SALMO-OO: A Process-based Simulation Library for Lake Ecosystems

Lydia T. Cetin

A thesis submitted for the award of Doctor of Philosophy

2007

Ecoinformatics and Watershed Ecology Laboratory
School of Earth and Environmental Sciences
Environmental Biology Discipline
The University of Adelaide, Australia

CONTENTS

Thesis Contents i

Abstract v

Declaration vi

Acknowledgements vii

Publications and Scientific Communications During Candidature viii

List of Tables ix

List of Figures x

CHAPTER 1. GENERAL INTRODUCTION 1

1.1. Introduction of the main concepts and contributions of this project 1

CHAPTER 2. LITERATURE REVIEW 4

2.1. The establishment of simulation models in freshwater ecology 4

2.1.1. Deterministic ecological models 5

2.1.2. Current trends in dynamic freshwater ecosystem and water quality Modelling 6

2.1.3. Problems and limitations of current water quality models 9

2.1.3.1 Data availability and quality 9

2.1.3.2 Complexity 10

2.1.3.3 Duplication of effort: “reinventing” the ecosystem model 11

2.2. Process-based Model Libraries for the Simulation of Phytoplankton Dynamics 12

2.3. Adopting the Object-oriented Paradigm for Ecological Modelling 16

2.3.1. Key principles in object-oriented modelling 17

2.3.2. Advantages of adopting the object-oriented approach to ecological Modelling 19

2.3.3. Application of object-oriented modelling to ecology 22

CHAPTER 3. MATERIALS AND METHODS 26

3.1. SALMO: Dynamic Water Quality Model for Freshwater Lakes 26

3.1.1. Description of SALMO 26

3.1.2. Phytoplankton growth process as simulated by SALMO-OO 28

3.1.3. Phytoplankton grazing by Zooplankton process as simulated by SALMO-OO 31

3.2. Data Requirements and Study Sites 32

3.2.1. Data requirements for the SALMO-OO simulation library 32

3.2.2 Study sites 34

3.2.2.1 Bautzen reservoir, Germany 34

3.2.2.2 Lake Arendsee, Germany 34

3.2.2.3 Lake Roodeplaat, South Africa 35

3.2.2.4 Lake Hartbeespoort, South Africa 35

3.2.2.5 Lake Klipvoor, South Africa 36

3.2.2.6 Saidenbach reservoir, Germany 37

3.2.2.7 Lake Weida, Germany 38

3.2.2.8 Lake Stechlin, Germany 38

3.2.2.9 Lake Soyang, South Korea 39

3.2.3 A comparison of trophic states 39

3.3. Selection criteria for literature model evaluation 42

3.4. Initial "Testing Frameworks" for Model Analysis 43

3.4.1 Phytoplankton growth process models 43

3.4.2 Phytoplankton grazing process models 44

3.5. Description of alternative process models for phytoplankton growth and grazing dynamics 47

3.5.1 Phytoplankton growth process models 48

3.5.2 Phytoplankton grazing process models 51

3.6 Design and Implementation of the SALMO-OO simulation Library 53

3.6.1 Design of simulation library structure using the object-oriented paradigm 53

3.6.2 Implementation of the SALMO-OO simulation library 56

3.6.3 Selection criteria and assessment of the SALMO-OO simulation library performance 58

CHAPTER 4. RESULTS 60

4.1. Experimental Results from SALMO-OO and the simulation library for lakes with different environmental conditions 60

4.1.1 Eutrophic and hypereutrophic conditions 60

4.1.1.1 Bautzen reservoir, Germany 60

4.1.1.2 Lake Arendsee, Germany 66

4.1.1.3 Lake Roodeplaat, South Africa 72

4.1.1.4 Lake Hartbeespoort, South Africa 78

4.1.1.5 Lake Klipvoor, South Africa 84

4.1.2 Mesotrophic conditions 89

4.1.2.1 Saidenbach reservoir, Germany 89

4.1.2.2 Lake Weida, Germany 95

4.1.3 Oligotrophic conditions 100

4.1.3.1 Lake Stechlin, Germany 100

4.1.3.2 Lake Soyang, South Korea 106

4.2. Generic model structures for lakes with different environmental conditions 111

CHAPTER 5. DISCUSSION AND CONCLUSIONS 118

5.1. The SALMO-OO Simulation Library as a Tool for Ecosystem Analysis and Management 118

5.1.1. Outcomes of the experiments using the phytoplankton growth and grazing simulation library for lakes with different environmental conditions 118

5.1.2. The SALMO-OO simulation library as a validation tool 122

5.2. Generic models for the simulation of lake ecosystems 131

5.2.1. The benefits of the object-oriented paradigm for generic model development and implementation 134

5.3. Conclusions 136

APPENDIX A: Lists all phytoplankton growth and grazing parameter and function definitions for the original SALMO-OO model and the three alternative models from Arhonditsis and Brett (2005), Hongping and Jianyi (2002) and CLEANER. 138

APPENDIX B: Calibrated parameter values for the SALMO-OO simulation library 140

APPENDIX C: Java code for the AlgaeLibrary.class 141

APPENDIX D: Tabulated results of the statistical analysis for each water body investigated. 149

REFERENCES 155

Abstract

Over the past three decades numerous lake ecosystem models incorporating algal population dynamics have been developed and published. However, most of these models have been constructed, calibrated and validated *ad hoc* to suit one specific lake application. Even though many models, including SALMO (Benndorf and Recknagel, 1982; Recknagel and Benndorf, 1982), were designed and validated as being generic for a range of lake properties they were always rigid in their process equations and parameter values. This study discusses the concept, implementation and testing of SALMO-OO towards a more generic simulation library for lakes by taking advantage of object-oriented design and Java programming. A library of three phytoplankton growth and three grazing process models have been implemented in SALMO-OO, with the aim to increase the generality and flexibility of SALMO-OO for simulations of lakes with different trophic states and mixing conditions.

The initial focus was on phytoplankton models that were of the form of ordinary differential equations (ODEs) that displayed a similar model rationale to the original SALMO model. Three phytoplankton growth and three grazing models implemented in the full object-oriented version of the model (SALMO-OO) as a simulation library of alternative process models. Combinations of different growth and grazing functions were tested within the simulation library to find generic model structures for lakes with different trophic state and mixing conditions. The validation of the SALMO-OO simulation library was based on comparison between the simulation library experiments and the results produced by the original SALMO-OO growth and grazing functions for phytoplankton biomass, zooplankton biomass, phosphate concentration and algal functional groups abundances. Root-mean square error (RMSE) and r^2 values are given as a quantitative measure of fit between the measured data and the model outputs for each state variable.

The results demonstrate the ability of the SALMO-OO model to simulate a variety of trophic and mixing conditions for freshwater lakes using a generic approach, and the ability of the simulation library to improve the validation results for each lake simulated. Generic model structures were found for different categories of lakes based on trophic state (eu-/hyper-, meso- and oligotrophic) and mixing conditions (dimictic and warm monomictic). A key factor that has determined a particular generic model structure has been the realistic simulation of phytoplankton functional groups dynamics. By providing the simulation library as an additional validation toolbox this has improved the overall model performance to give more accurate and realistic results for phytoplankton dynamics. As a result, the SALMO-OO model is a more comprehensive decision support tool for lake and reservoir management, which can be used to support the ranking of management scenarios and to base decisions on understanding and expert knowledge.

Future research for the SALMO-OO simulation library includes the integration of a multiple parameter optimisation option based on evolutionary algorithms. This will calibrate parameter values within their range of variance to improve the accuracy of simulation results. It is concluded that the object-oriented implementation of ODE based ecosystem models significantly improves its knowledge base, functionality and accuracy.

Declaration

I declare that this work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text.

I give consent to this copy of my thesis, when deposited in the University Libraries, being made available in all forms of media, now or hereafter known.

Lydia T. Cetin

June, 2007

Acknowledgements

I would like to thank the following people for their guidance and contribution to my PhD project:

- The Environmental Biology Discipline staff and fellow postgraduate students. It's comforting to know that other people have experienced similar situation, good and bad, during their own postgraduate studies, and to have the ability to learn from them.
- To my principle supervisor, A/Proff. Friedrich Recknagel, who has instructed me well, and has guided me in becoming a better researcher and scientist. I thank him for his patience and mentoring throughout my four years as a PhD student. I am forever grateful for his encouragement, his belief in me to pull through and do well, and for allowing me to broaden my experiences in the world of academia.
- To Byron Zhang for his timely arrival into the Ecoinformatics and Watershed Ecology Group as a Master postgraduate during my second year of candidature. Byron developed the SALMO-OO modelling environment, and created a piece of software that I have used consistently throughout my PhD. Originally I intended to develop the model myself, but little did I know what was in store for me. Byron saved the day and produced an excellent software package, which enabled him to achieve his Masters degree. I enjoyed collaborating with Byron and I thank him for teaching me the finer points of object-oriented and Java programming and software design. Many thanks.
- To my fellow postgraduate colleagues, who have entertained and supported me during my time as a PhD student in the Ecoinformatics and Watershed Ecology Group: Young-Kil Kim, Grace Wai, Tumi Bjornsson, Huge Wilson, and a warm thank you to our postdoctoral fellow, Dr. Hongqing Cao, for being so friendly and handling everything with a smile.
- I would especially like to thank my fellow PhD office mates, Anita Talib and Amber Welk, for always providing friendship, mateship and for their moral support in the day to day happenings during all of our PhD years. These close friendships that are developed with fellow postgraduates are the key resource in surviving a PhD, and Anita and Amber made my time that much more enjoyable and rewarding.
- I would like to express my gratitude to my family and friends whom have had to endure my neuroses and stresses during my PhD, in particular to my Mum (Myrta Cetin), Rachel Howard, Nerissa Haby and Virginia Holt.
- Finally, I would like to thank the most important person in the world to me, my partner in life, Shaun Howard. If anyone needs an acknowledgement for living with and loving someone who is perusing a postgraduate degree it is the spouse/partner. Shaun has supported me in so many ways, and has sacrificed his own goals and interests to allow me to build a career. I am eternally grateful for all he has done for me; his commitment to my well being, his understanding and patience when times were stressful and finally for his encouragement for me to achieve all that I can.
  jIH Par'mach SoH.

Publications and Scientific Communications During Candidature

Conference Presentations

Cetin, L., Zhang, B. and F. Recknagel, 2005. *Process-based simulation library SALMO-OO for lake ecosystems. Proceedings of the International Congress on Modelling and Simulation MODSIM*, Melbourne, Australia, December 12-15, 2005 (2005).

Recknagel, F., Cetin, L. and Zhang, B. (2006). Process-based Simulation Library SALMO-OO for Lake Ecosystems Implemented by Object-oriented Programming. *Ecological Informatics* (submitted).

Peer reviewed papers

Cetin, L., Zhang, B. and F. Recknagel, 2005. *Process-based simulation library SALMO-OO for lake ecosystems. Proceedings of the International Congress on Modelling and Simulation MODSIM*, Melbourne, Australia, December 12-15, 2005 (2005).

Recknagel, F., Cetin, L. and Zhang, B. (2006). Process-based Simulation Library SALMO-OO for Lake Ecosystems Implemented by Object-oriented Programming. *Ecological Informatics* (submitted).

Cao, H., Recknagel, F., Cetin, L. and Zhang, B. (2006). Embodiment of the Process-based Simulation Library SALMO-OO for lake Ecosystems by Evolutionary Algorithms. *Ecological Informatics* (submitted).

Recknagel F., Van Ginkel C., Cao H., Cetin L. & Zhang B., H (2006) Generic Limnological Models on the Touchstone: Testing the Lake Simulation library SALMO-OO and the rule-based Microcystis Agent for warm-monomictic hypertrophic lakes in South Africa. *Ecological Modelling* (submitted).

List of Tables

Table 2.1. Commonly used mathematical functions for the description of the phytoplankton photosynthetic rate dependence on light intensity. Graphs are shown only to give a general idea of the shape of each function, which defines the behaviour of the PI-curve. 8

Table 3.1. List of parameter values, definitions and units specific to the SALMO-OO phytoplankton growth and grazing process models. 33

Table 3.2. List of parameter definitions, units and values used in the SALMO-OO simulation library, in addition to the overall SALMO-OO model. 33

Table 3.3. Key morphological data and trophic status of the data sets used to develop and validate the SALMO-OO simulation library. 37

Table 3.4. German lake classification standard (Ryding & Rast, 1989). 40

Table 3.5. OCED lake classification standard (Vollenweider & Kerekes, 1982). 40

Table 3.6. Trophic levels according to (Forsberg & Ryding, 1980). 40

Table 3.7. Trophic State Index (TSI) according to Carlson (1977). 40

Table 3.8. Trophic state classification of the study sites used to test the SALMO-OO simulation library according to four different indices. 41

Table 4.1. Summary of generic model structures found by the SALMO-OO simulation library for different categories of lakes and reservoirs based on trophic state and mixing conditions. 111

Table 5.1. Summary of generic model structures found by the SALMO-OO simulation library for different categories of lakes and reservoirs based on trophic state and mixing conditions. 119

Table 5.2. List of various modellers/author's that have elected to use either the multiplicative or minimum function for the calculation of gross phytoplankton photosynthesis rate. 121

List of Figures

Figure 2.1. Different mathematical functions for temperature-limited phytoplankton growth, such as (a) linear, (b) optimal and (c) exponential functions. Example equations, which give the shape of the corresponding graphs, are also given. 13

Figure 2.2. Lagramge automated modelling framework based on the integration of domain-specific modeling knowledge in the process of equation discovery (Atanasova *et al.*, 2006). 14

Figure 2.3. An example of the object-oriented paradigm applied to a simple primary production model. 18

Figure 2.4. A key difference between object-oriented programming and the conventional programming approach is through encapsulation (Khebbal & Shamhong, 1995). 20

Figure 2.5. Hierarchical structure of two object-oriented dynamic aquatic models. 25

Figure 3.1. Model structure diagram of SALMO-OO illustrating all the state variables and key processes simulated by the model. 27

Figure 3.2. Bautzen reservoir linearly interpolated measured data for — phosphate concentration, — phytoplankton and — zooplankton biomasses. X-axis is in Julian days. 34

Figure 3.3. Lake Arendsee linearly interpolated measured data for — phosphate concentration and — phytoplankton biomass. X-axis is in Julian days. 35

Figure 3.4. Lake Roodeplaat linearly interpolated measured data for — phosphate concentration and — phytoplankton biomass. X-axis is in Julian days. 35

Figure 3.5. Lake Hartbeesooprt linearly interpolated measured data for — phosphate concentration and — phytoplankton biomass. X-axis is in Julian days. 36

Figure 3.6. Lake Klipvoor linearly interpolated measured data for — phosphate concentration; — phytoplankton biomass; — blue-green algae; — green algae and — diatoms. X-axis is in Julian days. 36

Figure 3.7. Saidenbach reservoir linearly interpolated measured data for — phosphate concentration, — phytoplankton and — zooplankton biomasses. X-axis is in Julian days. 37

Figure 3.8. Lake Weida linearly interpolated measured data for — phosphate concentration, — phytoplankton and — zooplankton biomasses. X-axis is in Julian days. 38

Figure 3.9. Lake Stechlin linearly interpolated measured data for — phosphate concentration, — phytoplankton and — zooplankton biomasses. X-axis is in Julian days. 38

Figure 3.10. Lake Soyang linearly interpolated measured data for — phosphate concentration and — phytoplankton biomass. X-axis is in Julian days. 39

Figure 3.11. Flow chart illustrating criteria for the selection of literature models to be included in the SALMO-OO simulation library. 42

Figure 3.12. Testing framework structure using STELLA software for alternative phytoplankton growth models. 45

Figure 3.13. Testing framework structure using STELLA software for alternative phytoplankton grazing models. 46

Figure 3.14. UML class diagram for the model components of SALMO-OO and the simulation library (`AlgaeLibrary`) (Zhang, 2006). 53

Figure 3.15. An example of the Java code for the growth method from Hongping and Jianyi (2002). Replacement of growth limiting functions, photosynthesis and respiration calculations can be made to customise for other growth models. 55

Figure 3.16. An example of the Java code for the grazing method from Hongping and Jianyi (2002). Replacement of phytoplankton grazing and detritus grazing functions can be made to customise for other growth models. 56

Figure 3.17. Graphical user interface (GUI) for the SALMO-OO simulation library. 57

Figure 3.18. Visual output of simulation results within the SALMO-OO application of each state variable and the measured data. 57

Figure 3.19. Selection criteria and assessment procedures for analyses of alternative growth and/or grazing model structures to improve the validation of the SALMO-OO model. 59

Figure 4.1a. Bautzen Reservoir (1978) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 63

Figure 4.1b. Bautzen Reservoir (1978) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 64

Figure 4.1c. Bautzen Reservoir (1978) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 65

Figure 4.2a. Lake Arendsee (1979) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 69

Figure 4.2b. Lake Arendsee (1979) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 70

Figure 4.2c. Lake Arendsee (1979) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 71

Figure 4.3a. Lake Roodeplaat (2003) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 75

Figure 4.3b. Lake Roodeplaat (2003) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 76

Figure 4.3c. Lake Roodeplaat (2003) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 77

Figure 4.4a. Lake Hartbeespoort (2003) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 81

Figure 4.4b. Lake Hartbeespoort (2003) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 82

Figure 4.4c. Lake Hartbeespoort (2003) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 83

Figure 4.5a. Lake Klipvoor (2003) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 86

Figure 4.5b. Lake Klipvoor (2003) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 87

Figure 4.5c. Lake Klipvoor (2003) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 88

Figure 4.6a. Saidenbach Reservoir (1975) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 92

Figure 4.6b. Saidenbach Reservoir (1975) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 93

Figure 4.6c. Saidenbach Reservoir (1975) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 94

Figure 4.7a. Lake Weida (1984) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 97

Figure 4.7b. Lake Weida (1984) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 98

Figure 4.7c. Lake Weida (1984) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 99

Figure 4.8a. Lake Stechlin (1975) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 103

Figure 4.8b. Lake Stechlin (1975) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 104

Figure 4.8c. Lake Stechlin (1975) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 105

Figure 4.9a. Lake Soyang (1998) simulation results from the SALMO-OO model and alternative phytoplankton growth process models from the simulation library. 108

Figure 4.9b. Lake Soyang (1998) simulation results from the SALMO-OO model and alternative phytoplankton grazing process models from the simulation library. 109

Figure 4.9c. Lake Soyang (1998) simulation results from combinations of alternative growth and grazing process models from the SALMO-OO simulation library. 110

Figure 4.10. The best combination model results for (a) Bautzen reservoir and (b) Lake Arendsee produced by the SALMO-OO simulation library for eutrophic/hypertrophic, dimictic water bodies. Comparisons are made with the simulations from the SALMO-OO model without any changes to the growth or grazing process equations. 112

Figure 4.11. The best combination model results for (a) Lake Roodeplaat, (b) Lake Hartbeespoort and (c) Lake Klipvoor produced by the SALMO-OO simulation library for eutrophic/hypertrophic, monomictic water bodies. Comparisons are made with the simulations from the SALMO-OO model without any changes to the growth or grazing process equations. 115

Figure 4.12. The best combination model results for (a) Saidenbach reservoir and (b) Lake Weida produced by the SALMO-OO simulation library for mesotrophic, dimictic water bodies. Comparisons are made with the simulations from the SALMO-OO model without any changes to the growth or grazing process equations. 116

Figure 4.13. The best combination model results for (a) Lake Stechlin and (b) Lake Soyang produced by the SALMO-OO simulation library for oligotrophic, dimictic water bodies. Comparisons are made with the simulations from the SALMO-OO model without any changes to the growth or grazing process equations. 117

Figure 5.1. Selection criteria and assessment procedures for analyses of alternative growth and/or grazing model structures to improve the validation of the SALMO-OO model. 123

Figure 5.2. SALMO-OO simulation library results for Bautzen Reservoir and Lake Stechlin. Comparisons are made with the simulations from the SALMO-OO model without any changes to the growth or grazing process equations. 124