0.3529	0.3725	0.0566	0.1783	0.0304	0.1226	0.0810	0.1206	-0.1707	-0.1176	-0.0142	-0.1010	0.9742	0.9686	0.9620	0.9834	0.9675	0.9527	0.9178	0.9400	0.9436	0.9126
256	Grid 1	Sparse	IDW	1.0254	0.3687	0.5479	0.4537	0.6605	0.5680	0.3376	0.9388	0.4274	0.6988	0.2330	0.0838	0.1245	0.1031	0.1501	0.1291	0.0767	0.2133	0.0971	0.1588	0.5285	0.1938	0.3543	0.2581	0.4081	0.3479	0.2136	0.4700	0.2926	0.4184	-0.3459	-0.0767	0.0088	-0.0259	-0.1065	-0.0710	-0.0088	-0.2420	-0.0009	-0.1579	0.8363	0.9788	0.9533	0.9679	0.9321	0.9498	0.9823	0.8628	0.9716	0.9240
256	Grid 1	Sparse	OK	0.6440	0.3687	0.3852	0.4537	0.2894	0.3519	0.3376	0.7280	0.2313	0.3334	0.1464	0.0838	0.0875	0.1031	0.0658	0.0800	0.0767	0.1654	0.0526	0.0758	0.2902	0.1938	0.2378	0.2581	0.1978	0.2210	0.2136	0.3250	0.1493	0.1995	-0.1759	-0.0767	-0.0090	-0.0259	-0.0031	-0.0236	-0.0088	-0.1867	-0.0008	-0.0515	0.9354	0.9788	0.9769	0.9679	0.9870	0.9807	0.9823	0.9175	0.9917	0.9827
256	Grid 1	Random	IDW	0.2122	0.2308	0.2493	0.1567	0.2504	0.2010	0.2045	0.2437	0.3048	0.2156	0.0482	0.0524	0.0567	0.0356	0.0569	0.0457	0.0465	0.0554	0.0693	0.0490	0.1329	0.1485	0.1522	0.0846	0.1543	0.1198	0.1360	0.1560	0.1805	0.1394	0.0065	-0.0246	0.0146	-0.0114	-0.0013	0.0082	0.0129	0.0102	-0.0415	-0.0007	0.9930	0.9917	0.9903	0.9962	0.9902	0.9937	0.9935	0.9908	0.9855	0.9928
256	Grid 1	Random	OK	0.1788	0.1603	0.1789	0.1567	0.1694	0.1392	0.1332	0.1599	0.1736	0.1444	0.0406	0.0364	0.0407	0.0356	0.0385	0.0316	0.0303	0.0363	0.0394	0.0328	0.0872	0.0967	0.1036	0.0846	0.1046	0.0799	0.0780	0.0989	0.1055	0.0890	0.0054	-0.0084	0.0168	-0.0114	0.0064	0.0063	0.0046	0.0119	-0.0100	0.0025	0.9950	0.9960	0.9950	0.9962	0.9955	0.9970	0.9972	0.9960	0.9953	0.9968
256	Grid 1	Regular	IDW	0.1749	0.1749	0.1749	0.1749	0.1749	0.1749	0.1749	0.1749	0.1749	0.1749	0.0397	0.0397	0.0397	0.0397	0.0397	0.0397	0.0397	0.0397	0.0397	0.0397	0.1061	0.1061	0.1061	0.1061	0.1061	0.1061	0.1061	0.1061	0.1061	0.1061	-0.0085	-0.0085	-0.0085	-0.0085	-0.0085	-0.0085	-0.0085	-0.0085	-0.0085	-0.0085	0.9952	0.9952	0.9952	0.9952	0.9952	0.9952	0.9952	0.9952	0.9952	0.9952
256	Grid 1	Regular	OK	0.0938	0.0938	0.0938	0.0938	0.0938	0.0938	0.0938	0.0938	0.0938	0.0938	0.0213	0.0213	0.0213	0.0213	0.0213	0.0213	0.0213	0.0213	0.0213	0.0213	0.0528	0.0528	0.0528	0.0528	0.0528	0.0528	0.0528	0.0528	0.0528	0.0528	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.9986	0.9986	0.9986	0.9986	0.9986	0.9986	0.9986	0.9986	0.9986	0.9986
256	Grid 2	Cluster	IDW	0.8258	0.7529	0.7074	0.5500	1.0064	0.9954	0.9974	0.9663	0.8152	0.7932	0.1627	0.1483	0.1393	0.1083	0.1982	0.1961	0.1965	0.1903	0.1606	0.1562	0.5803	0.4285	0.4826	0.3536	0.6990	0.6668	0.6835	0.6273	0.5640	0.5317	0.1715	0.0136	0.0261	0.1533	0.0892	0.2725	0.2491	-0.1647	-0.0122	0.0309	0.8353	0.8631	0.8791	0.9269	0.7554	0.7607	0.7598	0.7745	0.8395	0.8481
256	Grid 2	Cluster	OK	0.5769	0.7529	0.5973	0.5500	0.7405	0.7489	0.6515	0.7846	0.6278	0.7114	0.1136	0.1483	0.1176	0.1083	0.1459	0.1475	0.1283	0.1545	0.1237	0.1401	0.3759	0.4285	0.3078	0.3536	0.4850	0.4360	0.4034	0.4546	0.4095	0.4207	0.1004	0.0136	0.0687	0.1533	0.0708	0.1578	0.1447	-0.1151	0.0390	0.0805	0.9196	0.8631	0.9139	0.9269	0.8676	0.8646	0.8975	0.8513	0.9048	0.8778
256	Grid 2	Sparse	IDW	0.9022	0.4951	0.7336	0.5216	0.7135	0.7353	0.9179	0.7791	0.6713	0.7745	0.1777	0.0975	0.1445	0.1027	0.1405	0.1448	0.1808	0.1535	0.1322	0.1526	0.6469	0.3397	0.5733	0.3696	0.5572	0.5669	0.6638	0.6074	0.5257	0.5856	-0.0978	-0.0890	0.1270	0.1164	0.1306	0.0365	-0.1517	-0.1269	0.1218	-0.0668	0.8034	0.9408	0.8700	0.9343	0.8771	0.8694	0.7965	0.8534	0.8912	0.8551
256	Grid 2	Sparse	OK	0.5825	0.4951	0.5619	0.5216	0.4221	0.4192	0.5264	0.5873	0.4345	0.4533	0.1147	0.0975	0.1107	0.1027	0.0831	0.0826	0.1037	0.1157	0.0856	0.0893	0.3635	0.3397	0.3558	0.3696	0.3067	0.2773	0.3338	0.4327	0.3331	0.3328	-0.0838	-0.0890	0.1295	0.1164	0.0295	-0.0198	-0.0347	-0.1106	0.0890	0.0407	0.9181	0.9408	0.9237	0.9343	0.9570	0.9576	0.9331	0.9167	0.9544	0.9504
256	Grid 2	Random	IDW	0.3329	0.2194	0.4320	0.2362	0.4172	0.3444	0.3826	0.3771	0.4400	0.3617	0.0656	0.0432	0.0851	0.0465	0.0822	0.0678	0.0754	0.0743	0.0867	0.0713	0.2530	0.1511	0.3107	0.1531	0.2982	0.2587	0.2881	0.2740	0.3102	0.2736	0.0050	-0.0092	0.0483	-0.0133	0.0272	-0.0156	-0.0120	-0.0225	0.0285	0.0494	0.9732	0.9884	0.9549	0.9865	0.9580	0.9714	0.9646	0.9657	0.9532	0.9684
256	Grid 2	Random	OK	0.1777	0.2194	0.2270	0.2362	0.2899	0.2314	0.2281	0.2179	0.2487	0.2185	0.0350	0.0432	0.0447	0.0465	0.0571	0.0456	0.0449	0.0429	0.0490	0.0430	0.1257	0.1511	0.1545	0.1531	0.2016	0.1557	0.1559	0.1469	0.1625	0.1558	0.0037	-0.0092	0.0265	-0.0133	0.0265	-0.0196	-0.0135	-0.0039	0.0231	0.0263	0.9924	0.9884	0.9876	0.9865	0.9797	0.9871	0.9874	0.9885	0.9851	0.9885
256	Grid 2	Regular	IDW	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009	0.0593	0.0593	0.0593	0.0593	0.0593	0.0593	0.0593	0.0593	0.0593	0.0593	0.2178	0.2178	0.2178	0.2178	0.2178	0.2178	0.2178	0.2178	0.2178	0.2178	-0.0078	-0.0078	-0.0078	-0.0078	-0.0078	-0.0078	-0.0078	-0.0078	-0.0078	-0.0078	0.9781	0.9781	0.9781	0.9781	0.9781	0.9781	0.9781	0.9781	0.9781	0.9781
256	Grid 2	Regular	OK	0.1520	0.1520	0.1520	0.1520	0.1520	0.1520	0.1520	0.1520	0.1520	0.1520	0.0299	0.0299	0.0299	0.0299	0.0299	0.0299	0.0299	0.0299	0.0299	0.0299	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944	0.9944
256	Grid 3	Cluster	IDW	1.2784	1.4956	1.7026	1.0825	1.6473	1.2467	1.6818	1.4247	1.2660	1.5156	0.3470	0.4059	0.4621	0.2938	0.4471	0.3384	0.4565	0.3867	0.3436	0.4113	0.9873	0.9721	1.2305	0.7444	1.2215	0.9743	1.2128	1.0885	0.9475	1.1584	-0.0373	-0.3687	-0.4998	-0.1033	-0.4998	-0.1146	-0.4333	-0.2642	-0.0205	-0.2931	0.5304	0.3572	0.1669	0.6633	0.2202	0.5534	0.1872	0.4167	0.5394	0.3399
256	Grid 3	Cluster	OK	1.1063	1.4956	1.5007	1.0825	1.5746	1.1394	1.6982	1.2289	1.2148	1.4461	0.3003	0.4059	0.4073	0.2938	0.4274	0.3092	0.4609	0.3335	0.3297	0.3925	0.7628	0.9721	1.0357	0.7444	1.0997	0.8259	1.2404	0.8329	0.8145	1.1128	0.0853	-0.3687	-0.3554	-0.1033	-0.2779	-0.1281	-0.4412	-0.0915	-0.0383	-0.1822	0.6483	0.3572	0.3528	0.6633	0.2875	0.6270	0.1713	0.5660	0.5759	0.3990
256	Grid 3	Sparse	IDW	1.6432	1.2651	1.4861	1.2054	1.3626	1.4752	1.5421	1.4166	1.3000	1.4354	0.4460	0.3434	0.4033	0.3272	0.3698	0.4004	0.4185	0.3845	0.3528	0.3896	1.2916	0.9170	1.2369	0.9215	1.1351	1.2129	1.2544	1.1418	1.0693	1.1574	-0.3208	0.0430	-0.0574	-0.3159	-0.0508	-0.3000	-0.4097	0.0770	0.1608	0.0797	0.2241	0.5400	0.3653	0.5824	0.4665	0.3747	0.3166	0.4233	0.5144	0.4079
256	Grid 3	Sparse	OK	1.5833	1.2651	1.3592	1.2054	1.2758	1.1809	1.3249	1.3712	1.1379	1.3187	0.4297	0.3434	0.3689	0.3272	0.3463	0.3205	0.3596	0.3722	0.3088	0.3579	1.2565	0.9170	1.0605	0.9215	1.0636	0.9167	1.0133	1.0471	0.8226	0.9977	-0.2958	0.0430	0.1161	-0.3159	0.0375	-0.0973	-0.2102	0.2065	0.1763	0.1365	0.2797	0.5400	0.4691	0.5824	0.5323	0.5993	0.4956	0.4597	0.6279	0.5003
256	Grid 3	Random	IDW	1.0638	0.7611	1.0123	0.9564	1.0081	0.9925	1.0387	0.9788	1.0514	1.0372	0.2887	0.2066	0.2748	0.2596	0.2736	0.2694	0.2819	0.2657	0.2854	0.2815	0.8174	0.5419	0.7562	0.6982	0.7818	0.7609	0.7886	0.7614	0.7992	0.7968	-0.1351	-0.0313	0.0557	0.0226	-0.1241	-0.0170	-0.1010	-0.0262	-0.1675	0.0472	0.6748	0.8335	0.7055	0.7371	0.7080	0.7169	0.6900	0.7247	0.6823	0.6909
256	Grid 3	Random	OK	0.8951	0.7611	0.8598	0.9564	0.8259	0.8068	0.8797	0.8645	0.7554	0.9134	0.2429	0.2066	0.2333	0.2596	0.2241	0.2190	0.2388	0.2346	0.2050	0.2479	0.6824	0.5419	0.5830	0.6982	0.5739	0.5872	0.5961	0.6657	0.5433	0.6880	-0.0790	-0.0313	0.0356	0.0226	-0.0513	0.0198	-0.0386	-0.0315	-0.0549	0.0717	0.7698	0.8335	0.7876	0.7371	0.8040	0.8129	0.7776	0.7852	0.8360	0.7602
256	Grid 3	Regular	IDW	0.8936	0.8936	0.8936	0.8936	0.8936	0.8936	0.8936	0.8936	0.8936	0.8936	0.2425	0.2425	0.2425	0.2425	0.2425	0.2425	0.2425	0.2425	0.2425	0.2425	0.7062	0.7062	0.7062	0.7062	0.7062	0.7062	0.7062	0.7062	0.7062	0.7062	-0.0703	-0.0703	-0.0703	-0.0703	-0.0703	-0.0703	-0.0703	-0.0703	-0.0703	-0.0703	0.7705	0.7705	0.7705	0.7705	0.7705	0.7705	0.7705	0.7705	0.7705	0.7705
256	Grid 3	Regular	OK	0.5798	0.5798	0.5798	0.5798	0.5798	0.5798	0.5798	0.5798	0.5798	0.5798	0.1574	0.1574	0.1574	0.1574	0.1574	0.1574	0.1574	0.1574	0.1574	0.1574	0.4093	0.4093	0.4093	0.4093	0.4093	0.4093	0.4093	0.4093	0.4093	0.4093	-0.0234	-0.0234	-0.0234	-0.0234	-0.0234	-0.0234	-0.0234	-0.0234	-0.0234	-0.0234	0.9034	0.9034	0.9034	0.9034	0.9034	0.9034	0.9034	0.9034	0.9034	0.9034
256	Grid 4	Cluster	IDW	1.8787	1.7613	1.8931	1.9522	1.7840	1.9414	2.0264	1.7399	2.0507	1.9223	0.3057	0.2866	0.3080	0.3176	0.2903	0.3159	0.3297	0.2831	0.3337	0.3128	1.1471	1.0689	1.2102	1.1807	1.2350	1.3666	1.3188	1.1414	1.4580	1.2891	0.0715	0.0400	-0.0622	-0.2515	-0.2915	-0.4487	-0.2810	-0.0865	-0.6734	-0.2694	0.2006	0.2974	0.1883	0.1368	0.2791	0.1463	0.0699	0.3143	0.0475	0.1630
256	Grid 4	Cluster	OK	1.9936	1.7613	1.9784	1.9522	1.8878	2.0555	2.0055	1.8003	2.1261	2.0357	0.3244	0.2866	0.3219	0.3176	0.3072	0.3345	0.3263	0.2929	0.3459	0.3312	1.2393	1.0689	1.2687	1.1807	1.2961	1.3450	1.2054	1.1820	1.5122	1.2630	-0.0019	0.0400	-0.0709	-0.2515	-0.2833	-0.3495	-0.2024	-0.1107	-0.6351	-0.2697	0.0998	0.2974	0.1135	0.1368	0.1928	0.0430	0.0890	0.2659	-0.0238	0.0614
256	Grid 4	Sparse	IDW	1.8958	2.0112	1.8081	2.0128	1.5716	1.8856	1.8539	1.8591	1.8709	1.8283	0.3085	0.3272	0.2942	0.3275	0.2557	0.3068	0.3016	0.3025	0.3044	0.2975	1.3495	1.5588	1.1954	1.4043	0.9270	1.3718	1.2880	1.1851	1.3020	1.2417	-0.1565	-0.5662	0.1282	-0.0774	-0.1303	-0.2140	0.0075	0.2735	0.0702	0.1265	0.1860	0.0838	0.2596	0.0824	0.4406	0.1947	0.2215	0.2171	0.2072	0.2429
256	Grid 4	Sparse	OK	1.9924	2.0112	1.8999	1.9293	1.5716	2.0065	1.8925	1.9405	1.9453	1.8754	0.3242	0.3272	0.3091	0.3139	0.2557	0.3265	0.3079	0.3157	0.3165	0.3051	1.3063	1.5588	1.2468	1.2051	0.9270	1.4625	1.2721	1.2488	1.2128	1.2831	-0.1768	-0.5662	0.1698	0.1078	-0.1303	-0.2123	0.0714	0.2427	0.1185	0.1271	0.1009	0.0838	0.1825	0.1570	0.4406	0.0882	0.1888	0.1471	0.1429	0.2034
256	Grid 4	Random	IDW	1.5330	1.7275	1.6126	1.6324	1.6441	1.5479	1.6413	1.6000	1.5119	1.6058	0.2494	0.2811	0.2624	0.2656	0.2675	0.2519	0.2671	0.2603	0.2460	0.2613	1.0092	1.0960	1.0095	1.0019	1.0428	1.0031	0.9967	1.0349	0.9579	1.0209	-0.1403	0.1046	-0.0765	-0.0022	-0.0386	-0.0397	0.1422	-0.0931	-0.0537	-0.1355	0.4677	0.3241	0.4110	0.3965	0.3878	0.4573	0.3899	0.4202	0.4823	0.4159
256	Grid 4	Random	OK	1.6766	1.7275	1.5984	1.7427	1.5599	1.6741	1.5889	1.5769	1.6676	1.5393	0.2728	0.2811	0.2601	0.2836	0.2538	0.2724	0.2585	0.2566	0.2713	0.2505	1.1173	1.0960	0.9331	1.0798	0.8978	1.0950	0.8990	0.9369	1.0694	0.8873	-0.1676	0.1046	-0.1284	0.0135	0.0201	-0.0694	0.1095	-0.0828	-0.0608	-0.0786	0.3633	0.3241	0.4213	0.3121	0.4489	0.3652	0.4282	0.4368	0.3701	0.4633
256	Grid 4	Regular	IDW	1.4284	1.4284	1.4284	1.4284	1.4284	1.4284	1.4284	1.4284	1.4284	1.4284	0.2324	0.2324	0.2324	0.2324	0.2324	0.2324	0.2324	0.2324	0.2324	0.2324	0.9417	0.9417	0.9417	0.9417	0.9417	0.9417	0.9417	0.9417	0.9417	0.9417	-0.1134	-0.1134	-0.1134	-0.1134	-0.1134	-0.1134	-0.1134	-0.1134	-0.1134	-0.1134	0.5379	0.5379	0.5379	0.5379	0.5379	0.5379	0.5379	0.5379	0.5379	0.5379
256	Grid 4	Regular	OK	1.3275	1.3275	1.3275	1.3275	1.3275	1.3275	1.3275	1.3275	1.3275	1.3275	0.2160	0.2160	0.2160	0.2160	0.2160	0.2160	0.2160	0.2160	0.2160	0.2160	0.7696	0.7696	0.7696	0.7696	0.7696	0.7696	0.7696	0.7696	0.7696	0.7696	-0.1158	-0.1158	-0.1158	-0.1158	-0.1158	-0.1158	-0.1158	-0.1158	-0.1158	-0.1158	0.6009	0.6009	0.6009	0.6009	0.6009	0.6009	0.6009	0.6009	0.6009	0.6009

Number of Data Points	Grid Complexity	Data Distribution	Algorithm	Root Mean Square Error (RMSE)										Relative Root Mean Square Error (rRMSE)										Mean Average Error (MAE)										Bias Error (BE)										Correlation Coefficient (r2)									
676	Grid 1	Cluster	IDW	0.4595	1.0553	0.7918	0.9748	0.5269	0.4915	0.9825	1.1402	0.3436	1.0433	0.1044	0.2398	0.1799	0.2215	0.1197	0.1117	0.2233	0.2591	0.0781	0.2371	0.2693	0.5393	0.4108	0.4617	0.3141	0.3361	0.4999	0.4994	0.2239	0.5453	0.0913	-0.0640	-0.2525	-0.1867	0.0197	0.1455	-0.3152	-0.3435	0.0535	-0.1229	0.9671	0.8266	0.9024	0.8520	0.9568	0.9624	0.8497	0.7976	0.9816	0.8305
676	Grid 1	Cluster	OK	0.3349	0.9560	0.1739	0.8824	0.4615	0.3569	0.8808	1.0685	0.3103	0.8239	0.0761	0.2173	0.0395	0.2005	0.1049	0.0811	0.2002	0.2428	0.0705	0.1872	0.1859	0.4185	0.1207	0.3814	0.2727	0.2280	0.4369	0.4308	0.1973	0.3914	0.0703	-0.0992	0.0025	-0.1656	0.0186	0.0841	-0.2806	-0.3080	0.0454	-0.0990	0.9825	0.8577	0.9953	0.8787	0.9668	0.9802	0.8792	0.8222	0.9850	0.8943
676	Grid 1	Sparse	IDW	0.3786	0.2468	0.2751	0.2651	0.2644	0.3278	0.3027	0.2861	0.2864	0.4176	0.0860	0.0561	0.0625	0.0602	0.0601	0.0745	0.0688	0.0650	0.0651	0.0949	0.2479	0.1593	0.1705	0.1779	0.1629	0.2121	0.2000	0.1753	0.1884	0.2097	0.0040	-0.0082	-0.0245	-0.0033	0.0124	0.0073	-0.0020	-0.0330	0.0412	-0.0585	0.9777	0.9905	0.9882	0.9891	0.9891	0.9833	0.9857	0.9873	0.9872	0.9729
676	Grid 1	Sparse	OK	0.1808	0.1694	0.1908	0.2018	0.1734	0.1865	0.2212	0.2101	0.1870	0.3103	0.0411	0.0385	0.0434	0.0459	0.0394	0.0424	0.0503	0.0477	0.0425	0.0705	0.1145	0.1055	0.1225	0.1350	0.1070	0.1237	0.1465	0.1206	0.1225	0.1492	0.0094	-0.0063	-0.0107	-0.0047	0.0137	0.0125	0.0040	-0.0289	0.0338	-0.0455	0.9949	0.9955	0.9943	0.9937	0.9953	0.9946	0.9924	0.9931	0.9946	0.9850
676	Grid 1	Random	IDW	0.1401	0.1766	0.1739	0.1690	0.1804	0.1383	0.1658	0.1628	0.1810	0.1594	0.0318	0.0401	0.0395	0.0384	0.0410	0.0314	0.0377	0.0370	0.0411	0.0362	0.0789	0.1184	0.1207	0.1159	0.1204	0.0801	0.1155	0.1084	0.1213	0.1115	-0.0031	-0.0101	0.0025	0.0048	0.0013	-0.0083	0.0080	-0.0066	-0.0020	0.0033	0.9969	0.9951	0.9953	0.9956	0.9949	0.9970	0.9957	0.9959	0.9949	0.9960
676	Grid 1	Random	OK	0.0900	0.1553	0.1409	0.1515	0.1623	0.1681	0.0849	0.1349	0.1564	0.1369	0.0205	0.0353	0.0320	0.0344	0.0369	0.0382	0.0193	0.0307	0.0355	0.0311	0.0437	0.1058	0.0989	0.1051	0.1076	0.1140	0.0456	0.0915	0.1077	0.0973	-0.0008	-0.0087	0.0030	0.0042	0.0019	-0.0061	0.0063	-0.0045	0.0019	0.0058	0.9987	0.9962	0.9969	0.9964	0.9959	0.9956	0.9989	0.9972	0.9962	0.9971
676	Grid 1	Regular	IDW	0.0921	0.0921	0.0921	0.0921	0.0921	0.0921	0.0921	0.0921	0.0921	0.0921	0.0209	0.0209	0.0209	0.0209	0.0209	0.0209	0.0209	0.0209	0.0209	0.0209	0.0488	0.0488	0.0488	0.0488	0.0488	0.0488	0.0488	0.0488	0.0488	0.0488	-0.0062	-0.0062	-0.0062	-0.0062	-0.0062	-0.0062	-0.0062	-0.0062	-0.0062	-0.0062	0.9987	0.9987	0.9987	0.9987	0.9987	0.9987	0.9987	0.9987	0.9987	0.9987
676	Grid 1	Regular	OK	0.0714	0.0714	0.0714	0.0714	0.0714	0.0714	0.0714	0.0714	0.0714	0.0714	0.0162	0.0162	0.0162	0.0162	0.0162	0.0162	0.0162	0.0162	0.0162	0.0162	0.0357	0.0357	0.0357	0.0357	0.0357	0.0357	0.0357	0.0357	0.0357	0.0357	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	-0.0046	0.9992	0.9992	0.9992	0.9992	0.9992	0.9992	0.9992	0.9992	0.9992	0.9992
676	Grid 2	Cluster	IDW	0.7328	0.8109	0.6816	0.5731	0.7243	0.7393	0.6605	0.4957	0.6861	0.9770	0.1443	0.1597	0.1343	0.1129	0.1427	0.1456	0.1301	0.0976	0.1351	0.1924	0.4708	0.5442	0.4621	0.3926	0.4964	0.5098	0.4603	0.3608	0.4792	0.6655	0.0494	-0.0228	-0.0938	-0.0890	-0.1495	0.0579	-0.0252	0.0931	0.2366	-0.2062	0.8703	0.8412	0.8878	0.9207	0.8733	0.8680	0.8946	0.9407	0.8863	0.7695
676	Grid 2	Cluster	OK	0.5844	0.7443	0.5859	0.3984	0.5961	0.5606	0.5094	0.3332	0.5540	0.7675	0.1151	0.1466	0.1154	0.0785	0.1174	0.1104	0.1003	0.0656	0.1091	0.1512	0.3551	0.4640	0.3697	0.2666	0.3852	0.3628	0.3439	0.2487	0.3697	0.4817	0.0803	-0.0075	-0.0462	-0.0483	-0.0664	0.0916	0.0247	0.0643	0.1833	-0.2221	0.9175	0.8662	0.9171	0.9617	0.9142	0.9241	0.9373	0.9732	0.9259	0.8577
676	Grid 2	Sparse	IDW	0.4829	0.5055	0.5132	0.4389	0.4353	0.4472	0.4971	0.5091	0.5995	0.4530	0.0951	0.0996	0.1011	0.0864	0.0857	0.0881	0.0979	0.1003	0.1181	0.0892	0.3688	0.3794	0.3666	0.3243	0.3247	0.3280	0.3670	0.3468	0.4287	0.3461	-0.0215	-0.0390	-0.0354	-0.0924	-0.0215	-0.0162	0.0295	0.0576	0.0023	0.0686	0.9437	0.9383	0.9364	0.9535	0.9542	0.9517	0.9403	0.9374	0.9132	0.9504
676	Grid 2	Sparse	OK	0.2955	0.3091	0.3237	0.4389	0.2569	0.2863	0.2973	0.3510	0.3604	0.2945	0.0582	0.0609	0.0638	0.0864	0.0506	0.0564	0.0586	0.0691	0.0710	0.0580	0.2089	0.2199	0.2282	0.3243	0.1870	0.2092	0.2078	0.2157	0.2481	0.2096	0.0145	-0.0200	-0.0102	-0.0924	-0.0188	0.0007	0.0191	0.0387	0.0150	0.0595	0.9789	0.9769	0.9747	0.9535	0.9841	0.9802	0.9787	0.9702	0.9686	0.9791
676	Grid 2	Random	IDW	0.2504	0.2950	0.2948	0.2656	0.2807	0.2854	0.2864	0.2737	0.2866	0.2765	0.0493	0.0581	0.0581	0.0523	0.0553	0.0562	0.0564	0.0539	0.0564	0.0545	0.1745	0.2231	0.2212	0.2022	0.2140	0.2143	0.2166	0.2083	0.2137	0.2099	-0.0007	0.0089	-0.0105	-0.0134	-0.0131	-0.0105	0.0012	-0.0210	-0.0098	0.0089	0.9849	0.9790	0.9790	0.9830	0.9810	0.9803	0.9802	0.9819	0.9802	0.9815
676	Grid 2	Random	OK	0.1733	0.2073	0.2245	0.2016	0.2317	0.2102	0.2121	0.2039	0.2161	0.1818	0.0341	0.0408	0.0442	0.0397	0.0456	0.0414	0.0418	0.0402	0.0426	0.0358	0.1065	0.1585	0.1689	0.1530	0.1773	0.1574	0.1586	0.1555	0.1618	0.1273	-0.0016	0.0096	-0.0101	-0.0073	-0.0085	-0.0052	0.0026	-0.0140	-0.0078	0.0031	0.9927	0.9896	0.9878	0.9902	0.9870	0.9893	0.9891	0.9900	0.9887	0.9920
676	Grid 2	Regular	OK	0.1868	0.1868	0.1868	0.1868	0.1868	0.1868	0.1868	0.1868	0.1868	0.1868	0.0368	0.0368	0.0368	0.0368	0.0368	0.0368	0.0368	0.0368	0.0368	0.0368	0.1247	0.1247	0.1247	0.1247	0.1247	0.1247	0.1247	0.1247	0.1247	0.1247	-0.0063	-0.0063	-0.0063	-0.0063	-0.0063	-0.0063	-0.0063	-0.0063	-0.0063	-0.0063	0.9916	0.9916	0.9916	0.9916	0.9916	0.9916	0.9916	0.9916	0.9916	0.9916
676	Grid 2	Regular	OK	0.0990	0.0990	0.0990	0.0990	0.0990	0.0990	0.0990	0.0990	0.0990	0.0990	0.0195	0.0195	0.0195	0.0195	0.0195	0.0195	0.0195	0.0195	0.0195	0.0195	0.0566	0.0566	0.0566	0.0566	0.0566	0.0566	0.0566	0.0566	0.0566	0.0566	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	-0.0013	0.9976	0.9976	0.9976	0.9976	0.9976	0.9976	0.9976	0.9976	0.9976	0.9976
676	Grid 3	Cluster	IDW	1.0819	1.3972	1.4010	1.2679	1.3872	1.0872	1.2542	1.4781	1.0121	1.1437	0.2936	0.3792	0.3802	0.3441	0.3765	0.2951	0.3404	0.4012	0.2747	0.3104	0.7277	1.0473	0.9971	0.9289	0.9813	0.8103	0.9101	1.0140	0.7470	0.8680	-0.0770	-0.4368	-0.3429	-0.1419	-0.3142	-0.1066	-0.2169	-0.1407	0.0081	-0.1899	0.6636	0.4390	0.4360	0.5381	0.4470	0.6604	0.5480	0.3721	0.7056	0.6241
676	Grid 3	Cluster	OK	0.9998	1.2161	1.3460	1.2304	1.1935	1.0284	1.2931	1.4795	0.9081	0.9901	0.2714	0.3301	0.3653	0.3340	0.3239	0.2791	0.3510	0.4016	0.2465	0.2687	0.6529	0.8457	0.9093	0.8778	0.8452	0.7160	0.9850	0.9133	0.6569	0.6392	-0.0336	-0.2716	-0.3946	-0.1660	-0.1793	-0.0590	0.1088	-0.1514	0.0053	-0.1532	0.7127	0.5750	0.4794	0.5649	0.5907	0.6961	0.5195	0.3710	0.7630	0.7183
676	Grid 3	Sparse	IDW	1.2035	1.0261	1.1475	1.1017	1.0928	1.0598	1.1639	1.0902	1.2728	1.1323	0.3266	0.2785	0.3114	0.2990	0.2966	0.2876	0.3159	0.2959	0.3455	0.3073	0.9627	0.8203	0.9170	0.8538	0.8586	0.8441	0.8836	0.8773	0.9608	0.8906	-0.1586	-0.1844	-0.1839	0.0074	-0.0346	-0.1175	-0.0353	0.0350	-0.2704	-0.0232	0.5838	0.6974	0.6216	0.6512	0.6568	0.6772	0.6107	0.6584	0.5345	0.6316
676	Grid 3	Sparse	OK	0.9868	0.9165	1.0304	1.0435	0.9389	0.9775	1.0291	1.0018	1.1557	1.1161	0.2678	0.2487	0.2797	0.2832	0.2548	0.2653	0.2793	0.2719	0.3137	0.3029	0.7554	0.7090	0.7621	0.8232	0.6988	0.7459	0.7333	0.8114	0.8766	0.8861	-0.0883	-0.1713	-0.1332	0.0248	-0.0127	-0.0964	0.0083	-0.0021	-0.2146	-0.0258	0.7201	0.7586	0.6949	0.6871	0.7467	0.7254	0.6957	0.7116	0.6162	0.6420
676	Grid 3	Random	IDW	0.7359	0.7527	0.7188	0.7490	0.7131	0.7775	0.7503	0.7343	0.7987	0.7259	0.1997	0.2043	0.1951	0.2033	0.1935	0.2110	0.2036	0.1993	0.2168	0.1970	0.5023	0.5823	0.5804	0.5705	0.5742	0.6090	0.5865	0.5796	0.5873	0.5552	0.0011	0.0260	-0.0676	-0.0657	-0.0141	0.0042	0.0031	-0.0624	0.0705	-0.0301	0.8444	0.8372	0.8515	0.8388	0.8539	0.8263	0.8382	0.8451	0.8167	0.8486
676	Grid 3	Random	OK	0.5201	0.6397	0.5783	0.7346	0.5897	0.6824	0.5939	0.5950	0.6849	0.6055	0.1411	0.1736	0.1570	0.1994	0.1601	0.1852	0.1612	0.1615	0.1859	0.1643	0.3190	0.4849	0.4514	0.5643	0.4678	0.5246	0.4503	0.4577	0.4883	0.4590	0.0078	0.0182	-0.0512	-0.0620	-0.0237	0.0077	0.0026	-0.0502	0.0563	-0.0192	0.9223	0.8824	0.9039	0.8449	0.9001	0.8662	0.8986	0.8983	0.8652	0.8947
676	Grid 3	Regular	IDW	0.5496	0.5496	0.5496	0.5496	0.5496	0.5496	0.5496	0.5496	0.5496	0.5496	0.1492	0.1492	0.1492	0.1492	0.1492	0.1492	0.1492	0.1492	0.1492	0.1492	0.3861	0.3861	0.3861	0.3861	0.3861	0.3861	0.3861	0.3861	0.3861	0.3861	-0.0358	-0.0358	-0.0358	-0.0358	-0.0358	-0.0358	-0.0358	-0.0358	-0.0358	-0.0358	0.9132	0.9132	0.9132	0.9132	0.9132	0.9132	0.9132	0.9132	0.9132	0.9132
676	Grid 3	Regular	OK	0.3665	0.3665	0.3665	0.3665	0.3665	0.3665	0.3665	0.3665	0.3665	0.3665	0.0995	0.0995	0.0995	0.0995	0.0995	0.0995	0.0995	0.0995	0.0995	0.0995	0.2487	0.2487	0.2487	0.2487	0.2487	0.2487	0.2487	0.2487	0.2487	0.2487	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	-0.0166	0.9614	0.9614	0.9614	0.9614	0.9614	0.9614	0.9614	0.9614	0.9614	0.9614
676	Grid 4	Cluster	IDW	1.8824	2.0004	1.6759	1.7106	1.7178	1.8648	1.7543	1.5794	1.7789	1.7543	0.3063	0.3255	0.2727	0.2783	0.2795	0.3034	0.2854	0.2570	0.2894	0.2854	1.1931	1.3718	1.0562	1.2109	1.0926	1.3103	1.3380	0.9808	1.1059	1.3380	-0.4054	-0.3730	0.1028	-0.2935	-0.0707	-0.4555	-0.5073	0.1191	-0.0578	-0.5073	0.1974	0.0936	0.3638	0.3372	0.3317	0.2124	0.3030	0.4350	0.2833	0.3030
676	Grid 4	Cluster	OK	1.9922	2.0182	1.6298	1.5747	1.7825	1.9345	1.8339	1.5181	1.6884	1.7707	0.3242	0.3284	0.2652	0.2562	0.2900	0.3148	0.2984	0.2470	0.2747	0.2881	1.2868	1.3815	0.9647	1.0212	1.1236	1.3398	1.3806	0.8513	1.0016	1.0320	-0.4256	-0.3730	0.1106	-0.1281	-0.0753	-0.4369	-0.5373	0.2570	-0.0036	0.1558	0.1011	0.0775	0.3983	0.4384	0.2804	0.1524	0.2383	0.4780	0.3543	0.2898
676	Grid 4	Sparse	IDW	1.6891	1.6400	1.8240	1.7788	1.6453	1.6467	1.6557	1.7528	1.6382	1.7567	0.2748	0.2668	0.2968	0.2894	0.2677	0.2679	0.2694	0.2852	0.2665	0.2858	1.1205	1.1230	1.2009	1.0967	1.1515	1.0712	1.0953	1.1924	1.0883	1.0550	0.0885	-0.2540	-0.1363	0.0969	-0.1777	0.1107	-0.1064	-0.3143	-0.1123	0.2323	0.3538	0.3908	0.2464	0.2833	0.3869	0.3858	0.3791	0.3041	0.3922	0.3011
676	Grid 4	Sparse	OK	1.8250	1.6479	1.8717	1.7658	1.6161	1.7857	1.8030	1.8585	1.8032	1.7814	0.2969	0.2681	0.3045	0.2873	0.2630	0.2906	0.2934	0.3024	0.2934	0.2898	1.2173	1.0746	1.1702	1.0354	1.0444	1.2032	1.2215	1.2921	1.2178	1.0580	0.0983	-0.2364	-0.1019	0.1402	-0.0965	0.0971	-0.1350	-0.3541	-0.1281	0.2504	0.2456	0.3850	0.2065	0.2938	0.4084	0.2777	0.2637	0.2177	0.2635	0.2812
676	Grid 4	Random	IDW	1.2540	1.2981	1.2706	1.2958	1.2493	1.2411	1.3003	1.3818	1.3188	1.2551	0.2040	0.2112	0.2067	0.2108	0.2033	0.2019	0.2116	0.2000	0.2146	0.2042	0.7227	0.8577	0.8440	0.8437	0.8184	0.8200	0.8463	0.8200	0.8526	0.8210	-0.0698	-0.0574	-0.0720	-0.0366	-0.0417	-0.0771	-0.0293	-0.0457	-0.0411	-0.0509	0.6438	0.6183	0.6343	0.6197	0.6465	0.6511	0.6171	0.6233	0.6061	0.6432
676	Grid 4	Random	OK	1.0793	1.3577	1.1752	1.2027	1.1569	1.2769	1.2180	1.5181	1.2358	1.1080	0.1756	0.2209	0.1912	0.1957	0.1882	0.2078	0.1982	0.2470	0.2011	0.1803	0.5455	0.8471	0.7424	0.7453	0.7061	0.8229	0.7562	0.8513	0.7553	0.6370	-0.0528	-0.0597	-0.0528	-0.0344	-0.0287	-0.0703	-0.0289	0.2570	-0.0320	-0.0638	0.7361	0.5825	0.6872	0.6724	0.6969	0.6307	0.6640	0.4780	0.6541	0.7219
676	Grid 4	Regular	IDW	1.1116	1.1116	1.1116	1.1116	1.1116	1.1116	1.1116	1.1116	1.1116	1.1116	0.1809	0.1809	0.1809	0.1809	0.1809	0.1809	0.1809	0.1809	0.1809	0.1809	0.6342	0.6342	0.6342	0.6342	0.6342	0.6342	0.6342	0.6342	0.6342	0.6342	0.0030	0.0030	0.0030	0.0030	0.0030	0.0030	0.0030	0.0030	0.0030	0.0030	0.7201	0.7201	0.7201	0.7201	0.7201	0.7201	0.7201	0.7201	0.7201	0.7201
676	Grid 4	Regular	OK	1.2424	1.2424	1.2424	1.2424	1.2424	1.2424	1.2424	1.2424	1.2424	1.2424	0.2021	0.2021	0.2021	0.2021	0.2021	0.2021	0.2021	0.2021	0.2021	0.2021	0.7397	0.7397	0.7397	0.7397	0.7397	0.7397	0.7397	0.7397	0.7397	0.7397	0.0044	0.0044	0.0044	0.0044	0.0044	0.0044	0.0044	0.0044	0.0044	0.0044	0.6504	0.6504	0.6504	0.6504	0.6504	0.6504	0.6504	0.6504	0.6504	0.6504

Number of Data Points	Grid Complexity	Data Distribution	Algorithm	Root Mean Square Error (RMSE)										Relative Root Mean Square Error (rRMSE)										Mean Average Error (MAE)										Bias Error (BE)										Correlation Coefficient (r2)									
1600	Grid 1	Cluster	IDW	0.2794	0.3713	0.4731	0.9678	0.5948	0.7516	0.4099	0.3233	0.4975	0.6117	0.0635	0.0844	0.1075	0.2199	0.1352	0.1708	0.0931	0.0735	0.1131	0.1390	0.1256	0.2734	0.2147	0.4155	0.3874	0.3539	0.2133	0.1910	0.2180	0.2613	0.0531	0.1132	0.1001	-0.1836	0.1344	-0.0028	0.0225	0.1035	-0.0549	-0.0990	0.9878	0.9785	0.9651	0.8541	0.9449	0.9120	0.9738	0.9837	0.9615	0.9417
1600	Grid 1	Cluster	OK	0.2006	0.3408	0.4104	0.8997	0.4808	0.6408	0.3885	0.3507	0.5331	0.5382	0.0456	0.0774	0.0933	0.2044	0.1093	0.1456	0.0883	0.0797	0.1211	0.1223	0.0954	0.2514	0.2535	0.3847	0.3081	0.3343	0.2443	0.2711	0.2894	0.2988	0.0332	0.1025	0.1331	-0.2245	0.1122	-0.0118	-0.0109	0.1450	-0.0514	-0.0017	0.9937	0.9819	0.9738	0.8740	0.9640	0.9361	0.9765	0.9809	0.9557	0.9549
1600	Grid 1	Sparse	IDW	0.1976	0.1803	0.1925	0.2253	0.1953	0.1738	0.1990	0.1863	0.2261	0.1867	0.0449	0.0410	0.0437	0.0512	0.0444	0.0395	0.0452	0.0423	0.0514	0.0424	0.1183	0.1232	0.1264	0.1328	0.1260	0.1185	0.1270	0.1217	0.1396	0.1211	-0.0081	0.0102	-0.0048	-0.0312	-0.0028	0.0034	-0.0051	0.0038	-0.0081	-0.0107	0.9939	0.9949	0.9942	0.9921	0.9941	0.9953	0.9938	0.9946	0.9920	0.9946
1600	Grid 1	Sparse	OK	0.1370	0.1341	0.1348	0.1506	0.1314	0.1253	0.1518	0.1324	0.1827	0.1511	0.0311	0.0305	0.0306	0.0342	0.0299	0.0285	0.0345	0.0301	0.0415	0.0343	0.0784	0.0910	0.0898	0.0921	0.0856	0.0822	0.0987	0.0844	0.1146	0.0988	-0.0002	0.0096	-0.0061	-0.0154	-0.0014	0.0003	-0.0039	-0.0001	-0.0058	-0.0090	0.9971	0.9972	0.9972	0.9965	0.9973	0.9976	0.9964	0.9973	0.9948	0.9964
1600	Grid 1	Random	IDW	0.0864	0.2206	0.1178	0.2038	0.2152	0.2040	0.1988	0.2111	0.2113	0.2048	0.0196	0.0501	0.0268	0.0463	0.0489	0.0464	0.0452	0.0480	0.0480	0.0465	0.0421	0.1535	0.0592	0.1419	0.1491	0.1455	0.1442	0.1464	0.1493	0.1421	0.0016	-0.0108	-0.0042	-0.0090	-0.0088	-0.0023	0.0047	-0.0090	-0.0035	-0.0103	0.9988	0.9924	0.9978	0.9935	0.9928	0.9935	0.9938	0.9931	0.9930	0.9935
1600	Grid 1	Random	OK	0.0745	0.2140	0.1998	0.1990	0.2080	0.1946	0.1913	0.2049	0.2016	0.1991	0.0169	0.0486	0.0454	0.0452	0.0473	0.0442	0.0435	0.0466	0.0458	0.0452	0.0364	0.1502	0.1409	0.1401	0.1457	0.1407	0.1395	0.1435	0.1441	0.1393	-0.0003	-0.0103	-0.0067	-0.0090	-0.0079	-0.0021	0.0024	-0.0088	-0.0045	-0.0100	0.9991	0.9929	0.9938	0.9938	0.9933	0.9941	0.9943	0.9935	0.9937	0.9938
1600	Grid 1	Regular	IDW	0.0588	0.0588	0.0588	0.0588	0.0588	0.0588	0.0588	0.0588	0.0588	0.0588	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0254	0.0254	0.0254	0.0254	0.0254	0.0254	0.0254	0.0254	0.0254	0.0254	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.0054	0.9995	0.9995	0.9995	0.9995	0.9995	0.9995	0.9995	0.9995	0.9995	0.9995
1600	Grid 1	Regular	OK	0.0601	0.0601	0.0601	0.0601	0.0601	0.0601	0.0601	0.0601	0.0601	0.0601	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0278	0.0278	0.0278	0.0278	0.0278	0.0278	0.0278	0.0278	0.0278	0.0278	-0.0068	-0.0068	-0.0068	-0.0068	-0.0068	-0.0068	-0.0068	-0.0068	-0.0068	-0.0068	0.9994	0.9994	0.9994	0.9994	0.9994	0.9994	0.9994	0.9994	0.9994	0.9994
1600	Grid 2	Cluster	IDW	0.3309	0.8674	0.7397	0.7109	0.6351	0.7076	0.7874	0.6311	0.5223	0.7990	0.0652	0.1709	0.1457	0.1400	0.1251	0.1394	0.1551	0.1243	0.1029	0.1574	0.1910	0.5687	0.4210	0.3930	0.3860	0.3936	0.4619	0.3607	0.2987	0.4753	-0.0604	-0.2145	-0.1585	-0.0422	-0.0682	0.0833	-0.1623	0.0270	-0.0209	-0.1589	0.9736	0.8183	0.8679	0.8779	0.9026	0.8791	0.8503	0.9038	0.9341	0.8459
1600	Grid 2	Cluster	OK	0.2155	0.7404	0.6158	0.6466	0.5161	0.5787	0.6555	0.5370	0.3944	0.5922	0.0424	0.1458	0.1213	0.1274	0.1017	0.1140	0.1291	0.1058	0.0777	0.1166	0.1162	0.4695	0.3928	0.4064	0.3575	0.3684	0.4334	0.3600	0.2851	0.3873	-0.0310	-0.1826	-0.1333	0.0337	-0.0305	0.0376	-0.1224	0.0927	-0.0397	-0.0707	0.9888	0.8676	0.9084	0.8990	0.9357	0.9191	0.8962	0.9304	0.9624	0.9153
1600	Grid 2	Sparse	IDW	0.3414	0.3277	0.3190	0.3229	0.3359	0.3256	0.3412	0.3150	0.3278	0.3201	0.0672	0.0645	0.0628	0.0636	0.0662	0.0641	0.0672	0.0620	0.0646	0.0630	0.2430	0.2401	0.2406	0.2358	0.2466	0.2425	0.2521	0.2353	0.2415	0.2397	-0.0089	-0.0053	-0.0049	-0.0082	-0.0079	0.0001	-0.0090	-0.0006	-0.0019	0.0102	0.9719	0.9741	0.9754	0.9748	0.9728	0.9744	0.9719	0.9760	0.9741	0.9753
1600	Grid 2	Sparse	OK	0.1888	0.2185	0.2247	0.2252	0.2127	0.2108	0.2190	0.2329	0.2157	0.1982	0.0372	0.0430	0.0443	0.0444	0.0419	0.0415	0.0431	0.0459	0.0425	0.0390	0.1271	0.1565	0.1663	0.1594	0.1556	0.1547	0.1608	0.1725	0.1568	0.1471	0.0023	0.0036	0.0068	0.0047	-0.0246	0.0087	-0.0114	0.0085	-0.0012	0.0089	0.9914	0.9885	0.9878	0.9878	0.9891	0.9893	0.9884	0.9869	0.9888	0.9905
1600	Grid 2	Random	IDW	0.1527	0.2907	0.2839	0.3024	0.2922	0.2887	0.2879	0.2961	0.3072	0.3027	0.0301	0.0573	0.0559	0.0596	0.0576	0.0569	0.0567	0.0583	0.0605	0.0596	0.0970	0.2290	0.2234	0.2351	0.2293	0.2292	0.2248	0.2337	0.2393	0.2344	-0.0046	-0.0155	0.0106	-0.0119	0.0098	-0.0141	-0.0153	-0.0040	-0.0203	0.0073	0.9944	0.9796	0.9805	0.9779	0.9794	0.9799	0.9800	0.9788	0.9772	0.9779
1600	Grid 2	Random	OK	0.1422	0.2633	0.2578	0.2715	0.2674	0.2647	0.2660	0.2673	0.2746	0.2718	0.0280	0.0519	0.0508	0.0535	0.0527	0.0521	0.0524	0.0526	0.0541	0.0535	0.0864	0.2074	0.2042	0.2124	0.2101	0.2102	0.2089	0.2121	0.2162	0.2128	-0.0025	-0.0123	0.0083	-0.0091	0.0080	-0.0117	-0.0122	-0.0016	-0.0149	0.0067	0.9951	0.9833	0.9839	0.9822	0.9827	0.9831	0.9829	0.9827	0.9818	0.9822
1600	Grid 2	Regular	IDW	0.1026	0.1026	0.1026	0.1026	0.1026	0.1026	0.1026	0.1026	0.1026	0.1026	0.0202	0.0202	0.0202	0.0202	0.0202	0.0202	0.0202	0.0202	0.0202	0.0202	0.0611	0.0611	0.0611	0.0611	0.0611	0.0611	0.0611	0.0611	0.0611	0.0611	0.0017	0.0017	0.0017	0.0017	0.0017	0.0017	0.0017	0.0017	0.0017	0.0017	0.9975	0.9975	0.9975	0.9975	0.9975	0.9975	0.9975	0.9975	0.9975	0.9975
1600	Grid 2	Regular	OK	0.0678	0.0678	0.0678	0.0678	0.0678	0.0678	0.0678	0.0678	0.0678	0.0678	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0134	0.0324	0.0324	0.0324	0.0324	0.0324	0.0324	0.0324	0.0324	0.0324	0.0324	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.9989	0.9989	0.9989	0.9989	0.9989	0.9989	0.9989	0.9989	0.9989	0.9989
1600	Grid 3	Cluster	IDW	0.7128	1.0655	1.1951	1.0193	1.0974	1.1094	1.1966	1.0478	1.1412	1.0140	0.1935	0.2892	0.3244	0.2767	0.2978	0.3011	0.3248	0.2844	0.3097	0.2752	0.4392	0.8197	0.6983	0.6268	0.6856	0.6404	0.7510	0.6665	0.6899	0.6387	-0.0654	-0.2270	-0.1500	-0.2432	-0.2346	-0.0936	-0.2352	-0.5000	0.1369	-0.0004	0.8540	0.6737	0.5895	0.7014	0.6540	0.6463	0.5885	0.6845	0.6258	0.7045
1600	Grid 3	Cluster	OK	0.5854	0.9874	1.1392	0.9945	1.0195	1.1520	1.2027	0.9340	1.0442	0.9852	0.1589	0.2680	0.3092	0.2699	0.2767	0.3127	0.3264	0.2535	0.2834	0.2674	0.3354	0.7358	0.7909	0.7160	0.7602	0.7992	0.8292	0.6884	0.7503	0.6956	-0.0229	-0.2403	-0.1600	-0.1937	-0.1656	-0.1101	0.0088	-0.2181	0.1061	0.0313	0.9015	0.7198	0.6271	0.7158	0.7013	0.6186	0.5843	0.7493	0.6867	0.7211
1600	Grid 3	Sparse	IDW	0.8776	0.8628	0.8962	0.8452	0.8337	0.8915	0.8934	0.8390	0.8151	0.9283	0.2382	0.2342	0.2432	0.2294	0.2263	0.2420	0.2425	0.2277	0.2212	0.2520	0.6473	0.6650	0.6890	0.6703	0.6549	0.6922	0.6875	0.6551	0.6573	0.7165	-0.0550	-0.0459	-0.0800	0.0011	-0.0852	-0.0100	-0.0420	-0.0520	-0.0244	-0.0140	0.7787	0.7861	0.7692	0.7947	0.8003	0.7716	0.7706	0.7977	0.8091	0.7524
1600	Grid 3	Sparse	OK	0.7092	0.6845	0.7699	0.7996	0.6895	0.8002	0.7949	0.6727	0.7848	0.8606	0.1925	0.1858	0.2090	0.2170	0.1871	0.2172	0.2158	0.1826	0.2130	0.2336	0.4851	0.5029	0.5693	0.6239	0.5135	0.6062	0.5999	0.4927	0.6243	0.6642	-0.0210	-0.0301	-0.1056	0.0073	-0.0784	0.0088	-0.0256	-0.0494	-0.0252	-0.0041	0.8555	0.8654	0.8297	0.8163	0.8634	0.8160	0.8184	0.8699	0.8230	0.7872
1600	Grid 3	Random	IDW	0.4463	0.6257	0.6488	0.6224	0.6335	0.6251	0.6137	0.6425	0.6368	0.6271	0.1211	0.1698	0.1761	0.1689	0.1719	0.1696	0.1666	0.1744	0.1728	0.1702	0.2752	0.5133	0.5204	0.5083	0.5174	0.5157	0.5105	0.5223	0.5172	0.5125	-0.0163	-0.0314	-0.0060	-0.0093	-0.0134	-0.0233	-0.0312	-0.0358	-0.0210	-0.0306	0.9428	0.8875	0.8790	0.8887	0.8847	0.8877	0.8918	0.8814	0.8835	0.8870
1600	Grid 3	Random	OK	0.3180	0.5700	0.5598	0.5642	0.5625	0.5451	0.5553	0.5536	0.5349	0.5372	0.0863	0.1547	0.1519	0.1531	0.1527	0.1479	0.1507	0.1502	0.1452	0.1458	0.1838	0.4673	0.4482	0.4603	0.4588	0.4504	0.4601	0.4506	0.4377	0.4377	0.0000	-0.0258	-0.0115	-0.0076	-0.0113	-0.0201	-0.0259	-0.0296	-0.0124	-0.0280	0.9709	0.9066	0.9099	0.9085	0.9091	0.9146	0.9114	0.9119	0.9178	0.9171
1600	Grid 3	Regular	IDW	0.3316	0.3316	0.3316	0.3316	0.3316	0.3316	0.3316	0.3316	0.3316	0.3316	0.0900	0.0900	0.0900	0.0900	0.0900	0.0900	0.0900	0.0900	0.0900	0.0900	0.1964	0.1964	0.1964	0.1964	0.1964	0.1964	0.1964	0.1964	0.1964	0.1964	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.9684	0.9684	0.9684	0.9684	0.9684	0.9684	0.9684	0.9684	0.9684	0.9684
1600	Grid 3	Regular	OK	0.2154	0.2154	0.2154	0.2154	0.2154	0.2154	0.2154	0.2154	0.2154	0.2154	0.0585	0.0585	0.0585	0.0585	0.0585	0.0585	0.0585	0.0585	0.0585	0.0585	0.1075	0.1075	0.1075	0.1075	0.1075	0.1075	0.1075	0.1075	0.1075	0.1075	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.9867	0.9867	0.9867	0.9867	0.9867	0.9867	0.9867	0.9867	0.9867	0.9867
1600	Grid 4	Cluster	IDW	1.3828	1.5094	1.6429	1.7873	1.9759	1.4066	1.4564	1.7135	1.5463	1.6295	0.2250	0.2456	0.2673	0.2908	0.3215	0.2289	0.2370	0.2788	0.2516	0.2651	0.7851	0.8109	0.8963	1.0439	1.3225	0.7087	0.8851	0.9627	0.8525	0.9387	-0.1491	0.0138	-0.2084	-0.4196	-0.3855	0.1435	-0.3049	-0.1765	-0.2072	-0.2400	0.5669	0.4840	0.3887	0.2765	0.1157	0.5519	0.5196	0.3350	0.4584	0.3986
1600	Grid 4	Cluster	OK	1.4628	1.5032	1.5050	1.7856	1.9932	1.4963	1.5439	1.6510	1.5442	1.6044	0.2380	0.2446	0.2449	0.2905	0.3243	0.2435	0.2512	0.2686	0.2513	0.2611	0.8549	0.9625	0.9928	1.1691	1.2950	0.9119	1.1368	1.0175	0.9926	1.0645	-0.0956	-0.1228	-0.1596	-0.3703	-0.5227	0.1294	-0.3503	-0.1198	-0.1990	-0.1853	0.5153	0.4882	0.4870	0.2778	0.1002	0.4929	0.4601	0.3826	0.4599	0.4169
1600	Grid 4	Sparse	IDW	1.4975	1.4291	1.3956	1.3892	1.3978	1.5371	1.4284	1.4314	1.4082	1.3564	0.2437	0.2325	0.2271	0.2260	0.2274	0.2501	0.2324	0.2329	0.2291	0.2207	0.9163	0.9547	0.9134	0.9077	0.9006	0.9585	0.8905	0.9048	0.8842	0.9233	-0.0844	-0.2013	-0.0429	-0.0464	-0.0117	0.1292	0.0561	0.0119	0.0694	-0.1825	0.4921	0.5374	0.5589	0.5629	0.5574	0.4649	0.5379	0.5360	0.5508	0.5833
1600	Grid 4	Sparse	OK	1.3128	1.3938	1.3363	1.3665	1.3508	1.4812	1.3516	1.3813	1.4451	1.4893	0.2136	0.2268	0.2174	0.2223	0.2198	0.2410	0.2199	0.2248	0.2351	0.2423	0.7208	0.8647	0.8272	0.8286	0.8117	0.8638	0.7910	0.8154	0.8834	1.0076	-0.0433	-0.1570	-0.0873	-0.0459	-0.0158	0.1252	0.0496	0.0339	0.0588	-0.1972	0.6096	0.5600	0.5955	0.5771	0.5867	0.5031	0.5862	0.5678	0.5270	0.4976
1600	Grid 4	Random	IDW	0.9672	1.1724	1.1517	1.1317	1.1125	1.1204	1.1385	1.1147	1.1085	1.1326	0.1574	0.1908	0.1874	0.1841	0.1810	0.1823	0.1852	0.1814	0.1804	0.1843	0.4824	0.7455	0.7555	0.7465	0.7488	0.7410	0.7524	0.7327	0.7311	0.7378	-0.0180	0.0767	0.0111	-0.0089	-0.0316	-0.0033	-0.0052	-0.0075	0.0059	0.0088	0.7881	0.6887	0.6996	0.7099	0.7197	0.7157	0.7064	0.7186	0.7217	0.7095
1600	Grid 4	Random	OK	0.9014	1.0522	1.0441	1.0360	1.1329	1.0025	1.0549	1.0079	1.0030	1.0314	0.1467	0.1712	0.1699	0.1686	0.1843	0.1631	0.1716	0.1640	0.1632	0.1678	0.4298	0.6619	0.6699	0.6741	0.7534	0.6531	0.6789	0.6535	0.6518	0.6618	-0.0074	0.0642	0.0166	-0.0064	-0.0120	0.0034	0.0093	-0.0035	0.0117	0.0034	0.8160	0.7492	0.7531	0.7569	0.7093	0.7724	0.7480	0.7699	0.7722	0.7591
1600	Grid 4	Regular	IDW	0.7479	0.7479	0.7479	0.7479	0.7479	0.7479	0.7479	0.7479	0.7479	0.7479	0.1217	0.1217	0.1217	0.1217	0.1217	0.1217	0.1217	0.1217	0.1217	0.1217	0.3644	0.3644	0.3644	0.3644	0.3644	0.3644	0.3644	0.3644	0.3644	0.3644	-0.0103	-0.0103	-0.0103	-0.0103	-0.0103	-0.0103	-0.0103	-0.0103	-0.0103	-0.0103	0.8733	0.8733	0.8733	0.8733	0.8733	0.8733	0.8733	0.8733	0.8733	0.8733
1600	Grid 4	Regular	OK	0.5645	0.5645	0.5645	0.5645	0.5645	0.5645	0.5645	0.5645	0.5645	0.5645	0.0918	0.0918	0.0918	0.0918	0.0918	0.0918	0.0918	0.0918	0.0918	0.0918	0.2475	0.2475	0.2475	0.2475	0.2475	0.2475	0.2475	0.2475	0.2475	0.2475	-0.0093	-0.0093	-0.0093	-0.0093	-0.0093	-0.0093	-0.0093	-0.0093	-0.0093	-0.0093	0.9278	0.9278	0.9278	0.9278	0.9278	0.9278	0.9278	0.9278	0.9278	0.9278

CHAPTER 4

ASSESSING THE IMPACT OF PROGRAM SELECTION ON THE ACCURACY OF 3D GEOLOGIC MODELS

Abstract

As the field of 3D subsurface geological modelling develops at an increasingly rapid rate, so too does the number of available software programs catering to these applications, most of which offer very similar ensembles of algorithms for interpolating data. A few studies have analyzed the effect of algorithm selection on the accuracy and uncertainty of subsurface geologic models, but little consideration has been given to the uncertainty and variability introduced into the model by software program selection. In this study, inverse distance weighting (IDW) and ordinary kriging (OK) algorithms were used to interpolate identical datasets by three different software programs (ArcGIS, ROCKWORKS 2006, and VIEWLOG). The results indicate that the output of the OK and IDW interpolation algorithms are inconsistent between programs and that this variability should be considered when assessing the uncertainty associated with subsurface model results. This paper shows that program selection has a significant influence on model output results when modelling complex subsurface geological environments, particularly when interpolating clustered data, which are most commonly used in geological and environmental applications.

4.1 Introduction

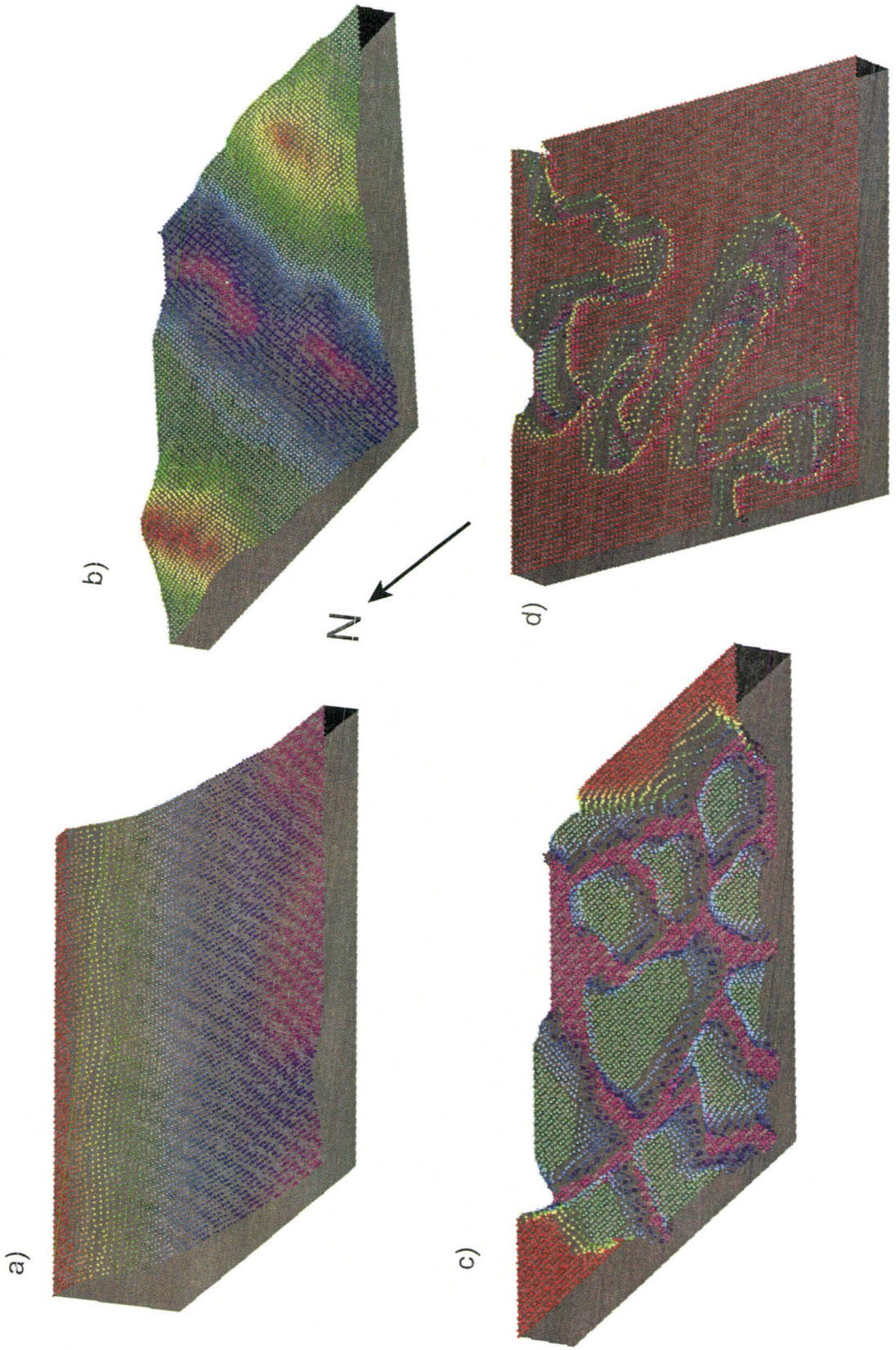
As the demand for three-dimensional (3D) models increases, so too does the number of software programs used for the generation of such models. The majority of these 3D modelling programs offer similar methods for data interpolation. The two most commonly used interpolation algorithms for subsurface modelling applications are Inverse Distance Weighting (IDW) and Ordinary Kriging (OK; Kravchenko and Bullock, 1999; Johnston, et al., 2001; Jones et al., 2003; Kravchenko, 2003; Mueller, et al., 2004). Each of these two algorithms have very different strengths for spatial data processing; IDW is often favoured for being computationally 'quick and easy', whereas kriging is favoured for its ability to provide the best linear unbiased estimates (Weber and Englund, 1992; Mueller et al., 2004). Several studies have evaluated the effectiveness of these algorithms in producing accurate models (Tabios and Salas, 1985; Weber and Englund, 1992; Weber and Englund, 1994; Brus et al., 1996; Walker and Loftis, 1997; Nalder and Wein, 1998; Zimmerman et al., 1999; Schloeder et al., 2001; Jones et al., 2003; Kravchenko, 2003; Dille et al., 2003; Lapen and Hayhoe; 2003). However, no studies to date have compared the effectiveness of the IDW and OK algorithms to create accurate models when run by different software programs. It is commonly assumed that data modelled using either algorithm in one program would produce identical results if modelled using the same algorithm in another program, providing that both programs were supplied with identical input datasets. The goal of this study is therefore to compare the output of models run using the IDW and OK algorithms using three different software

programs commonly used in 3D subsurface investigations (ArcGIS, ROCKWORKS 2006, and VIEWLOG). Models are created with each of the three programs using identical data sets extracted from synthetic grids of variable complexity and with varying numbers and distributions of data points. This will allow evaluation of the performance of IDW and OK under each program and assessment of the impact of program selection on model accuracy. The purpose is not to show that any one program is 'better' than another, but to identify the degree and nature of differences in the model outputs from each of the programs. Therefore, the programs will not be identified by name in the results, but will be referred to as program X, Y, and Z in order to conceal their identities.

4.2 Methods

To effectively test differences in the output models of the three 3D modelling programs selected for study, it was necessary to develop synthetic grids with known values at all point locations from which to extract input data. Four geologically realistic synthetic grids (Figure 4.1) were created that allowed the extraction of specific numbers and distributions of data in a controlled manner. The advantage of using synthetic datasets to conduct this evaluation is that the point values for each grid being modelled are known at every location, allowing quantitative analysis of the variability between actual and interpolated values across the entire grid. The accuracy of modelling natural surfaces has been tested elsewhere using previously interpolated grid surfaces (such as a

Figure 4.1: Synthetic grids created with 6400 known data points represent realistic geologic environments from which the data points for modelling were extracted. a) Grid 1 forms a gently sloping surface that may represent one element of a basin system or gently dipping bedrock valley wall, b) Grid 2 consists of two linear 'highs' separated by a central trough and represents a simple valley form, c) Grid 3 shows a series of interconnecting troughs separated by linear 'highs' and may represent an eroded bedrock surface or a braided river system, and d) Grid 4 consists of a flat surface incised by a highly sinuous channel and represents an incised meandering river system.


b)
N
d)
a)
c)

digital elevation model – DEM) that may include variable quantities of unknown errors (Zimmerman et al., 1999). These errors could then be propagated through all subsequent analyses, making it difficult to discriminate variations in the results produced by the processing mechanisms used by the various software programs from those due to errors propagated from the original model (Burrough, 2001).

The synthetic grids were sampled using three different sampling patterns (clustered, random, and regular) to determine if data distribution had any impact on the ability of each program to produce an accurate model. These sampling patterns were selected to represent the types of data distributions that may be encountered in various geoscientific and environmental applications. The number of data points used for interpolation was also varied (100, 256, and 676 points) and modelled independently in order to determine the influence of data quantity on the output models from the three programs. This created 96 datasets that were modelled by all three programs using both the IDW and OK algorithms. The data subsets extracted from the four synthetic grids were interpolated, and then re-imported into MATLAB to allow comparison of the interpolated results with the original synthetic models. The accuracy of the modelled grids generated by each software program was quantified using a variety of statistical measures including root mean square error (RMSE) and bias error (BE). The RMSE results were used to determine how accurately each of the programs was able to interpolate the original grids and the BE was used to show where the models created under- or over-estimations of the original data.

In order to assess the relative influence of each variable included in the modelling tests (i.e. number and distribution of data points, grid complexity, and algorithm and program selection) on model accuracy, a multi-way (n-way) ANOVA (analysis of variance) was calculated in MATLAB (Appendix 4.1). The results obtained from the ANOVA tests are used to quantify the influence of program selection relative to grid complexity, number and distribution of data points, and algorithm selection in producing the most accurate 3D subsurface model.

4.2.1 Grid Creation

Four synthetic grids were created to represent realistic geological environments of variable spatial complexity using ROCKWORKS 2006 software (Figure 4.1). The method used to create the synthetic grids is described by MacCormack et al., (submitted 2010; Chapter 3) and was developed to test the impact of data quantity, distribution, and algorithm selection on the accuracy of 3D subsurface models. Each synthetic grid was constructed using identical 80x80 grid dimension templates. The grid spacing was set to 1 arbitrary unit, which resulted in 6400 grid cells for each model. This allows each grid to contain sufficient detail to test each interpolation process while not being computationally exhausting. Each grid cell was assigned a value (thickness/elevation) value of between 1 and 9 in order to create the topographic variation shown in each of the four synthetic models. The 3D models are shown here with flat lower surfaces for ease of illustration (Figure 4.1).

The first synthetic grid (grid 1) was created to represent a simple, gently sloping unidirectional surface with lateral continuity in the direction perpendicular to the slope (grid 1; Figure 4.1a). The second synthetic grid surface is slightly more complex, consisting of a linear trough between areas of relatively high elevation (grid 2; Figure 4.1b). This surface shows undulating topography with alternating highs and lows. The third synthetic grid surface shows more spatial and topographic complexity, and consists of a series of interconnected troughs separated by irregularly spaced 'highs' (grid 3; Figure 4.1c). The fourth grid is characterised by a sinuous trough, with a high degree of directional variability, cut into a flat surface and will likely be the most difficult for the various software programs to accurately model (grid 4; Figure 4.1d). For more detailed descriptions of the four synthetic grids, refer to MacCormack et al., (submitted 2010; Chapter 3).

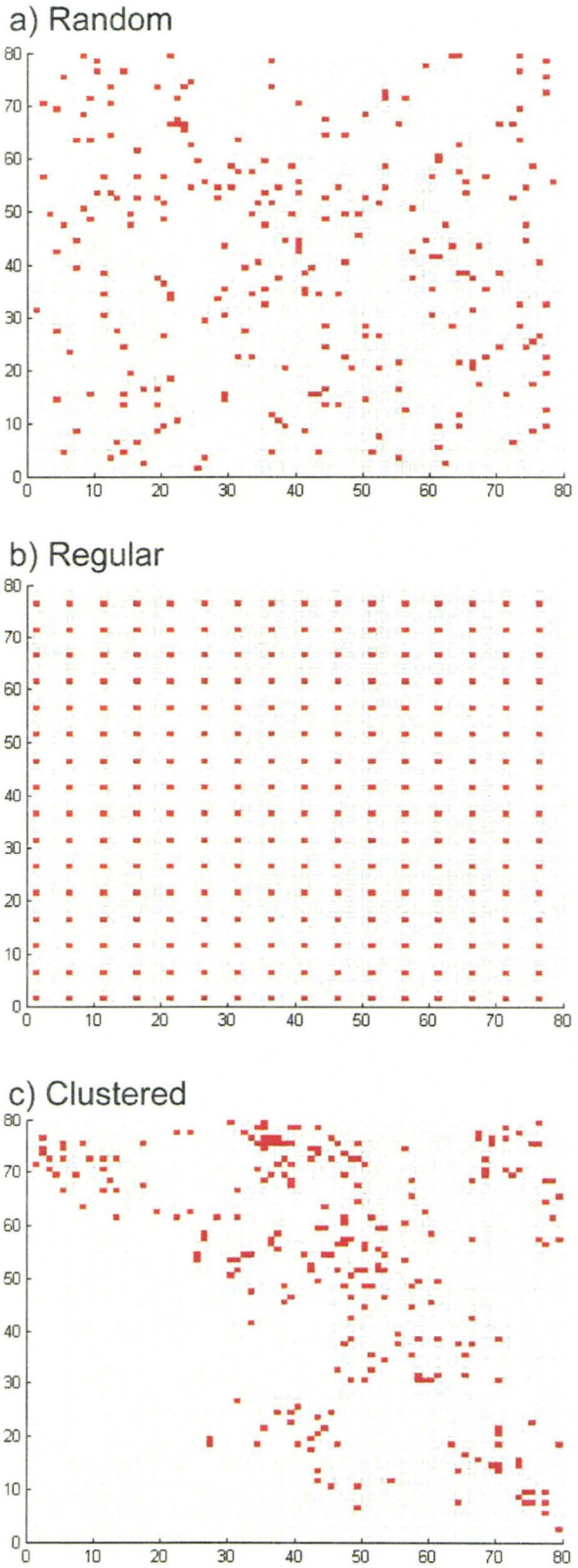
4.2.2 Data Extraction

To allow quantitative analysis of differences between the model outputs from the three modelling software programs, data were extracted from the four synthetic grids in a consistent and un-biased manner. A study by Bond et al. (2007) showed that data selection can be unintentionally biased by prior knowledge of the user. Hence, the points used for interpolation were selected using MATLAB scripts to eliminate the introduction of user bias into the analysis. The MATLAB scripts were designed to extract points from each of the four synthetic grids with specified quantities and distributions of data. The quantities and distributions of the data points within each data subset were varied in order to assess whether the quantity of data points, distribution of the data, and/or complexity of

the modelled surface had any impact on the ability of each of the software programs to consistently produce an accurate model. Four separate data point datasets were created, each containing 100, 256, 676 or 1600 cells (representing 1.6, 4, 10.5 and 25% surface coverage, respectively). The points included in each data point dataset were extracted in three common sampling distribution patterns: a) random, b) regular, and c) clustered (Zimmerman et al., 1999; Davis, 2002; Figure 4.2).

Random sample distributions (Figure 4.2a), were created for the desired quantity of data points by repeating computer-generated random assignment of x and y grid locations without replacement on each synthetic surface. Regular sample distributions (Figure 4.2b) were produced by imposing a square-grid of equally-spaced sample points on the synthetic grids. The spacing between sample points was universally adjusted to accommodate the specified amount of data points; this ensured maximum spatial coverage of the surface, while preserving the equal spacing and distribution (number of rows and columns) of sample points. The clustered sampling distributions (Figure 4.2c), were generated by establishing data clusters of sampling points by randomly assigning 'cluster centres' on the synthetic grid, and then equally distributing the desired number of sample points between each cluster (MacCormack et al., submitted 2010; Chapter 3).

Figure 4.2: Data points were extracted from the four synthetic grids in 3 spatial distribution patterns a) random, b) regular, and c) clustered. Sample distribution patterns for the 256 point dataset are illustrated.


a) Random
b) Regular
c) Clustered
0
10
20
30
40
50
60
70
80

4.2.3 Data Formatting

Each of the extracted data subsets were exported from MATLAB as text document (.txt) files in a 3-column format, containing x and y-coordinates, and z values respectively. These files were copied three times so that each software program received the same data for interpolation. However, the three programs (ArcGIS, ROCKWORKS 2006, and VIEWLOG) were unable to directly import the data in this format and each dataset required reformatting to meet the specific requirements of each program. Once all the data subsets were formatted appropriately and saved, they were imported into each software program for interpolation.

4.2.4 Establishing Unbiased Interpolation Settings

Each of the data subsets were modelled using both IDW and OK gridding algorithms available in all three software programs. Each software program provided numerous options for selection or adjustment of parameters that provide the user some control over the interpolation process. Deciding how to include or adjust these parameters requires user input and expert knowledge, and can introduce user bias and uncertainty into the model output results (Englund, 1990; Bond et al., 2007). In order to minimize the impact of user bias on the model output results, standard settings were applied within each program. For IDW, the number of user options was relatively small and only required determination of the number of points utilized for interpolation, set to 8 for all models run in this study. Many more options are available to influence the performance of the OK algorithm but only two were available for all three programs; variogram type and number of neighbours included for interpolation. The variogram type

was set to spherical (the default settings for two of the programs), and the number of neighbours included for interpolation was also set to 8 (to be consistent with the IDW parameters). All other parameters were left as the default settings of the program. Although using a 'black box' approach to modelling is less than ideal and does not allow the user to adjust settings to best accommodate the data being modelled, this was the only way to minimize the impact of external variables that may bias the results and obscure the effect of the internal workings of each program on the interpolation results. Minimizing external inputs into the modelling process allowed any deviations in the output results to be considered as a result of the software program and not confused with user bias/influence.

4.2.5 Comparing the Output Models

Once the 96 data subsets were interpolated by each of the three programs, they were converted from Excel files into text document (.txt) files and re-imported into MATLAB to allow comparison of results. To identify the differences between the models interpolated by the three programs, the interpolated model outputs were compared with the original synthetic grids. This was done by creating custom MATLAB functions developed to provide a quantitative comparison of each interpolated grid with the original synthetic grid. Assessment of the differences between the interpolated and original grids was then possible using a number of statistical measures such as Root Mean Square Error (RMSE), relative RMSE (rRMSE), Mean Average Error (MAE), and the Correlation Coefficient (r2). The bias error (BE) was also calculated to determine whether the interpolated grids were either under or over-estimating the original synthetic values due to

the various sampling treatments. Although all of these statistical measures were compared during initial assessment of the impacts of software selection, RMSE was determined to provide the best overall comparative statistic as it provides an un-biased indication of how similar the interpolated values are to the original values from the synthetic grids. When analyzing the RMSE statistics, a small RMSE value indicates that the interpolated values for the output model are more similar to the original synthetic values, whereas a large RMSE value suggests that the interpolated model produced by the software program is less similar to the original synthetic grid. Thus, RMSE values are used here to determine the accuracy of the model output with low RMSE values indicting a high degree of model accuracy (Zimmerman et al., 1999; Davis, 2002; Dille et al., 2003; Jones et al., 2003; Mueller et al., 2004).

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}\left(\hat{Z}\,(s_i) - z(s_i)\right)^2}{n}}$$

Where $\hat{Z}\,(s_i)$ is the interpolated value at the point (s_i), and $z(s_i)$ is the observed (true) value from the synthetic dataset at that same location, and n is the number of points within the input dataset.

The bias error (BE) results identify the extent to which the modelling programs are under- or over-estimating the prediction of subsurface unit geometries and/or volumes (see section 4.3.5).

$$BE = \frac{\sum_{i=1}^{n}(\hat{Z}(s_i) - z(s_i))}{n}$$

The RMSE results produced by all 96 models (Appendix 4.1) were compared with one another using a series of graphs, and through a multi-way (n-way) analysis of the variance (ANOVA) for each variable (grid complexity, distribution of data, number of data points, algorithm, and program selection). ANOVA is often used to quantify the differences between results of multiple trials in which one variable is altered at a time in order to assess its singular influence on the results (Appendix 4.2; Carr, 2002; Davis, 2002; Borradaile, 2003). The benefit of using a multi-way ANOVA is the ability to determine if and/or how the results differ with respect to the influence of individual variables, or a combination of variables (Davis, 2002; Borradaile, 2003).

The ANOVA was performed in MATLAB to statistically assess which variables had most influence on the accuracy of the synthetic grids modelled by the three software programs (Appendix 4.3). For this study, all of the ANOVA results were based on a significance of 95% (α=0.05), which is a commonly used confidence level (Issaks and Srivastava, 1989; Cressie, 1993; Carr, 2002; Davis, 2002; Haneberg, 2004).

4.3 Results and Discussion

The model outputs from the three software programs under investigation (ArcGIS, ROCKWORKS 2006, and VIEWLOG) of the four synthetic grids using the OK and IDW

algorithms were quantitatively assessed using Root Mean Square Error (RMSE) and Bias Error (BE). Any differences between the RMSE and BE results produced by the three programs were analyzed graphically, and the significance of RMSE differences were quantified in the multi-way ANOVA (Table 4.1-4.5; Appendix 4.3). The statistical tests were used to establish the amount of influence that each of the variables (i.e. data point distribution, grid complexity, number of data points, algorithm selection and program selection) have on the accuracy of models created by each of the three programs.

4.3.1 Influence of Grid Complexity

To evaluate the impact of grid complexity on the ability of the three programs (X, Y, Z) to produce accurate models, RMSE values were compared for models of the four synthetic grids produced by interpolation of 100, 256, and 676 regularly distributed data points (Figure 4.3). The RMSE results clearly show that the value and range of RMSE values increase with greater grid complexity for all programs and algorithms (Figure 4.3). For grids 1 and 2, the RMSE values are all very similar to one another regardless of the number of data points used to generate the model or which software program and interpolation algorithm was used (Figure 4.3). RMSE values for the more complex grids (grids 3 and 4) are higher than those for grids 1 and 2 but decrease as more data points are used to create the models (Figure 4.3). When modelling the more complex subsurface

Table 4.1: Summary ANOVA results for RMSE values averaged for all model simulations. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3.

Source of Variability	Sum of Squares	'F' Statistic	p-value	% influence
Grid Complexity	51.78	4277.5	0	**60.81**
Data Distribution	14.74	1827.0	0	**17.32**
Algorithm Selection	1.32	327.28	1.78E-15	**1.55**
Number of Data Points	8.13	1007.89	0	**9.55**
Program Selection	0.36	45.46	6.87E-09	**0.43**
Total	85.15	-	-	-

Table 4.2: Summary ANOVA table of RMSE results for grid 1 showing the influence of individual variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3.

Source of Variability	Sum of Squares	'F' Statistic	p-value	% influence
Data Distribution	5.28	936.83	0	**61.73**
Algorithm Selection	0.69	122.42	1.86E-10	**8.07**
Number of Data Points	1.64	145.25	2.11E-13	**19.14**
Program Selection	0.030	2.64	0.094	**0.35**
Total	8.55	-	-	-

Table 4.3: Summary ANOVA table of RMSE results for grid 2 showing the influence of individual variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3.

Source of Variability	Sum of Squares	'F' Statistic	p-value	% influence
Data Distribution	7.41	4343.61	0	**50.70**
Algorithm Selection	0.75	439.25	5.55E-16	**5.13**
Number of Data Points	5.27	1543.99	0	**36.05**
Program Selection	0.022	6.53	0.005952	**0.15**
Total	14.61	-	-	-

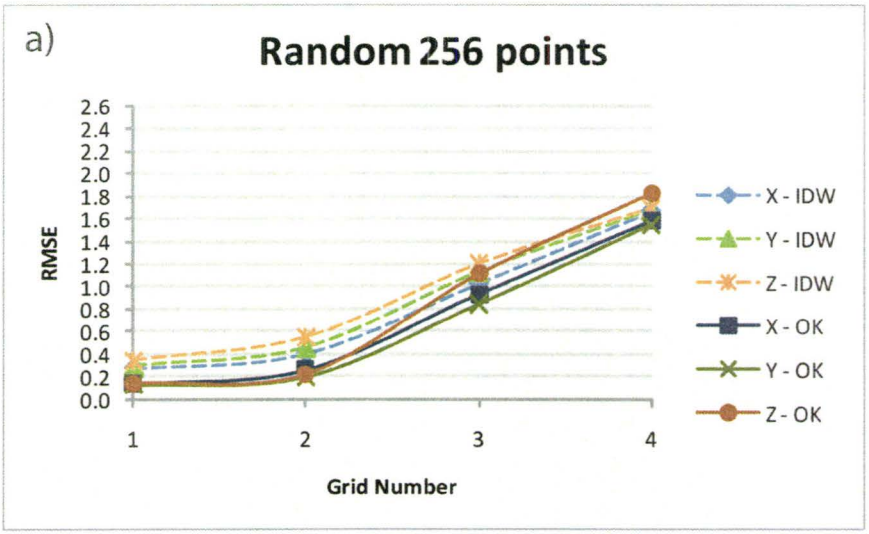
Table 4.4: Summary ANOVA table of RMSE results for grid 3 showing the influence of individual variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3.

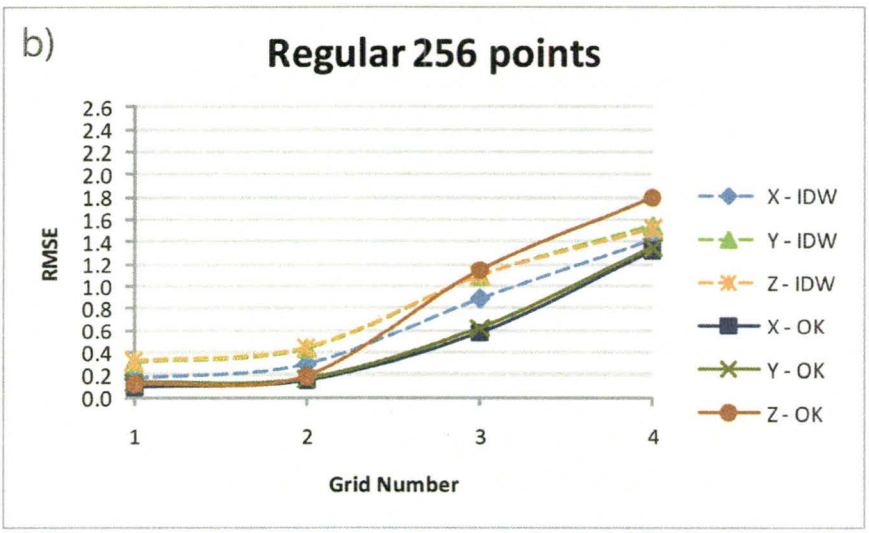
Source of Variability	Sum of Squares	'F' Statistic	p-value	% influence
Data Distribution	2.34	274.97	6.43E-14	**39.26**
Algorithm Selection	0.32	37.04	3.99E-06	**5.29**
Number of Data Points	1.88	110.63	3.31E-12	**31.59**
Program Selection	0.24	14.04	0.00012	**4.01**
Total	5.96	-	-	-

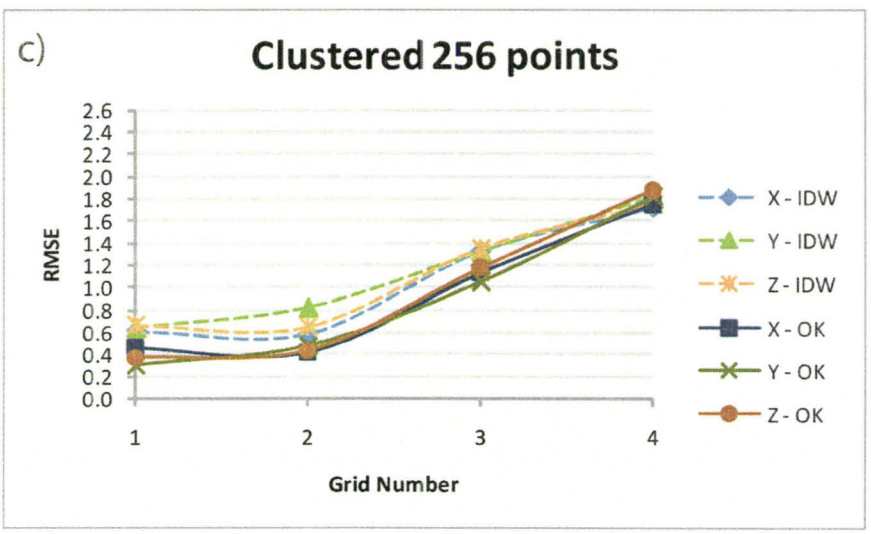
Table 4.5: Summary ANOVA table of RMSE results for grid 4 showing the influence of individual and selected combinations of variables on model accuracy. See Appendix 4.2 for description of parameters shown. Data extracted from Appendix 4.3.

Source of Variability	Sum of Squares	'F' Statistic	p-value	% influence
Data Distribution	1.21	97.42	1.53E-09	**28.31**
Algorithm Selection	0.0080	0.65	0.429997	**0.19**
Number of Data Points	1.78	71.80	2.28E-10	**41.72**
Program Selection	0.079	3.18	0.048	**1.85**
Distribution and Number of Data Points	0.09	3.67	0.04	**2.13**
Distribution and Program Selection	0.09	3.63	0.04	**2.11**
Total	4.26	-	-	-

Figure 4.3: Graphs of RMSE results for datasets modelled with 256 data points in a) random, b) regular, and c) clustered distributions. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.


a)
Random 256 points
RMSE
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
Grid Number
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK


b)
Regular 256 points
RMSE
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
Grid Number
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK


c)
Clustered 256 points
RMSE
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
Grid Number
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK

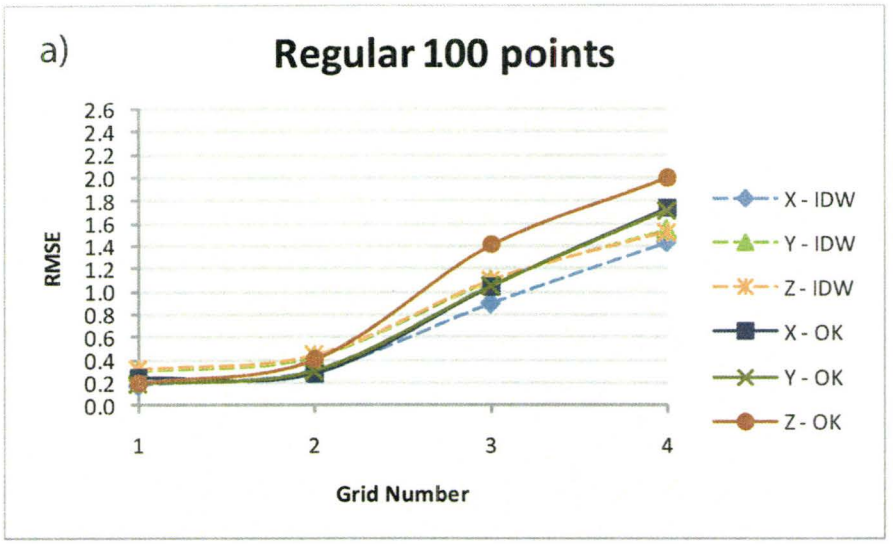
environments represented by grids 3 and 4, program X typically produced the lowest RMSE using either IDW or OK, followed by program Y, and then Z (Figure 4.3). Program X also generated the most accurate model of grid 4 (lowest RMSE values) when both 256 and 676 data points were interpolated using the OK algorithm (Figure 4.3 b,c).

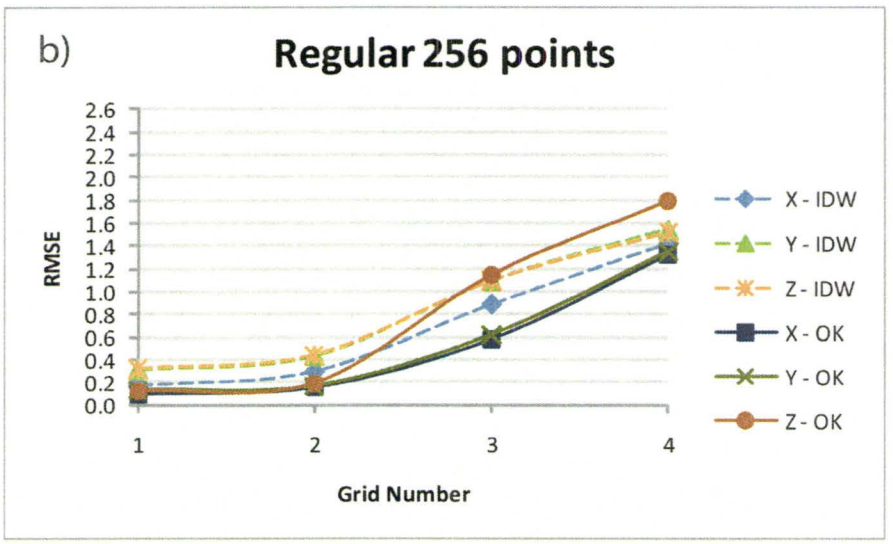
The ANOVA based on the RMSE results showed that grid complexity had by far the greatest influence on how accurately the synthetic grids were modelled and accounted for most of the variation in the RMSE results (Table 4.1). Data point distribution and number of data points accounted for the second and third highest amounts of variability respectively, followed by algorithm and program selection, which both had relatively low influences on model accuracy (Table 4.1). Grid complexity had such an overwhelming influence (60.81%) on the RMSE variance, that in order to better assess the influence of the other variables, four separate n-way ANOVAs were run on the RMSE results for each of the four synthetic grids (Tables 4.2-4.5). For grids 1and 2, that represent relatively simple subsurface conditions, data distribution had the greatest individual influence (highest SS_T; Appendix 4.2) on RMSE, followed by number of data points, algorithm selection, and program selection respectively (Tables 4.2,4.3). For grid 3 the order of influence was the same as grids 1 and 2, with the exception that algorithm and program selection had essentially equal influence on model accuracy (Table 4.4). Interestingly, the relative influence of each individual variable was different for the grid 4 ANOVA, which showed that the number of points used for interpolation had the greatest influence on model accuracy, closely followed by data point distribution, program selection, and algorithm selection (Table 4.5). In addition, when the combination of variables were

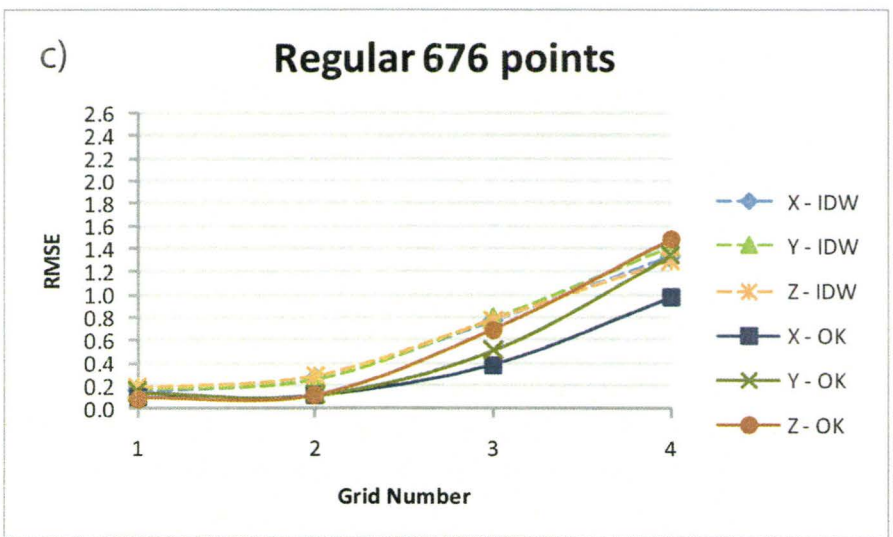
analyzed for grid 4 (representing an extremely complex subsurface unit), the distribution and number of data points (two variables shown to have a substantial impact on the model accuracy of complex grids individually; Table 4.5) ranked only slightly higher than the combination of program selection and data point distribution in controlling model accuracy (Table 4.5). This is an important finding as it shows that when interpolating complex environments, program selection and data distribution can have as significant an influence on the accuracy of the model output as the number and distribution of data points used in modelling, and have more influence than algorithm selection on model accuracy.

These results suggest that program selection has little influence on model accuracy when modelling relatively simple grids (e.g. grids 1 and 2; Figure 4.3, Figure 4.4 b,e), but has a stronger impact, noted by the greater differences in RMSE values between the three programs (e.g. grids 3 and 4; Figure 4.3, Figure 4.4 h,k), when modelling more complex grids. The ANOVA results support these conclusions by showing that the influence of program selection increased with increasing grid complexity (Tables 4.2-4.5). This is especially true in the case of grid 4, where program selection was shown to have a greater influence on model accuracy than algorithm selection (Table 4.5). Therefore, when modelling complex subsurface environments, program selection should be carefully considered as it can have a statistically significant impact on model accuracy.

Figure 4.4: Graphs showing the change in RMSE produced by the software programs (X, Y, Z) using algorithms IDW and OK, as increasing numbers of regularly distributed data a) 100, b) 256, and c) 676 were modelled. RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.


a)
Regular 100 points
RMSE
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
Grid Number
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK


b)
Regular 256 points
RMSE
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
Grid Number
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK

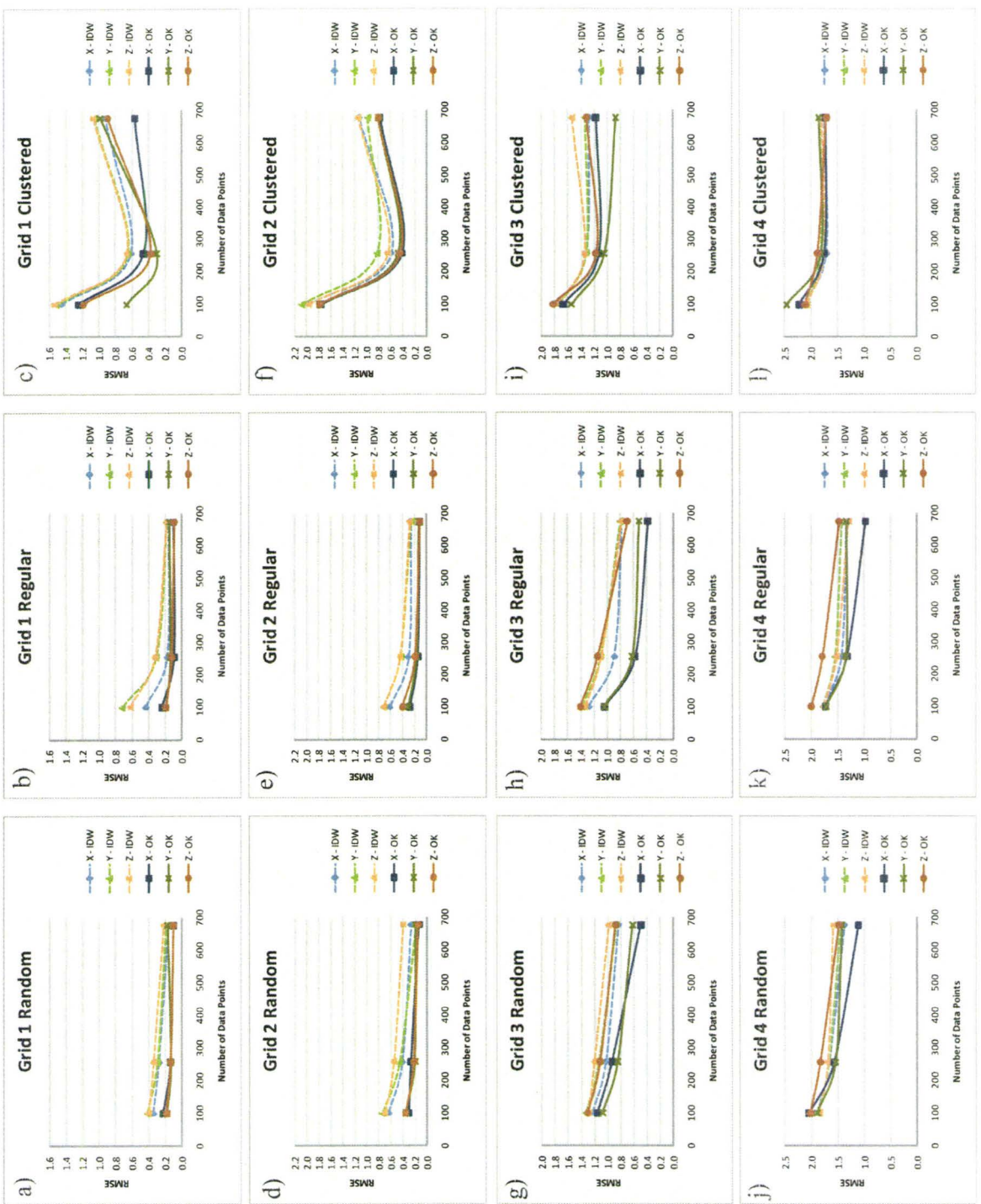

c)
Regular 676 points
RMSE
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
Grid Number
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK

4.3.2 Influence of Data Point Distribution

Data were extracted from the original synthetic grids in three distribution patterns (random, regular, and clustered) and interpolated using OK and IDW by the three software programs. Analysis of the results from the models run with 256 data points showed that grids 1 and 2 were modelled most accurately (lowest RMSE values) by randomly and regularly distributed data using OK by all three programs (Figure 4.5 a,b). However, when more complex grids were modelled using random and regularly distributed data, the RMSE values show considerable increase, regardless of algorithm or program used (grids 3 and 4; Figure 4.5). Clustered data produced the largest RMSE values when modelling all four grids, regardless of program or algorithm selection (Figure 4.5c). It is interesting to note that the most variation in the RMSE results between program and algorithm selection occurred when clustered data were used to model grids 1 and 2, and became more similar when interpolating grids 3 and 4 (Figure 4.5c). Program Z produced the highest RMSE values when the OK algorithm was used, but was the least impacted by the spatial distribution of the data (Figure 4.5). This contrasts with the performance of programs X and Y that showed high levels of accuracy (low RMSE) when modelling random and regularly spaced data, but performed with similar accuracy to program Z when modelling clustered data (Figure 4.5).

Of all distributions, the RMSE results for randomly distributed datasets were the least susceptible to variation between the three programs, followed by regular and clustered distributions (Figure 4.4). The increased range of RMSE results for clustered datasets may reflect how the individual programs manage the irregular distributions of

Figure 4.5: Graphs showing the change in RMSE values produced by the software programs (X, Y, Z) as increasing numbers (100, 256, 676) of data points in random (a,d,g,j), regular (b,e,h,k), and clustered (c,f,i,l) distributions are used to interpolate synthetic grids 1 (a,b,c), 2 (d,e,f), 3 (g,h,i) and 4 (j,k,l). RMSE values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.


a)
Grid 1 Random
b)
Grid 1 Regular
c)
Grid 1 Clustered
d)
Grid 2 Random
e)
Grid 2 Regular
f)
Grid 2 Clustered
g)
Grid 3 Random
h)
Grid 3 Regular
i)
Grid 3 Clustered
j)
Grid 4 Random
k)
Grid 4 Regular
l)
Grid 4 Clustered
RMSE
Number of Data Points
X - IDW
Y - IDW
Z - IDW
X - OK
Y - OK
Z - OK

high data point densities, which can produce large amounts of variability over short distances, and how this variability is propagated through the model. This is an important finding as most geological studies use clustered data to interpret their results (Paulen et al., 2006; Bond et al., 2007; Keefer, 2007). Overall, program X produced slightly lower RMSE results, followed by programs Y and Z (Figure 4.4 c,f,i,l). The large variation in RMSE results for clustered datasets produced by the three programs indicates that clustered data were most susceptible to introducing increased uncertainty into the model output due to software selection.

The ANOVA results showed that overall, data distribution had the second greatest influence on RMSE (model accuracy) when all models were analyzed (Table 4.1). When the influence of data point distribution was analyzed independently for each of the four grids, the ANOVA results showed that data point distribution had the greatest influence of any variable when interpolating grids 1, 2 and 3 (Tables 4.2-4.4). When modelling complex surfaces (grid 4), data point distribution had the second-most influence after the number of points being modelled (Table 4.5).

These results indicate that data point distribution has a significant influence on the accuracy of model results. In particular, program selection should be carefully considered when interpolating clustered data in order to ensure that all sources of uncertainty and variability to the model output are appropriately identified.

4.3.3 Impact of Data Quantity

A common assumption made by 3D modelers is that incorporating more data in the interpolation process will provide a more accurate model. In order to assess whether the number of data points used in the modelling process had any impact on the effectiveness of the different programs to create accurate models, the RMSE values were graphed based on the number of data points used for interpolation (Figure 4.4). Overall, the RMSE values drop as the number of data points used for interpolation increases, with the exception of the clustered datasets modelled for grids 1, 2 and 3(Figure 4.4 c,f,i). The OK algorithms applied within the X and Z software programs produced the lowest RMSE values (i.e. the most accurate model results) when grids 1 and 2 were modelled using a large number of data points (676; Figure 4.4 a,b,d,e). Differences in RMSE values computed for grids 1 and 2 modelled by the three programs also reduced with the addition of data points and models run with 676 points show remarkably similar RMSE results for all three programs (Figure 4.4 a,b,d,e). In contrast, the RMSE results for grids 3 and 4 modelled using random and regularly distributed data (Figure 4.4 g,h,j,k) show an increased range of values produced by the three programs as the number of data points increases. Overall, program X produces the lowest RMSE results for models of grids 3 and 4 using the OK algorithm (Figure 4.4 g,h,j,k).

The RMSE results for the clustered datasets show a decrease for all programs and algorithms when the number of clustered data points increases from 100 to 256 indicating that the additional data points have increased the accuracy of the model. However, when the number of data points increase from 256 to 676, the RMSE results for all programs

and algorithms increased for grids 1 and 2 (Figure 4.4 c,f) indicating an increase in error values and a reduction in model accuracy. When interpolating grid 3 with 676 data points, the RMSE results increased for all programs except Y using the OK algorithm (Figure 4.4i). The increased variability in RMSE results when additional data points were used for interpolation was originally thought to be due to differences between the OK and IDW algorithms, but numerous graphs (Figure 4.4 c,f,g,h,i,j,k) show substantial variability within the RMSE results when OK and IDW outputs are considered independently.

To relate these results to other studies, the number of points used for interpolation can also be translated into % area covered. The synthetic grids were composed of a total of 6400 data points (Figure 4.1), therefore 100, 256, and 676 data points can also be considered to represent 1.6%, 4%, 10.6% area covered respectively. These results indicate that it is more important to consider the impact of program selection on model accuracy for studies with greater than 4% data coverage.

ANOVA results for RMSE indicate that the number of data points used for interpolation became increasingly important as the grid complexity increased (Tables 4.2-4.5). When all models were considered in the ANOVA, data quantity had the third most influence on model accuracy, behind grid complexity and data distribution respectively (Table 4.1). When separate ANOVAs were calculated for each synthetic grid, data quantity had the second most influence on RMSE for grids 1, 2 and 3, and was the most influential variable when modelling complex environments such as grid 4 (Tables 4.2-4.5).

4.3.4 Influence of Algorithm Selection

The influence of algorithm selection on the accuracy of the modelled grids using random, regular and clustered datasets of between 100 and 676 points is shown in Figure 4.4. Overall, the OK algorithm produces the lowest RMSE results regardless of data distribution (Figure 4.4). When the OK algorithm was used to interpolate grids 1 and 2, the RMSE values produced by programs X, Y, and Z were very similar to one another. This indicates that program selection has little impact when using OK to interpolate relatively simple models (grids 1 and 2; Figure 4.4 a-f). However, when OK was used to interpolate the more complex grids (3 and 4), greater differences in the RMSE values were produced by the three programs (Figure 4.4 g-l). Overall, the variability of RMSE values for models interpolated with IDW were fairly consistent between the three programs, indicating that IDW is less susceptible to program selection than OK (Figure 4.4). When modelling grid 4, algorithm selection had little impact as there were minimal differences between the RMSE values produced by models interpolated with either IDW or OK (Figure 4.4 j-l). The ANOVA results reveal that algorithm selection was the third most influential variable on model accuracy for grids 1 through 3, and was the least important for grid 4 (Tables 4.2-4.5).

These results imply that the program-specific processes operating within the three programs are affected more strongly by the OK algorithm than IDW. These program-specific influences were shown to cause variability in model accuracy, and should be considered when attempting to quantify model variability and uncertainty. This is

especially important when modelling complex grids, for which program selection can have more influence on model accuracy than the algorithm chosen for interpolation.

4.3.5 Bias Error Analysis

Analyzing the bias errors associated with the interpolated results is useful for determining whether the predictions typically represent under- or over-estimations of the actual surface. Ideally, the bias errors should be as close to zero as possible, although the amount that they deviate from zero and whether they are positive or negative can provide valuable information about the accuracy of the predictions (Elith et al., 2002; Hengl et al., 2004). If the bias error is negative, the interpolated results are biased toward the production of under-estimations when compared to the observed values. A positive bias error reveals that the interpolated results are typically producing over-estimations when compared to the observed values (Elith et al., 2002; Mueller and Pierce, 2003).

In this study, bias errors were analyzed and graphed in two ways by calculating the average of the bias errors, and the absolute sum of the bias errors. The average bias error (AVBE) is used to assess whether the overall impact of each sampling treatment causes over or under-estimation. However, AVBE can provide misleading results if extreme high and low deviations both occur within the model as they will cancel each other out during the averaging process. Calculating the absolute bias error (ABBE) allows the total amount of deviation to be summed together which will identify the amount of error, regardless of whether the predictions are either over or under-estimating the actual values. If the ABBE results show high values, a large amount of error is

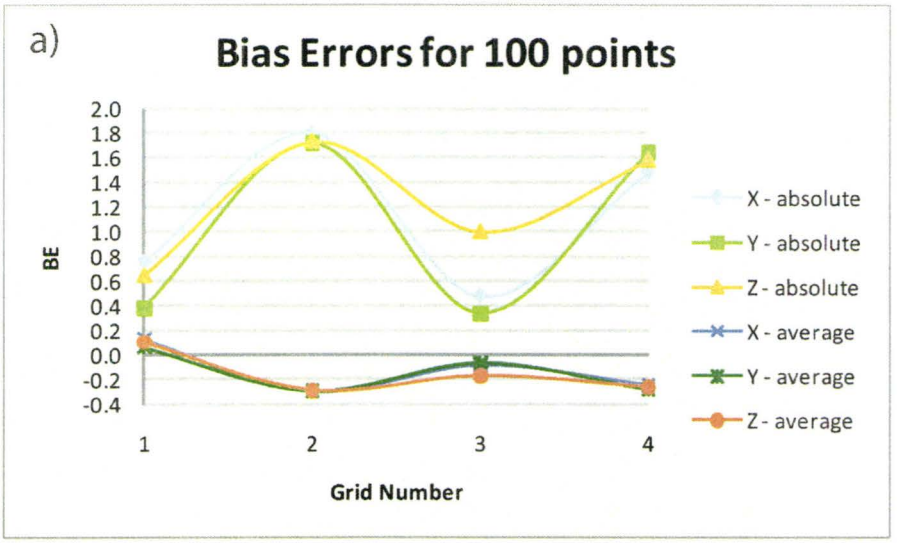
indicated, whereas low values indicate small deviation from the actual values and a more realistic result.

The ABBE and AVBE were calculated for the models produced by all three software programs using different numbers of points for all 4 synthetic grids (Figure 4.6). Comparison of the bias errors produced by the three software programs for the models created under the various conditions produced very interesting results. No one software program appeared to consistently outperform the others in terms of providing consistently low error values. This suggests that each program has certain conditions that favour their specific modelling procedures.

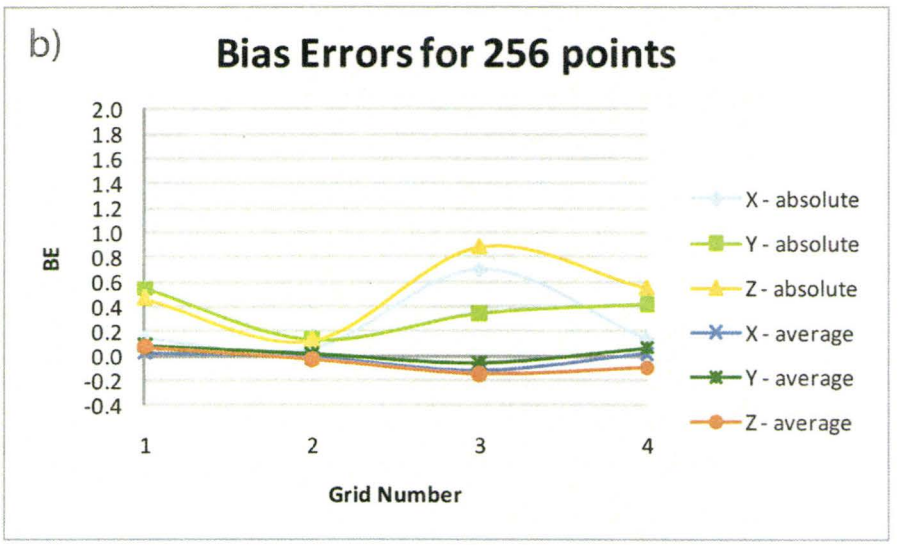
The models produced with 100 points produced the most similar ABBE and AVBE results among the three programs, which suggest that with low numbers of data points, the interpolation processes all have similar effects on the model output (Figure 4.6a). However, for models interpolated with additional data points (256 and 676), there was less variability in the bias errors produced by each program (Figure 4.6 b,c). Program X and Y produced similar AVBE results when interpolating with 256 and 676 data points, and similar ABBE results when interpolating with 100 and 676 results (Figure 4.6). Both the AVBE and ABBE results for program Z followed similar trends to those for program X and Y, but the actual values were quite different (Figure 4.6). These results suggest that programs X and Y may follow similar processes when interpolating data under certain conditions because they tend produce similar errors. Program Z is likely interpolating data using a different set of procedures because it produced distinctly different bias errors than programs X and Y (Figure 4.6). These results exemplify the

Figure 4.6: Graphs showing the change in the absolute sum of the bias errors (ABBE) and the average bias errors (AVBE) produced by the software programs (X, Y, Z) to interpolate Grids 1, 2, 3, and 4 using 100 (a), 256 (b) and 676 (c) data points. Bias error values are given in arbitrary units that relate to the thickness values (1-9) allocated to points on the synthetic grids.

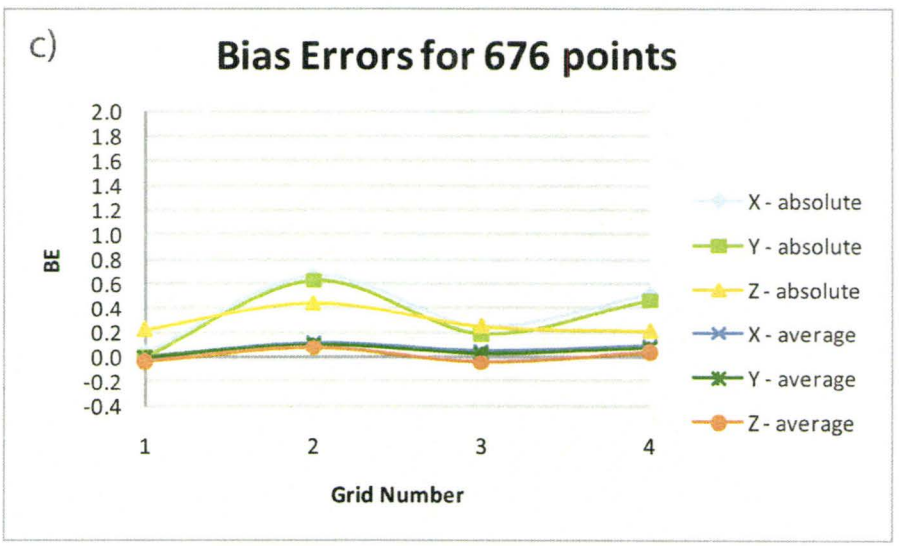
a)


Bias Errors for 100 points
BE
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
1
2
3
4
Grid Number
X - absolute
Y - absolute
Z - absolute
X - average
Y - average
Z - average

b)


Bias Errors for 256 points
BE
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
1
2
3
4
Grid Number
X - absolute
Y - absolute
Z - absolute
X - average
Y - average
Z - average

c)


Bias Errors for 676 points
BE
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
1
2
3
4
Grid Number
X - absolute
Y - absolute
Z - absolute
X - average
Y - average
Z - average

importance of considering program selection when quantifying variability or uncertainty, as program selection alone can impact whether a model represents an over- or under-estimation of the actual values.

4.4 Conclusions

This paper compares the ability of three commonly used 3D modelling programs to accurately interpolate grids of variable complexity, using different numbers and distributions of data points. This study demonstrates that, although certain software programs offer the same interpolation algorithms, they do not necessarily provide the same output results. In most 3D subsurface investigations, a substantial amount of time and effort is spent collecting and analyzing data, as well as assessing data parameters to ensure the most accurate model possible is produced. The results of this study suggest that program selection should also be seriously considered as a possible source of model uncertainty, the effects of which should be considered especially when modelling complex subsurface geological environments, interpolating with clustered data, or when relatively large quantities of data (more than 4 - 10.6% data coverage) are used for interpolation.

This study confirmed that the output of the OK and IDW interpolation algorithms is not consistent when used by different software programs and this variability should be considered when assessing the uncertainty associated with subsurface model results. These results do not suggest that any particular program is better than another, but do

show that software selection can impact the accuracy of the output model in a similar manner to that documented for algorithm selection (Tabios and Salas, 1985; Weber and Englund, 1992; Weber and Englund, 1994; Brus et al., 1996; Walker and Loftis, 1997; Nalder and Wein, 1998; Zimmerman et al., 1999; Schloeder, 2001; Jones et al., 2003; Kravchenko, 2003; Dille et al., 2003; Lapen and Hayhoe; 2003). In some instances program selection can actually have a greater impact on model accuracy than which algorithm is used perform the interpolation process.

Given that 3D modelling is increasingly used as an analytical tool for numerous applications in geo- and environmental sciences and may form the basis on which large scale, multi-million dollar decisions are made, serious attention should be paid to the many factors that control model accuracy. Numerous studies have documented the influence of algorithm selection on model output but none have quantified the impact of software selection. The results of this study indicate that program selection can have a significant influence on the accuracy of model results and therefore should be seriously considered as a potential source of uncertainty.

Reference List

Bond, C. E., Gibbs, A. D., Shipton, Z. K., & Jones, S. (2007). What do you think this is? "Conceptual uncertainty" in geoscience interpretation. *GSA Today, 17,* 4-10.

Borradaile, G. J. (2003). *Statistics of earth science data: their distribution in time, space and orientation.* Springer.

Brus, D. J., De Gruijter, J. J., Marsman, B. A., Visschers, R., Bregt, K. A., Breeuwsma, A. et al. (1996). The performance of spatial interpolation methods and choropleth maps to estimate properties at points: a soil survey case study. *Environmetrics, 7,* 1-16.

Burrough, P. A. (2001). GIS and geostatistics: Essential partners for spatial analysis. *Environmental and Ecological Statistics, 8,* 361-377.

Carr, J. R. (2002). *Data Visualization in the Geosciences.* New Jersey: Prentice Hall.

Cressie, N. A. (1993). *Statistics for Spatial Data.* Wiley Interscience.

Davis, J. C. (2002). *Statistics and data analysis and geology.* John Wiley and Sons.

Dille, J. A., Milner, M., Groeteke, J. J., Moretensen, D. A., & Williams, M. M. (2003). How good is your weed map? A comparison of spatial interpolators. *BioOne, 51,* 44-55.

Elith, J., Burgman, M. A., & Regan, H. M. (2002). Mapping epistemic uncertainties and vague concepts in predictions of species distribution. *Ecological Modelling, 157,* 313-329.

Englund, E. J. (1990). A variance of Geostatisticians. *Mathematical Geology, 22,* 417-455.

Haneberg, W. C. (2004). *Computational Geosciences with Mathematica.* (1 ed.) Springer.

Hengl, T., Heuvelink, G. B. M., & Stein, A. (2004). A generic framework for spatial prediction of soil variables based on regression-kriging. *Geoderma, 120,* 75-93.

Isaaks, E. H. & Srivistava, R. M. (1989). *An Introduction to Applied Geostatistics*. New York: Oxford University Press.

Johnston, K., Ver Hoef, J. M., Krivoruchko, K., & Lucas, N. (2001). *Using ArcGIS Geostatistical Analyst*. USA: ESRI.

Jones, N. L., Davis, R. J., & Sabbah, W. (2003). A comparison of Three-dimensional interpolation techniques for plume characterization. *Groundwater, 41,* 411-419.

Keefer, D. A. & Rittenhouse, S. (2005). Estimating the uncertainty of 3D geologic maps. *Three-Dimensional Geologic Mapping for Groundwater Applications - Workshop Extended Abstracts, Geological Survey of Canada, Open File 5048,* 31-35.

Kravchenko, A. N. (2003). Influence of spatial structure on accuracy of interpolation methods. *Soil Science Society of America Journal, 67,* 1564-1571.

Kravchenko, A. N. & Bullock, D. G. (1999). A comparative study of interpolation methods for mapping soil properties. *Agronomy Journal, 91,* 393-400.

Lapen, D. R. & Hayhoe, H. N. (2003). Spatial analysis of seasonal and annual temperature and precipitation normals in southern Ontario, Canada. *Journal of Great Lakes Research, 29,* 529-544.

Mueller, T. G. & Pierce, F. J. (2003). Soil carbon maps: Enhancing spatial estimates with simple terrain attributes at multiple scales. *Soil Science Society of America Journal, 67,* 258-267.

Mueller, T. G., Pusuluri, P. B., Mathias, K. K., Cornelius, P. L., Barnhisel, R. I., & Shearer, S. A. (2004). Map quality for ordinary kriging and inverse distance weighted interpolation. *Soil Science Society of America Journal, 68,* 2042-2047.

Nalder, I. A. & Wein, R. W. (1998). Spatial interpolation of climatic Normals: test of a new method in the Canadian boreal forest. *Agricultural and Forest Meteorology, 92,* 211-225.

Paulen, R. C., McClenaghan, M. B., & Harris, J. R. (2006). Bedrock topography and drift thickness models from the Timmins area, northeastern Ontario: An application of GIS to the Timmins overburden drillhole database. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 413-434). St. John's: Geological Association of Canada.

Schloeder, C. A., Zimmerman, N. E., & Jacobs, M. J. (2001). Comparison of methods for interpolating soil properties using limited data. *Soil Science Society of America Journal, 66,* 479.

Tabios, G. Q. & Salas, J. D. (1985). A comparative-analysis of techniques for spatial interpolation of precipitation. *Water Resources Bulletin, 21,* 365-380.

Walker, D. D. & Loftis, J. C. (1997). Alternative spatial estimators for ground-water and soil measurements. *Groundwater, 35,* 593-599.

Weber, D. & Englund, E. J. (1992). Evaluation and comparison of spatial interpolators. *Mathematical Geology, 24,* 381-391.

Weber, D. & Englund, E. J. (1994). Evaluation and comparison of spatial interpolators II. *Mathematical Geology, 26,* 589-603.

Zimmerman, D., Pavlik, C., Ruggles, A., & Armstrong, M. P. (1999). An experimental comparison of Ordinary and Universal Kriging and inverse distance weighting. *Mathematical Geology, 31,* 375-390.

APPENDIX 4.1: RMSE RESULTS

Grid Variables				Program X					Program Y					Program Z				
# Data Points	Grid #	Distribution	Algorithm	RMSE	rRMSE	MAE	BE	r2	RMSE	rRMSE	MAE	BE	r2	RMSE	rRMSE	MAE	BE	r2
100	1	Clustered	IDW	1.45495	0.33063	1.06572	0.21706	0.67037	1.50939	0.34300	1.14609	0.24684	0.64524	1.54147	0.35029	1.16480	0.27483	0.63000
100	1	Clustered	OK	1.24884	0.28379	0.89009	0.28031	0.75714	0.66621	0.15139	0.43936	0.06489	0.93089	1.19108	0.27067	0.83559	0.25247	0.77909
100	1	Random	IDW	0.34439	0.07826	0.25612	0.09191	0.98153	0.41916	0.09525	0.31455	0.06198	0.97264	0.40234	0.09143	0.28797	0.07219	0.97479
100	1	Random	OK	0.22645	0.05146	0.15497	0.09341	0.99201	0.18361	0.04172	0.12083	0.03873	0.99475	0.18625	0.04232	0.12092	0.05083	0.99460
100	1	Regular	IDW	0.43590	0.09905	0.30702	0.01042	0.97041	0.71977	0.16356	0.42806	-0.10809	0.91933	0.62186	0.14131	0.38756	-0.08212	0.93978
100	1	Regular	OK	0.23883	0.05427	0.16420	0.06408	0.99112	0.19354	0.04398	0.11416	0.08238	0.99417	0.19401	0.04409	0.12483	0.07839	0.99414
100	2	Clustered	IDW	1.97807	0.38962	1.42473	-1.02267	0.05511	2.08606	0.41089	1.52953	-1.02663	-0.05088	1.96527	0.38710	1.42050	-1.02062	0.06729
100	2	Clustered	OK	1.76505	0.34766	1.18127	-0.91652	0.24766	1.78429	0.35145	1.20966	-0.79009	0.23117	1.77950	0.35051	1.22034	-0.83325	0.23530
100	2	Random	IDW	0.63633	0.12534	0.50634	0.10963	0.90222	0.74393	0.14653	0.59259	0.10119	0.86635	0.69946	0.13777	0.55280	0.14023	0.88185
100	2	Random	OK	0.30186	0.05946	0.21920	0.04442	0.97800	0.35378	0.06968	0.25378	0.01147	0.96977	0.35563	0.07005	0.25727	0.02942	0.96946
100	2	Regular	IDW	0.61125	0.12040	0.46925	-0.02291	0.90977	0.71534	0.14090	0.56109	-0.02309	0.87643	0.71018	0.13988	0.53625	-0.07984	0.87820
100	2	Regular	OK	0.27699	0.05456	0.19581	0.00709	0.98147	0.30775	0.06062	0.21603	0.00638	0.97713	0.40083	0.07895	0.26983	0.03242	0.96120
100	3	Clustered	IDW	1.74554	0.47376	1.35077	-0.15036	0.12442	1.72535	0.46828	1.37763	-0.16941	0.14456	1.75027	0.47504	1.38578	-0.22266	0.11968
100	3	Clustered	OK	1.66966	0.45316	1.28067	-0.08605	0.19890	1.54900	0.42042	1.19841	0.07925	0.31050	1.82560	0.49549	1.46817	-0.27070	0.04226
100	3	Random	IDW	1.23588	0.33543	1.03017	-0.07255	0.56108	1.32714	0.36020	1.13802	-0.11286	0.49387	1.28998	0.35012	1.09844	-0.14506	0.52181
100	3	Random	OK	1.15469	0.31340	0.94544	-0.02563	0.61685	1.08178	0.29361	0.81116	0.00112	0.66371	1.30667	0.35465	1.12227	-0.05130	0.50936
100	3	Regular	IDW	1.28207	0.34797	1.06450	-0.10675	0.52766	1.37857	0.37416	1.16184	-0.11944	0.45387	1.33689	0.36285	1.12128	-0.13447	0.48640
100	3	Regular	OK	1.03992	0.28225	0.77595	-0.03905	0.68923	1.04648	0.28403	0.77450	-0.02159	0.68530	1.40699	0.38187	1.20459	-0.17734	0.43113
100	4	Clustered	IDW	2.12657	0.34601	1.68659	-0.54912	-0.02428	2.07683	0.33792	1.73516	-0.55578	0.02307	2.08614	0.33943	1.67823	-0.50592	0.01429
100	4	Clustered	OK	2.22458	0.36196	1.76881	-0.61384	-0.12087	2.45993	0.40025	2.01070	-0.72817	-0.37059	2.11529	0.34418	1.70342	-0.47842	-0.01344
100	4	Random	IDW	1.88467	0.30665	1.32839	-0.14183	0.19549	1.87343	0.30482	1.39713	-0.17903	0.20506	1.85293	0.30149	1.35256	-0.17309	0.22236
100	4	Random	OK	2.04788	0.33321	1.43425	-0.16650	0.05012	1.90018	0.30918	1.23752	-0.15198	0.18220	2.02384	0.32930	1.54759	-0.20975	0.07229
100	4	Regular	IDW	1.76590	0.28733	1.24775	0.00294	0.29369	1.77599	0.28897	1.28745	0.00198	0.28560	1.76538	0.28724	1.27250	-0.03081	0.29411
100	4	Regular	OK	1.73189	0.28179	1.11255	-0.01498	0.32064	1.71581	0.27918	1.09358	-0.02845	0.33319	2.00130	0.32563	1.56592	-0.17955	0.09284

Grid Variables				Program X					Program Y					Program Z				
# Data Points	Grid #	Distribution	Algorithm	RMSE	rRMSE	MAE	BE	r2	RMSE	rRMSE	MAE	BE	r2	RMSE	rRMSE	MAE	BE	r2
256	1	Clustered	IDW	0.61375	0.13947	0.34384	0.11472	0.94134	0.64656	0.14693	0.40562	0.28591	0.93490	0.66558	0.15125	0.38572	0.17534	0.93102
256	1	Clustered	OK	0.46306	0.10523	0.24033	0.07923	0.96661	0.30080	0.06835	0.18070	0.12892	0.98591	0.37599	0.08544	0.21362	0.13444	0.97799
256	1	Random	IDW	0.27512	0.06252	0.16261	-0.02964	0.98821	0.29870	0.06788	0.19902	0.01439	0.98611	0.34616	0.07866	0.21909	-0.00244	0.98134
256	1	Random	OK	0.14064	0.03196	0.07373	-0.01145	0.99692	0.13187	0.02997	0.07872	0.04441	0.99729	0.13890	0.03156	0.08306	0.04000	0.99700
256	1	Regular	IDW	0.17486	0.03974	0.10606	-0.00847	0.99524	0.30905	0.07023	0.20002	0.00889	0.98513	0.32264	0.07332	0.20872	0.05678	0.98379
256	1	Regular	OK	0.09381	0.02132	0.05277	0.00105	0.99863	0.13448	0.03056	0.08047	0.06866	0.99718	0.12511	0.02843	0.08080	0.06442	0.99756
256	2	Clustered	IDW	0.58634	0.11549	0.43170	-0.02008	0.91698	0.82307	0.16212	0.58203	0.09044	0.83640	0.64935	0.12790	0.48323	0.00117	0.89817
256	2	Clustered	OK	0.41880	0.08249	0.27056	-0.00891	0.95764	0.47783	0.09412	0.30009	0.05322	0.94486	0.44095	0.08685	0.29537	0.02294	0.95305
256	2	Random	IDW	0.40601	0.07997	0.31208	-0.01630	0.96019	0.45806	0.09022	0.34937	-0.00600	0.94933	0.54888	0.10811	0.41787	-0.08997	0.92725
256	2	Random	OK	0.26541	0.05228	0.17881	-0.00363	0.98299	0.20231	0.03985	0.14491	0.00753	0.99012	0.21742	0.04283	0.15333	0.00686	0.98858
256	2	Regular	IDW	0.30092	0.05927	0.21781	-0.00778	0.97813	0.43301	0.08529	0.32650	-0.00634	0.95472	0.44305	0.08727	0.32811	-0.07027	0.95260
256	2	Regular	OK	0.15201	0.02994	0.10281	-0.00463	0.99442	0.16779	0.03305	0.11684	-0.00512	0.99320	0.19449	0.03831	0.13308	-0.00058	0.99087
256	3	Clustered	IDW	1.32009	0.35829	0.97411	-0.13742	0.49923	1.32503	0.35963	1.04141	0.04172	0.49547	1.34482	0.36500	1.02927	-0.13348	0.48029
256	3	Clustered	OK	1.13320	0.30756	0.81422	-0.12178	0.63098	1.04982	0.28493	0.77825	-0.01909	0.68329	1.17350	0.31850	0.89166	-0.10688	0.60427
256	3	Random	IDW	1.02954	0.27943	0.79989	-0.19198	0.69541	1.13207	0.30726	0.94753	-0.19350	0.63172	1.20071	0.32589	0.98550	-0.25847	0.58570
256	3	Random	OK	0.93499	0.25377	0.72442	-0.15639	0.74878	0.84651	0.22975	0.62608	-0.10580	0.79408	1.11477	0.30256	0.92380	-0.16989	0.64289
256	3	Regular	IDW	0.89358	0.24253	0.70625	-0.07031	0.77054	1.09687	0.29770	0.91514	-0.08267	0.65427	1.09703	0.29775	0.89750	-0.11188	0.65416
256	3	Regular	OK	0.57984	0.15738	0.40927	-0.02336	0.90338	0.61920	0.16806	0.44833	0.01105	0.88982	1.14731	0.31139	0.96136	-0.10220	0.62174
256	4	Clustered	IDW	1.71477	0.27901	1.08364	0.02223	0.33400	1.81733	0.29570	1.22675	0.04756	0.25195	1.74618	0.28412	1.23375	-0.13184	0.30938
256	4	Clustered	OK	1.75597	0.28571	0.97844	0.10666	0.30162	1.82088	0.29627	1.07517	0.35927	0.24903	1.87865	0.30567	1.37827	-0.21855	0.20062
256	4	Random	IDW	1.66594	0.27106	1.02338	0.08928	0.37139	1.67501	0.27254	1.10384	0.09575	0.36453	1.69192	0.27529	1.10203	0.08072	0.35164
256	4	Random	OK	1.57862	0.25685	0.88238	0.15053	0.43557	1.54646	0.25162	0.87992	0.16736	0.45833	1.83084	0.29789	1.21983	0.07089	0.24080
256	4	Regular	IDW	1.42840	0.23241	0.94166	-0.11338	0.53787	1.54961	0.25213	1.09913	-0.11994	0.45612	1.52114	0.24750	1.08533	-0.15045	0.47592
256	4	Regular	OK	1.32748	0.21599	0.76964	-0.11577	0.60087	1.35070	0.21977	0.80733	-0.12545	0.58678	1.79316	0.29176	1.31297	-0.20119	0.27172

Grid Variables				Program X					Program Y					Program Z				
# Data Points	Grid #	Distribution	Algorithm	RMSE	rRMSE	MAE	BE	r2	RMSE	rRMSE	MAE	BE	r2	RMSE	rRMSE	MAE	BE	r2
676	1	Clustered	IDW	0.92286	0.20971	0.46005	-0.13770	0.86738	1.05860	0.24056	0.50336	-0.18258	0.82550	1.07086	0.24335	0.49920	-0.23948	0.82143
676	1	Clustered	OK	0.56597	0.12861	0.25739	-0.07920	0.95012	0.98665	0.22421	0.45236	-0.17633	0.84841	0.89245	0.20280	0.37147	-0.17378	0.87598
676	1	Random	IDW	0.15727	0.03574	0.10300	0.04531	0.99615	0.19343	0.04396	0.13953	0.09003	0.99417	0.22304	0.05068	0.13889	0.06036	0.99225
676	1	Random	OK	0.10449	0.02374	0.06348	0.05192	0.99830	0.17327	0.03938	0.11220	0.09792	0.99532	0.10556	0.02399	0.06414	0.05092	0.99826
676	1	Regular	IDW	0.15558	0.03536	0.09783	0.03217	0.99623	0.17942	0.04077	0.12806	0.08128	0.99499	0.18124	0.04118	0.11517	0.03098	0.99489
676	1	Regular	OK	0.10110	0.02297	0.06136	0.05033	0.99841	0.15033	0.03416	0.10230	0.08836	0.99648	0.09314	0.02116	0.05703	0.04562	0.99865
676	2	Clustered	IDW	1.11860	0.22033	0.71366	0.44294	0.69783	0.97786	0.19261	0.59839	0.36717	0.76909	1.14328	0.22519	0.76481	0.24791	0.68435
676	2	Clustered	OK	0.77656	0.15296	0.44608	0.24039	0.85437	0.80108	0.15779	0.42239	0.27227	0.84503	0.80714	0.15898	0.44566	0.27263	0.84268
676	2	Random	IDW	0.26092	0.05139	0.19084	0.00106	0.98356	0.28325	0.05579	0.20520	-0.00155	0.98063	0.39937	0.07866	0.26891	-0.04528	0.96148
676	2	Random	OK	0.13606	0.02680	0.09167	-0.00630	0.99553	0.18516	0.03647	0.12183	-0.00267	0.99172	0.14593	0.02874	0.09759	-0.00650	0.99486
676	2	Regular	IDW	0.26339	0.05188	0.18750	-0.00475	0.98325	0.25906	0.05103	0.18467	-0.00667	0.98379	0.28489	0.05611	0.19320	-0.02548	0.98040
676	2	Regular	OK	0.11542	0.02274	0.07047	-0.00163	0.99678	0.12284	0.02420	0.08131	0.00012	0.99636	0.11434	0.02252	0.07111	-0.00148	0.99684
676	3	Clustered	IDW	1.27705	0.34661	0.97947	0.08053	0.53135	1.34221	0.36429	0.95153	0.08966	0.48230	1.53803	0.41744	1.15014	-0.08811	0.32023
676	3	Clustered	OK	1.17367	0.31855	0.78103	0.21522	0.60416	1.29748	0.35215	0.88411	0.10845	0.51624	1.31957	0.35815	0.98850	0.07144	0.49962
676	3	Random	IDW	0.83564	0.22680	0.65555	0.00117	0.79933	0.87310	0.23697	0.67008	0.00211	0.78094	0.99011	0.26873	0.74102	-0.08998	0.71879
676	3	Random	OK	0.49857	0.13532	0.33216	0.00388	0.92857	0.61943	0.16812	0.39603	0.01697	0.88974	0.88018	0.23889	0.67922	-0.01350	0.77737
676	3	Regular	IDW	0.77193	0.20951	0.61141	-0.04803	0.82877	0.79976	0.21706	0.61569	-0.02350	0.81620	0.78078	0.21191	0.58242	-0.09814	0.82482
676	3	Regular	OK	0.38543	0.10461	0.24956	0.00306	0.95731	0.51557	0.13993	0.33712	-0.00169	0.92362	0.69290	0.18806	0.52041	-0.03325	0.86203
676	4	Clustered	IDW	1.74998	0.28474	1.03295	0.34220	0.30537	1.82799	0.29743	1.00739	0.38886	0.24315	1.79855	0.29264	1.04802	0.32377	0.26734
676	4	Clustered	OK	1.72332	0.28040	0.97661	0.39777	0.32735	1.85828	0.30236	1.02063	0.40853	0.21787	1.71432	0.27894	0.92556	0.36494	0.33435
676	4	Random	IDW	1.38152	0.22479	0.93506	-0.14388	0.56771	1.45663	0.23701	0.96758	-0.14745	0.51943	1.59422	0.25939	1.08972	0.20628	0.42435
676	4	Random	OK	1.11726	0.18179	0.63687	-0.07225	0.71727	1.41059	0.22952	0.86172	-0.15553	0.54932	1.48000	0.24081	0.96106	-0.18228	0.50388
676	4	Regular	IDW	1.32618	0.21611	0.85269	-0.01088	0.60045	1.42358	0.23163	0.90422	-0.01397	0.54099	1.29726	0.21108	0.86313	-0.06481	0.61883
676	4	Regular	OK	0.97638	0.15887	0.53211	0.00580	0.78408	1.33881	0.21784	0.80602	-0.01286	0.59403	1.47636	0.24022	0.95503	-0.02144	0.50632

APPENDIX 4.2: ANOVA DESCRIPTION

The first step in the ANOVA analysis is to generate a hypothesis about the variables, known as the null hypothesis (H_o), which implies that there is no difference (relationship) between the variables and the RMSE results.

$$H_o : \mu_1 = \mu_2 = \mu_3 \ldots\ldots \mu_n$$

H_1: at least one of the treatment means will be different

To identify a relationship between the variation in the variables and the variation in the RMSE results, the null hypothesis must be rejected. The p-value provides the probability that the null hypothesis could be rejected incorrectly (type 1 error) and the results were created by chance alone (Davis 2002; Borradaile, 2003). If the p-value in the ANOVA table is less than the accepted level of significance (α), then the H_o can be rejected, and a relationship between the variables is assumed (Davis, 2002; Borradaile, 2003). For this study, all of the ANOVA results are based on a significance of 95% (α=0.05), which is a commonly used confidence level (Issaks and Srivastava, 1989; Cressie, 1993; Carr, 2002; Davis, 2002; Haneberg, 2004). Therefore, only the results from the ANOVA test with p-values < α were considered to be significant, as there is a less than 5% chance that the H_o could be rejected incorrectly (type I error; Davis, 2002). Once the H_o has been rejected, the differences in variances amongst the variables are determined to be significant and to have an influence on the variance in the RMSE

results. The amount of variance attributed to each variable (and combination of variables) can be quantified by calculating the sum of squares for each treatment (SS_T; Davis, 2002).

$$SS_{TOT} = SS_E + SS_{T1} + SS_{T2} + SS_{T3} + SS_{T4} + SS_{T5}$$

Where SS_{TOT} is the total variation, SS_E is the variance that could not be explained by the variables, and SS_{Tn} is the variation attributed to each treatment. This information can be used to compare the variance in the mean values produced by each variable (SS_{Tn}) to the overall variability (SS_{TOT}), providing an indication of how much of the total variance (SS_{TOT}) can be attributed to each variable (SS_A).

$$(SS_{Tn}/SS_{TOT}) \times 100 = SS_A$$

The more variation that each variable accounts for (higher SS_A), the greater its influence is determined to be on results. Therefore, high SS_A values indicate that the variable of interest has a large influence on the RMSE results, while a small SS_A value indicates that the variable has less influence on the RMSE results. The ANOVA results will be used in a relative sense for this study to assess the order of influence for the variables impacting RMSE results. Therefore, there will not be much attention paid to the actual values of the ANOVA, but rather on their relative relationships to one another.

APPENDIX 4.3: ANOVA RESULTS

Grid	Source of Variability	Sum of Squares	F' Statistic	p-value	% Influence
all	Grid Complexity (Grid)	51.78	4277.54	0.00	60.81
all	Data Distribution (Dist)	14.75	1827.04	0.00	17.32
all	Algorithm Selection (Alg)	1.32	327.28	0.00	1.55
all	Number of Data Points (Num_pt)	8.13	1007.90	0.00	9.55
all	Program Selection (Pro)	0.37	45.47	0.00	0.43
all	'Grid*Dist'	1.73	71.50	0.00	2.03
all	'Grid*Alg'	0.55	45.41	0.00	0.65
all	"'Grid*Num_pt'	0.82	33.81	0.00	0.96
all	'Grid*Prog'	0.14	5.84	0.00	0.17
all	'Dist*Alg'	0.01	0.75	0.48	0.01
all	"'Dist*Num_pt'	2.37	146.55	0.00	2.78
all	'Dist*Prog'	0.06	3.71	0.02	0.07
all	"'Alg*Num_pt'	0.00	0.28	0.76	0.00
all	'Alg*Prog'	0.07	9.26	0.00	0.09
all	"'Num_pts*Pro'	0.06	3.70	0.02	0.07
all	"'Grid*Dist*Al'	0.10	4.19	0.01	0.12
all	"'Grid*Dist*Num_pt'	1.49	30.74	0.00	1.75
all	"'Grid*Dist*Pro'	0.11	2.25	0.04	0.13
all	"'Grid*Alg*Num_pt'	0.27	11.34	0.00	0.32
all	"'Grid*Alg*Pro'	0.14	5.77	0.00	0.16
all	"'Grid*Num_pts*Pro'	0.10	2.00	0.07	0.11
all	"'Dist*Alg*Num_pt'	0.02	1.16	0.35	0.02
all	"'Dist*Alg*Pro'	0.05	3.35	0.03	0.06
all	"'Dist*Num_pts*Pro'	0.07	2.15	0.07	0.08
all	"'Alg*Num_pts*Pro'	0.12	7.38	0.00	0.14
all	"'Grid*Dist*Alg*Num_pt'	0.05	1.12	0.39	0.06
all	"'Grid*Dist*Alg*Pro'	0.12	2.38	0.03	0.14
all	"'Grid*Dist*Num_pts*Pro'	0.17	1.77	0.09	0.20
all	"'Grid*Alg*Num_pts*Pro'	0.07	1.55	0.18	0.09
all	"'Dist*Alg*Num_pts*Pro'	0.01	0.21	0.99	0.01
all	'Error'	0.10	[]	[]	[]
all	'Total'	85.15	[]	[]	[]

Grid	Source of Variability	Sum of Squares	F' Statistic	p-value	% Influence
1	Data Distribution (Dist)	5.28	936.83	0.00	61.73
1	Algorithm Selection (Alg)	0.69	122.42	0.00	8.07
1	Number of Data Points (Num_pt)	1.64	145.25	0.00	19.14
1	Program Selection (Pro)	0.03	2.64	0.09	0.35
1	'Dist*Alg'	0.06	10.62	0.00	0.70
1	'"Dist*Num_pt'	0.83	73.31	0.00	9.66
1	'Dist*Prog'	0.02	2.10	0.15	0.28
1	'"Alg*Num_pt'	0.13	11.11	0.00	1.46
1	'Alg*Prog'	0.04	3.19	0.06	0.42
1	'"Num_pts*Pro'	0.10	4.31	0.01	1.14
1	'"Dist*Alg*Num_pt'	0.00	0.27	0.77	0.04
1	'"Dist*Alg*Pro'	0.01	1.21	0.32	0.16
1	'"Dist*Num_pts*Pro'	0.12	5.38	0.00	1.42
1	'"Alg*Num_pts*Pro'	0.09	3.91	0.02	1.03
1	'Error'	0.12	[]	[]	[]
1	'Total'	8.55	[]	[]	[]
2	Data Distribution (Dist)	7.41	4343.60	0.00	50.70
2	Algorithm Selection (Alg)	0.75	439.25	0.00	5.13
2	Number of Data Points (Num_pt)	5.27	1544.00	0.00	36.05
2	Program Selection (Pro)	0.02	6.53	0.01	0.15
2	'Dist*Alg'	0.00	0.07	0.80	0.00
2	'"Dist*Num_pt'	2.59	760.00	0.00	17.74
2	'Dist*Prog'	0.01	1.74	0.20	0.04
2	'"Alg*Num_pt'	0.01	3.49	0.05	0.08
2	'Alg*Prog'	0.00	1.29	0.29	0.03
2	'"Num_pts*Pro'	0.02	3.11	0.04	0.15
2	'"Dist*Alg*Num_pt'	0.03	9.13	0.00	0.21
2	'"Dist*Alg*Pro'	0.00	0.73	0.49	0.02
2	'"Dist*Num_pts*Pro'	0.02	2.79	0.05	0.13
2	'"Alg*Num_pts*Pro'	0.03	3.77	0.02	0.18
2	'Error'	0.04	[]	[]	[]
2	'Total'	14.61	[]	[]	[]

Grid	Source of Variability	Sum of Squares	F' Statistic	p-value	% Influence
3	Data Distribution (Dist)	2.34	274.97	0.00	39.26
3	Algorithm Selection (Alg)	0.32	37.04	0.00	5.29
3	Number of Data Points (Num_pt)	1.88	110.63	0.00	31.59
3	Program Selection (Pro)	0.24	14.04	0.00	4.01
3	'Dist*Alg'	0.01	1.38	0.25	0.20
3	"'Dist*Num_pt'	0.26	15.05	0.00	4.30
3	'Dist*Prog'	0.02	1.47	0.25	0.42
3	"'Alg*Num_pt'	0.03	1.54	0.24	0.44
3	'Alg*Prog'	0.06	3.73	0.04	1.06
3	"'Num_pts*Pro'	0.02	0.54	0.71	0.31
3	"'Dist*Alg*Num_pt'	0.01	0.52	0.60	0.15
3	"'Dist*Alg*Pro'	0.03	1.82	0.19	0.52
3	"'Dist*Num_pts*Pro'	0.02	0.71	0.59	0.41
3	"'Alg*Num_pts*Pro'	0.04	1.04	0.41	0.59
3	'Error'	0.19	[]	[]	[]
3	'Total'	5.96	[]	[]	[]
4	Data Distribution (Dist)	1.21	97.42	0.00	28.31
4	Algorithm Selection (Alg)	0.01	0.65	0.43	0.19
4	Number of Data Points (Num_pt)	1.78	71.80	0.00	41.72
4	Program Selection (Pro)	0.08	3.18	0.05	1.85
4	'Dist*Alg'	0.02	1.68	0.21	0.49
4	"'Dist*Num_pt'	0.09	3.67	0.04	2.13
4	'Dist*Prog'	0.09	3.63	0.04	2.11
4	"'Alg*Num_pt'	0.08	3.15	0.06	1.83
4	'Alg*Prog'	0.03	1.24	0.31	0.72
4	"'Num_pts*Pro'	0.06	1.20	0.34	1.40
4	"'Dist*Alg*Num_pt'	0.00	0.00	1.00	0.00
4	"'Dist*Alg*Pro'	0.07	2.64	0.09	1.53
4	"'Dist*Num_pts*Pro'	0.02	0.40	0.81	0.46
4	"'Alg*Num_pts*Pro'	0.04	0.90	0.48	1.05
4	'Error'	0.27	[]	[]	[]
4	'Total'	4.26	[]	[]	[]

CHAPTER 5
SUMMARY AND CONCLUSIONS

The objective of the research conducted for this thesis is to improve the accuracy of 3D geologic models by identifying, assessing, and quantifying the impact of data quality, grid complexity, data quantity and distribution, and algorithm and program selection on the modelling process. Ensuring that the model output is as accurate as possible is of great importance as 3D models are increasingly being used for decision making and geoscientific applications in many fields of study. The increased use of 3D models for a broad range of applications has raised concerns about the accuracy and reliability of model outputs (Weber and Englund, 1992; Weber and Englund, 1994; Zimmerman et al., 1999; Jones et al., 2003), and the relationships between output quality, input data, model parameters, and the interpolation mechanism employed in the modelling process.

This thesis has addressed these concerns by; 1) assessing the impact of variable quality data on the accuracy of model estimations and developing a 'Quality Weighting' methodology for incorporating data into the modelling process to enhance the accuracy of the model results (Chapter 2), 2) assessing and quantifying the variability and influence of data quantity, data distribution, and interpolation algorithm on the accuracy of models simulating environments of varying complexity (Chapter 3), and 3) assessing and quantifying the impact of program selection on the accuracy of 3D geologic models (Chapter 4).

The methodology developed to impose a quality weighting factor on the input data used for model interpolation was shown to enhance the accuracy of 3D models (Chapter 2). This methodology allowed all types of data to be incorporated in the interpolation of the model while enhancing the influence of the high quality data, which ultimately increased the reliability of the output model. This methodology was tested in a study of the McMaster University campus area and showed that a dataset composed of variable quality data produced significantly different 3D model outputs to that produced by either high or low quality data alone. Applying the Quality Weighting method for interpolation allowed all of the data points to be used in the modelling process, while also allowing the higher quality data to have a greater influence on the model than the lower quality data. Utilizing this method reduced the negative impacts of the lower quality data on the model output, while still utilizing these data to constrain the model in areas where high quality data were unavailable. Comparison of model outputs created for the McMaster University campus area indicates that the Quality Weighted model outputs more closely conform to the available high quality data points and proxy data than un-weighted model outputs.

This research shows that the quality of the data used to create 3D models can have a substantial impact on the accuracy of the models produced. In cases where it is necessary to create models with variable quality data, the data should be weighted using a differential weighting mechanism, such as the Quality Weighted methodology proposed here, in order to assure the most accurate modelling results.

One of the reasons that lower quality data are often included in 3D modelling studies is in order for the models to be interpolated using the maximum number of data points. A common saying in 3D modelling is "You can never have too much data". However, analysis of the impact of data quantity on the accuracy of 3D models reported in this thesis (Chapter 3) suggests that increased numbers of data points do not always improve model accuracy. The research presented here showed that when modelling relatively complex grids, increasing the number of data points used for interpolation had the greatest impact on improving model accuracy. The model accuracy of relatively simple grids was less impacted by the addition of data points. These results were used to present a cost-benefit analysis that showed the optimum number of data points (data coverage) required for accurate and cost-effective interpolation of units of varying complexity. This analysis identified the point at which collecting additional data (increasing cost) produced a diminishing return (minimal increase in model accuracy) for models of varying complexity.

The distribution of the data points was also determined to be an extremely important factor affecting interpolation accuracy (Chapter 3). Regularly and randomly distributed data points produce the most accurate models, followed by sparse and clustered data respectively. The relationship between data quantity and distribution in the modelling process is also explored in this thesis (Chapters 3 and 4). The results of this research suggest that the relative importance of data distribution and data quantity on model accuracy are a function of the geologic complexity within the model. When modelling relatively simple geological environments, the model accuracy was more heavily

influenced by the distribution of data than the number of data points. In contrast, when modelling more complex geological environments, the number of data points had a greater influence on model accuracy than the spatial distribution of data. This research showed that contrary to popular belief, more data does not necessarily produce a more accurate model and that when modelling relatively simple surfaces it is more important to consider the distribution of the data than the actual number of data used for interpolation.

Although a large portion of this research focused on assessing the impacts of the data parameters on model accuracy, the methods by which the models are produced were also evaluated. Assessment of the impact of algorithm selection on model accuracy has been reported in the literature for over 10 years. The significance the assessments reported in this thesis is that not only was the overall performance of each algorithm assessed, but also their ability to produce accurate predictions given differences in modelling parameters (Chapters 3 and 4). Overall, the ordinary kriging (OK) algorithm produced more accurate results than inverse distance weighting (IDW). However, when their performances on individual grids were compared, IDW produced slightly more accurate results than OK in situations where complex grids were modelled with relatively low numbers of data points. The differences in model accuracy between OK and IDW were shown to decrease as the model complexity and number of data points used for modelling increased, implying that algorithm selection has the greatest impact on model accuracy when interpolating relatively simple grids with limited data.

Determining that there was a difference in the accuracy of results produced using OK and IDW to interpolate the models simulated in this study was not surprising, and is

in keeping with the findings of previous studies. However discovering that the model results, using identical algorithms by different software programs, are different is much more significant (Chapter 4). A major contribution of this study is to demonstrate that, although certain software programs offer the same interpolation algorithms for modelling, they do not necessarily provide the same output results. When modelling complex environments, program selection was shown to have a greater impact on model accuracy than the algorithm chosen to interpolate the data. These results indicate that program selection can have a significant influence on the accuracy of model results and should be seriously considered as a possible source of model uncertainty, especially when modelling complex subsurface geological environments, interpolating with clustered data, or when relatively large quantities of data (more than 4 - 10.6% data coverage) are used for interpolation.

Given that 3D models are increasingly used as analytical tools for numerous applications in geo- and environmental sciences and may form the basis on which large scale, multi-million dollar decisions are made, serious attention should be paid to the many factors that control model accuracy. When modelling spatial data there is always a high level of uncertainty, especially in subsurface environments where the unit(s) of interest are defined by data only available in select locations. Consequently, it is extremely difficult to validate the output of 3D subsurface models and to identify the many factors that may impact their reliability and accuracy. The results presented in this thesis can be used to guide the selection of modelling parameters used in 3D subsurface

investigations and will allow the more effective and efficient creation of accurate and reliable 3D models.

Future Work

The research presented in this thesis is just the 'tip of the iceberg'. There is much more that can be done to further assess and quantify the impacts of uncertainty on the accuracy of 3D geologic models. I believe that uncertainty is becoming such an important aspect of modelling that methods will soon be developed to visually incorporate uncertainty into models as the fifth dimension (5D). The technology has been in place for years to create 4D models with attributes that span time and space, and the assignation of values of uncertainty to these attributes will allow the development of 5D models. This will allow people to visualize how the values, as well as the uncertainty associated with the values, vary in both time and space.

The field of 3D modelling is expanding, not only in popularity, but quite literally as well. The size and scale of the 3D models being produced today are much larger than in the past. A few years ago, developing models the size of cities and townships was considered large scale (Bajc et al., 2004; Hansel et al., 2004; Logan et al., 2004). Today, models are being constructed at the provincial (Keller et al., 2009) and national scales (Kessler et al., 2007; Gunnink, 2009), and at global scales with projects such as OneGeology, designed to create a 'dynamic digital geological model' of the entire Earth.

I believe that research in geomodelling is moving past the creation of 3D models that only estimate the value of attributes in space, and is now focusing on quantifying and assessing the uncertainty associated with model predictions. Producing colourful 3D visualizations still has a digital 'wow factor' (Blewett and Henson, 2006), which implies a certain degree of confidence and authority. However, the recent development of applications such as GOOGLE EARTH ©, GOOGLE MAPS ©, and MAP QUEST © are raising legal issues surrounding the communication of spatial data (Onsrud, 2010). It is only a matter of time before these legal issues are extended to 3D geologic models, which will likely result in the quantification of uncertainty being more important than the actual model itself. Hence, a major field of future research will be in the development of effective mechanisms for uncertainty analysis in the modelling of multi-dimensional parameters.

References

Bajc, A. F., Endres, A. L., Hunter, J. A., Pullen, S. E., & Shirota, J. (2004). Three-Dimensional Mapping of Quaternary Deposits in the Waterloo Region, Southwestern Ontario. *Illinois State Geological Survey (IGSG) Open File Series 2004-2008,* 12-15.

Blewett, R. & Henson, P. (2006). Beyond the boardroom "wow factor": the utility of 3D maps/models for scale-integrated target generation, an example from the gold mineral system in the Yilgarn Craton - Western Australia. In K. McCaffrey, J. Imber, N. Holliman, R. Holdsworth, & T. Wawrzyeniec (Eds.), *Penrose Conference Abstracts* (pp. 15).

Gunnink, J. L. (2005). Geological mapping in the Netherlands: the case of the shallow subsurface (- 500 m). In *2005 Annual Meeting Geological Society of America.*

Hansel, A. K., Stiff, B. J., & Barhhardt, M. L. (2004). Three-dimensional Geologic Mapping in Rapid Growth Areas: A Case from Lake County, Northeastern Illinois. *Illinois State Geological Survey (IGSG) Open File Series 2004-2008,* 23-27.

Jones, N. L., Davis, R. J., & Sabbah, W. (2003). A comparison of Three-dimensional interpolation techniques for plume characterization. *Groundwater, 41,* 411-419.

Keller, G., Matile, G., & Thorleifson, H. (2009). Progress in 3D geological mapping in the eastern prairies of Canada and the USA. In *2009 Annual Meeting Geological Society of America.*

Kessler, H., Mathers, S., Lelliott, M., Hughes, A., & Macdonald, D. (2007). Rigorous 3D geological models as the basis for groundwater modelling. In *Minnesota Geological Survey Open-Report 07-4* (pp. 27-32).

Logan, C., Russel, H. A. J., Sharpe D.R., & Kenny, F. M. (2006). The role of GIS and expert knowledge in 3-D modelling, Oak Ridges Moraine, southern Ontario. In J.R.Harris (Ed.), *GAC Special Paper 44: GIS for the Earth Sciences* (pp. 519-542). St. John's: Geological Association of Canada.

Onsrud, H. J. (2010). Liability for Spatial Data Quality. In R.Devillers & H. Goodchild (Eds.), *Spatial Data Quality: From Process to Decisions* (pp. 1-222). Boca Raton, FL: CRC Press.

Weber, D. & Englund, E. J. (1992). Evaluation and comparison of spatial interpolators. *Mathematical Geology, 24,* 381-391.

Weber, D. & Englund, E. J. (1994). Evaluation and comparison of spatial interpolators II. *Mathematical Geology, 26,* 589-603.

Zimmerman, D., Pavlik, C., Ruggles, A., & Armstrong, M. P. (1999). An experimental comparison of Ordinary and Universal Kriging and inverse distance weighting. *Mathematical Geology, 31,* 375-390.