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Limno-physikalische Modellierung möglicher Folgen des Klimawandels für den Ammersee auf Basis regionaler Klimamodelldaten

vorgelegt von
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Vorwort und Danksagung

Hier möchte ich allen sehr herzlich danken, die mich von Beginn der Forschungsarbeit an bis zur Fertigstellung dieser Dissertation unterstützt haben. Die Arbeit entstand im Rahmen des Forschungsprojekts LAGO (Limnologische Auswirkungen des Globalen Wandels in Oberbayern), welches hauptsächlich vom Bayerischen Landesamt für Umwelt (LfU) finanziert wird. Für diese Förderung danke ich sehr, da sie entscheidend zum Erhalt der guten Arbeitsbedingungen beitrug. Das Projekt ist am Lehrstuhl für Geographie und Landschaftsökologie des Departments für Geographie der LMU München angesiedelt.

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Kurzzusammenfassung

Der klimawandelbedingte Anstieg der Lufttemperaturen und die daraus resultierende Erwärmung der Wassertemperatur an der Oberfläche von Seen beeinflussen sowohl die physikalischen, als auch die biologischen und chemischen Prozesse im Gewässer. Durch hydrodynamische Modellierung in Verbindung mit regionalen Klimamodellen ist es möglich, diese zukünftigen Einflüsse abzuschätzen. Die vorliegende Studie beleuchtet limno-physikalische Veränderungen am peri-Alpinen, 83 m tiefen und momentan dimiktischen Ammersee, ca. 30 km südwestlich von München gelegen. Ziel soll dabei sein, einerseits die Sensibilität von Seen gegenüber einem sich verändernden Klima zu unterstreichen und andererseits eine umfangreiche Grundlage zur weitergehenden limnologischen Forschung zu schaffen.

Den ersten zeitlichen Abschnitt dieses Promotionsvorhabens bildete die Kalibrierung und Validierung des hydrodynamischen Modells DYRESM, um die vertikale Verteilung der Temperatur in der Wassersäule zu simulieren. Des Weiteren wurden meteorologische Daten aus dem regionalen Klimamodell REMO biaskorrigiert und aufbereitet, um darauf basierend eine Modellierung der zukünftigen Periode 2041-2050 zu ermöglichen. Das verwendete IPCC A1B-Emissionsszenario, welches in Zukunft von einer ausgeglichenen Nutzung aller verfügbaren Ressourcen auf der Erde ausgeht, simuliert einen Anstieg der globalen Luftmitteltemperatur um etwa 3 Kelvin (K) bis zum Jahr 2100. Zur sorgfältigen Kalibrierung und Validierung des Modells DYRESM wurden die Zeiträume 2004-2007 sowie 1993-1999 gewählt. Dabei traten während der Kalibrierung, beim Vergleich der modellierten Temperaturen in der Wassersäule mit Felddaten, lediglich geringe Fehlerwerte auf. Der MAE (Mean Absolute Error) lag zwischen 0,96 und 1,61 K, der RMSE (Root Mean Square Error) zwischen 1,42 und 1,96 K und das Bestimmtheitsmaß (R^2) unter Berücksichtigung sämtlicher Wassertiefen zwischen 0,71 und 0,96.

Die anschließende Ableitung limno-physikalischer Variablen für die Periode 2041-2050 am Ammersee zeigt eine Erhöhung des Wärmeinhalts in den oberen 3 m des Epilimnions von Ende März bis Mitte November. Bezüglich des Gesamtwärmeinhalts ist dagegen von Januar bis Dezember eine Abnahme gegenüber 1997-2007 zu erwarten. Dies hängt mit der thermischen Stabilität des Sees zusammen, die laut Modell im Vergleich zum Zeitraum 1985-2007 zunehmen wird, wobei auch ein früherer Beginn und eine längere Dauer der sommerlichen, thermischen Schichtung zu erwarten sind. Nach Ableitung der mittleren Tiefe der Thermokline prognostiziert DYRESM von Mai bis Juni eine Abnahme gegenüber der Tiefe der Vergangenheit, wogegen die mittlere Tiefe im Zeitraum Anfang August bis Oktober zunehmen soll. Außerdem führte die Modellierung zu einer zukünftigen Zunahme der mittleren Mächtigkeit des Metalimnions zwischen Mai und Oktober.

Um den Prozess der hydrodynamischen Modellierung und der Ableitung limno-physikalischer Verhältnisse in der Zukunft unter Verwendung des regionalen Klimamodells REMO zu vereinfachen und zu beschleunigen, erfolgte im Rahmen dieser Dissertation darüber hinaus die Entwicklung eines Workflows auf Basis automatisierter IT-Tools. Somit ist es möglich, bei der Modellierung unterschiedlicher Untersuchungsgebiete, welche häufig deutliche geomorphologische, klimatische und landnutzungsbedingte Unterschiede aufweisen, die Wiederholung zeitraubender Arbeitsschritte zu vermeiden. Eines dieser Tools ist ein Linux Shell Script, welches zur automatisierten Konvertierung und Anpassung der REMO-Daten nach dem Download dient. Des Weiteren wurde ein Makro in Visual Basic for Applications (VBA) entwickelt, welches die meteorologischen Eingangsdaten für das hydrodynamische Modell DYRESM zusammenstellt und aufbereitet. Die automatisierte Berechnung der zur Modellierung notwendigen Volumen der verschiedenen horizontalen Wasserschichten erfolgte an Hand einer GIS (Geographisches Informationssystem)-Analyse auf Basis bathymetrischer Daten.

Hierzu wurde Esri ArcGIS zusammen mit den Erweiterungen 3D-Analyst und Spatial Analyst sowie der graphischen Programmieroberfläche ModelBuilder angewandt. Darüber hinaus wurden verschiedene weitere VBA-Makros entwickelt, um im Anschluss der Modellierung die limno-physikalischen Variablen im Gewässer automatisiert ableiten zu können.

Zusammenfassend betrachtet bietet die hydrodynamische Modellierung unter Verwendung von Eingangsdaten eines regionalen Klimamodells eine umfassende Basis, um die zukünftigen Herausforderungen in der Seenmodellierung zu bestehen. Dieser Modellierungsansatz ist in der Lage, mögliche limno-physikalische Auswirkungen des Klimawandels auf Seen zu simulieren und somit entscheidend zur weitergehenden erfolgreichen Forschung an Seeökosystemen beizutragen. Zu guter Letzt ist es auch in Zukunft wichtig, in der Community auf dem aktuellen Stand der Forschung automatisierte IT-Tools zu entwickeln, um Modellierungsansätze wie den vorliegenden weiter zu vereinfachen und zu verbessern und wertvolle Zeit einzusparen.

Summary

Climate change-derived higher air temperatures and the resulting increase in lake surface temperatures are known to influence the physical, biological and chemical processes of water bodies. By using hydrodynamic lake models coupled with regional climate models, the potential future impact of a changing climate can be investigated. The present study hence elucidates limno-physical changes at the peri-Alpine, 83-m deep, currently dimictic Ammersee in southeastern Germany, both to underline the role of lakes as sentinels of climate change and provide a sound basis for further limnological investigations.

The first step of this dissertation was to calibrate and validate the model DYRESM in order to simulate the vertical thermal distribution in Lake Ammersee and to prepare bias-corrected meteorological data from the model REMO to establish a hydrodynamic simulation run for the period 2041-2050. The IPCC A1B emission scenario, which assumes a balanced use of all available energy sources in the world, predicts the global mean temperature to increase by about 3 Kelvin from 1990 to the year 2100. To calibrate and validate the model DYRESM carefully, date from 2004–2007 and 1993–1999 was used. When comparing simulated and measured water temperatures regarding the calibration period, small mean absolute errors (0.96 K–1.61 K) and root mean square errors (1.42 K–1.96 K) were observed, as well as high coefficients of determination (0.71–0.96) at all depths.

In a second step, modelling of future heat content resulted in a projected increase of heat content in the upper 3 m of the epilimnion from end of March to mid-November, whereas a decrease in future total heat content (January-December) of the entire water column was simulated compared to that observed in 1997-2007. Lake thermal stability is projected to be higher in the period 2041-2050 than in 1985-2007. Stratification is expected to occur earlier and to last longer in the future than the pattern observed in the years 1985-2007. The future mean May-June depth of the thermocline is simulated to be situated above its past average vertical position, whereas an increase of mean thermocline depth is projected for the beginning of August to October. Furthermore, the mean May-October thickness of the metalimnion is simulated to increase.

As a last step, a workflow was developed, supported by information technology (IT), to facilitate and accelerate the use of results of the regional climate model REMO as input data for hydrodynamic lake models and the simulation of limnological conditions in the future. In this way, we can avoid repeating time-consuming steps when investigating the impact of climate change on different lakes and their catchment area, which are regionally different, owing to morphometric, climatologic and land-use conditions, etc. We created an application (Linux Shell script) to convert and customise REMO data automatically and provide a macro in Visual Basic for Applications (VBA) to assemble and pre-process the meteorological input data for the hydrodynamic model DYRESM. An automated, geographic information system (GIS)-based analysis was included to calculate the volumes of different horizontal layers on the basis of bathymetric lake data, using Esri ArcGIS together with the 3D Analyst and Spatial Analyst extensions and the visual coding language ModelBuilder. Finally, we generated auxiliary routines in VBA to deduce the limno-physical criteria of a lake.

In conclusion, the elucidation of physical changes at Ammersee by means of a regional climate model provides a sound basis on which to face the new challenges of ecological lake modelling. The hydrodynamic model can be used to identify potential drawbacks of climate change (e.g. extended duration of stratification, higher thermal stability, lack of mixing) on the lake ecosystem by higher water temperatures. Also it should be a future objective to develop additional automated tools, considering the particular state of the art. In this way, it is possible to simplify modelling within the community and to go on improving and accelerating integrated model approaches.

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1. Erweiterte Zusammenfassung

1.1 Einleitung

Untersuchungen zur Bestimmung, Sicherung und Verbesserung der Wasserqualität von stehenden Oberflächengewässern im Klimawandel und der damit verbundene Gewässerschutz stellen heute und in Zukunft ein äußerst wichtiges Forschungsfeld dar. Dies wurde bereits im Jahr 2008 in einem Technical Paper des Intergovernmental Panel on Climate Change (IPCC) festgehalten: „Observational records and climate projections provide abundant evidence that freshwater resources are vulnerable and have the potential to be strongly impacted by climate change, with wide-ranging consequences for human societies and ecosystems." (Bates et al., 2008). Vor dem Hintergrund dieser Tatsachen soll im Rahmen der vorliegenden Dissertation ein Beitrag dazu geleistet werden, auf dem neuesten Stand der Forschung den Einfluss des Klimawandels auf die physikalischen, chemischen und biologischen Eigenschaften von Seen abzuschätzen. Hierzu werden Methoden der hydrodynamischen Modellierung in stehenden Gewässern angewandt. Somit ist es möglich, Veränderungen der thermischen Struktur sowie des Wärmehaushalts der Gewässer zu simulieren, was wiederum als wichtige Grundlage zur weitergehenden ökologischen Modellierung aquatischer Systeme dient.
Der starke Einfluss eines klimawandelbedingten Anstiegs der Lufttemperatur auf die Wassertemperaturen von Seen (Livingstone, 2003; Adrian et al., 2009; Williamson et al., 2009; Ludovisi and Gaino, 2010; Schneider and Hook, 2010; Dokulil, 2013) wurde bereits in verschiedenen Studien aufgezeigt. Daraus resultiert eine Erwärmung der oberen Wasserschichten, die wiederum deutliche Veränderungen der limno-physikalischen Eigenschaften des Gewässers zur Folge hat (Gaiser et al., 2009; Ambrosetti et al., 2010; Rempfer et al., 2010; Hadley et al., 2013). Diese Veränderungen wurden sowohl für Durchmischungsprozesse und Schichtungsverhalten (Danis et al., 2004; Ambrosetti and Barbanti, 2005; Austin and Colman, 2008; MacIntyre et al., 2009; Rimmer et al., 2011) als auch für den Wärmeinhalt (Hondzo and Stefan, 1993; Dokulil et al., 2006; Vetter and Sousa, 2012) nachgewiesen. Besonders wichtig ist die Untersuchung eben genannter limno-physikalischer Variablen vor dem Hintergrund, dass sie nahezu alle biologischen und chemischen Prozesse im Seeökosystem direkt beeinflussen. Auch hierzu existieren umfangreiche Studien aus den letzten Jahren, beispielsweise zu klimabedingten möglichen Veränderungen von Trophie und Artenspektrum (Kirilova et al., 2009; Wagner and Adrian, 2009; Rinke et al., 2010; Gallina et al., 2011) sowie zur Beeinflussung der Verteilung von Nährstoffen oder Sauerstoff im Gewässer (Rempfer et al., 2010; Vetter and Sousa, 2012; Riverson et al., 2013).
Um zu einem besseren Verständnis eben genannter physikalischer, biologischer und chemischer Prozesse im aquatischen Ökosystem beizutragen, ist es dringend notwendig, bisherige Felduntersuchungen und statistische Auswertungen historischer Messdaten (Peeters et al., 2002) durch hydrodynamische und ökologische Modelle zu ergänzen (Huber et al., 2008; Fang and Stefan, 2009; Trolle et al., 2012). Diese Modelle sind in der Lage, den zukünftigen Einfluss eines sich verändernden Klimas auf Seeökosysteme und die Wasserqualität zu simulieren (Perroud et al., 2009). Somit stellen entsprechende Modellierungsstudien ein aktuelles, umfangreiches Gebiet der hydrologischen Forschung dar. Allerdings existieren noch deutliche Wissenslücken in der Modellierung konkreter Klimawandelauswirkungen auf Seen (Bates et al., 2008; Huang et al. 2010; Dibike et al., 2011), die es im Rahmen weiterer, umfassender Forschungsarbeiten zu schließen gilt (MacKay et al., 2009). Besonders relevant ist hierbei die Nutzung simulierter Daten regionaler Klimamodelle wie beispielsweise REMO (Jacob et al., 2007; Teichmann et al., 2013), welche auf Basis verschiedener IPCC Emissions-Szenarien (Nakicenovic et al., 2000; Solomon et al., 2007) für die Zukunft erstellt und in der Vergangenheit kaum als Eingangsdaten bei der Seenmodellierung verwendet wurden. Diese Klimamodelle sind eine sehr gute Möglichkeit,

zufriedenstellende Prognosen zukünftiger Klimaveränderungen als Antrieb hydrodynamischer Modelle zu erhalten (Samuelsson, 2010).
Die grundlegenden Ziele dieses Promotionsvorhabens sind somit (1) die Kalibrierung und Validierung des eindimensionalen hydrodynamischen Modells DYRESM, (2) die Nutzung und Anpassung simulierter meteorologischer Eingangsvariablen aus dem regionalen Klimamodell REMO zur Modellierung der möglichen zukünftigen, vertikalen Temperaturverteilung im Gewässer, (3) die Ableitung limno-physikalischer Werte für Vergangenheit und Zukunft zur Identifikation möglicher klimawandelbedingter Veränderungen sowie (4) die Entwicklung eines automatisierten IT-Workflows, um den Modellierungsprozess zu verbessern und zu beschleunigen und den Modellierungsansatz innerhalb der Community auf weitere Gewässer übertragen zu können.
Als Untersuchungsgebiet dieser Studie dient der voralpine, 83 Meter tiefe und momentan dimiktische Ammersee, welcher 30 km südwestlich von München liegt (Abbildung 1). Ein wichtiges Auswahlkriterium war hierbei, dass der Ammersee bezüglich seines geogenen, klimageographischen und limnologischen Charakters als repräsentativ für viele andere Seen im nördlichen Alpenvorland angesehen werden kann. Mit einer Ausdehnung von 46,6 km² und einem Wasservolumen von 1.750 Mio. m³ ist der glazialmorphologisch geprägte Ammersee der flächenmäßig drittgrößte See in Bayern (Nixdorf et al., 2004).

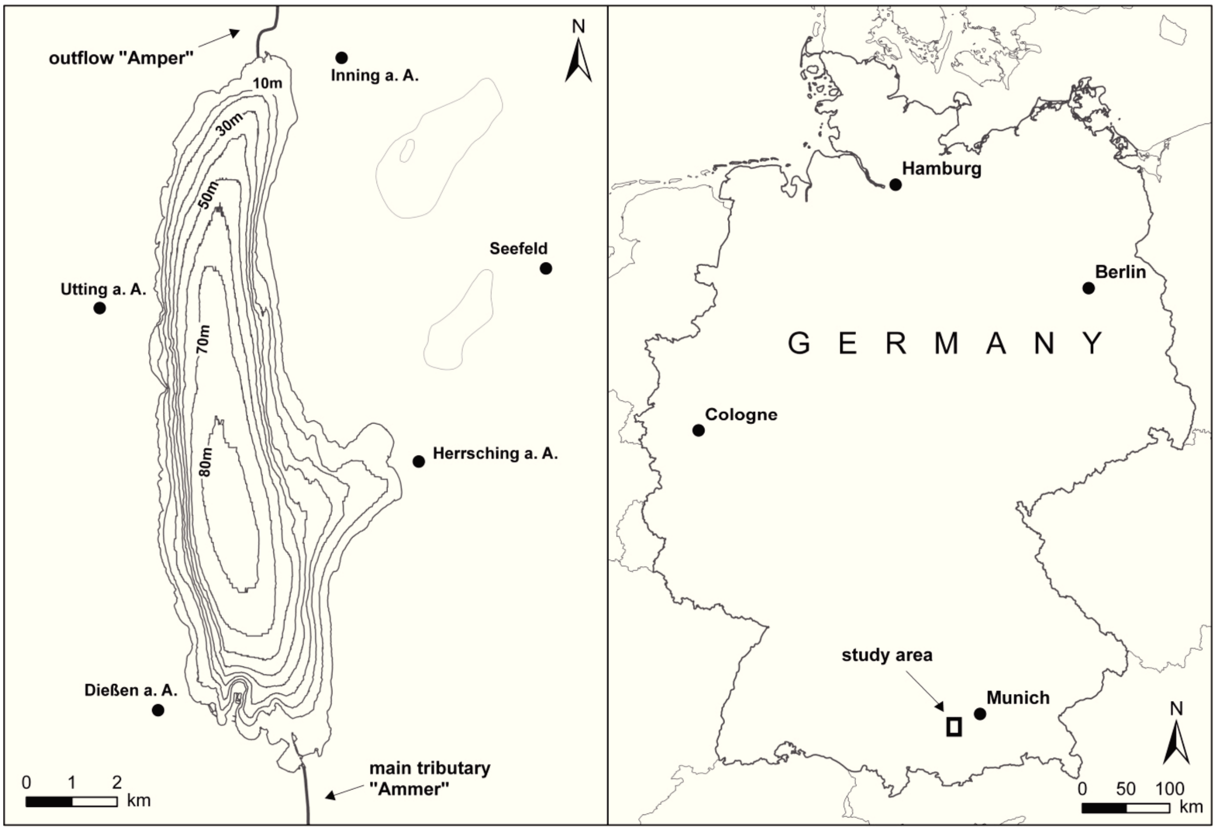

Abbildung 1: Darstellung des Untersuchungsgebietes am Ammersee (Weinberger and Vetter, 2012).

Der Hauptzufluss des Sees ist die Ammer, drei weitere kleinere Zuflüsse sind Windach, Rott und Kienbach. Der Abfluss des Sees erfolgt durch den Fluss Amper. Durch seine Nähe zur Metropole München ist der See besonders für den regionalen Tourismus von Bedeutung und auch Fischerei wird betrieben. Auf Grund seines natürlichen Zustandes wäre der Ammersee oligotroph (Kucklentz, 2001; Vetter and Sousa, 2012), doch aus der intensiven Landnutzung im Einzugsgebiet, welche um das Jahr 1950 einsetzte, resultierte ein mesotropher Zustand. In den letzten 20 Jahren allerdings, nach speziellen Kanalisierungsmaßnahmen, unterlag der See einer Re-Oligotrophierung (Ernst et al., 2009). Aktuelle Studien im Untersuchungsgebiet überprüfen momentan, in welchem Maße die im See erkennbaren Anzeichen eines Klimawandels diesen Trend beeinflussen könnten (Vetter und Sousa, 2012). Zu möglichen limno-physikalischen und daraus resultierenden ökologischen Konsequenzen als Folge anthropogener und klimatischer Einflüsse am Ammersee gab es bereits in der Vergangenheit Einschätzungen. Danis et al. (2004) prognostizierten dabei auf Basis ihrer Modellierungsstudie ein langanhaltendes Aussetzen der Durchmischung des Gewässers, beginnend um das Jahr 2020; dies würde zu einer Beeinträchtigung der Sauerstoffverteilung im Gewässer führen und die Fauna der tieferen Gewässerschichten irreversibel zerstören. Zuvor hatten Joehnk and Umlauf (2001) auf die Wichtigkeit von Modellierungsstudien am Ammersee hingewiesen. Eine solche Studie wurde von Brey (2013) vorgelegt, der im Rahmen seiner Dissertation an der LMU München ein hybrides Modell auf Basis des einfachen Zusammenhangs zwischen Lufttemperatur und Wasseroberflächentemperatur entwickeln und dieses auch unter Verwendung von REMO-Daten testen konnte. Dabei standen allerdings der methodische Aspekt der Modellgenerierung und technische Aspekte, wie das Data Mining und Machine Learning, im Vordergrund. Neben den Veröffentlichungen der vorliegenden kumulativen Promotion und der bereits genannten Studie von Vetter and Sousa (2012) wurde im LAGO-Projekt der LMU darüber hinaus auch zur Sensitivität klimatischer Modell-Eingangsdaten geforscht (Bueche and Vetter, 2014).

1.2 Modelle, Daten, Variablen und Parameter

1.2.1 Hydrodynamisches Modell DYRESM

Das eindimensionale hydrodynamische Modell DYRESM (DYnamic REservoir **S**imulation Model, Version v4.0.0-b2) wurde vom Centre for Water Research (CWR) an der University of Western Australia entwickelt, um die vertikale Verteilung von Temperatur, Salinität und Dichte in natürlichen Seen und Trinkwasserspeichern zu untersuchen. Es handelt sich um ein prozessbasiertes Modell mit einem sogenannten „Lagrangian layer scheme“. Dies bedeutet, dass im Modell horizontale Schichten übereinander liegen, deren Grenzen vom Nutzer selbst definiert werden. Diese Schichten werden dann während des Modellierungsprozesses auf Basis der berechneten Dichte des Wassers dynamisch angepasst, vereinigt oder geteilt (Imberger and Patterson, 1981; Antenucci and Horn, 2002). Eine Durchmischung der Schichten im Modell tritt auf sobald die kinetische Energie, welche durch Windeinfluss produziert wird, in der obersten Schicht der Wassersäule einen bestimmten Schwellenwert überschreitet. DYRESM wurde bereits in einer Vielzahl internationaler Studien erfolgreich angewendet (Han et al., 2000; Gal et al., 2003; Romero et al., 2004; Rinke et al., 2010; Trolle et al., 2011; Bayer et al., 2013). Hierbei schneidet das Modell im Vergleich zu anderen eindimensionalen Seemodellen besonders in Bezug auf seine Eignung zur Simulation längerer Zeiträume sowie in Bezug auf die Reproduktion der Variabilität von Wassertemperaturprofilen und der saisonalen Thermokline gut ab (Perroud et al., 2009). DYRESM kann darüber hinaus auch mit einem seeökologischen Modell, z.B. CAEDYM, gekoppelt werden, um biologische und chemische Prozesse im Gewässer abzubilden.
Zur Initialisierung des Simulationsprozesses benötigt DYRESM verschiedene Eingangsdaten. Diese werden vom Anwender in der meteorologischen (.met) und morphometrischen (.stg) Eingangsdatei sowie der hydrologischen Zufluss- (.inf) und Abfluss- (.wdr) Datei bereitgestellt. Darüber hinaus fließt die vertikale Verteilung von Temperatur und Salinität im See zu Beginn der Modellierung durch die Initialprofil-Datei (.pro) mit ein. Sämtliche spezifische Modellparameter, welche einen direkten Einfluss auf die komplexen Prozesse im Gewässer

haben und während der Kalibrierung des Modells als Stellschrauben vom Nutzer angepasst werden können, sind in der Parameterdatei (.par) und der Konfigurationsdatei (.cfg) organisiert. Abbildung 2 ermöglicht einen schematischen Überblick über die Datenstruktur und den Modellierungsprozess des hydrodynamischen Modells.

Von großer Bedeutung ist, dass die meteorologischen Bedingungen im Untersuchungsgebiet die dynamischen Prozesse im See, z.B. das Wassertemperaturprofil sowie Durchmischungsprozesse, direkt beeinflussen. Daher sind zur erfolgreichen hydrodynamischen Simulation sechs meteorologische Eingangsvariablen notwendig, welche in der oben erwähnten meteorologischen Eingangsdatei (.met) organisiert sind. Dies sind kurzwellige Sonneneinstrahlung (W/m²), Wolkenbedeckungsgrad (Okta), Lufttemperatur (°C), Sättigungsdampfdruck (hPa), Windgeschwindigkeit (m/s) und Niederschlag (m). Die ebenfalls benötigte langwellige Sonneneinstrahlung wird von einem im Modell integrierten Programmcode automatisch auf Basis des Wolkenbedeckungsgrades abgeschätzt (Imerito, 2007). Sämtliche meteorologischen Eingangsdaten zur Kalibrierung und Validierung des Modells wurden von der Station Raisting-Wielenbach des Deutschen Wetterdienstes (DWD) sowie der privat betriebenen Messstation Diessen-Obermühlhausen bereitgestellt, wobei die Daten der privaten Station durch eine Korrelationsanalyse mit Messdaten des DWD plausibilisiert wurden.

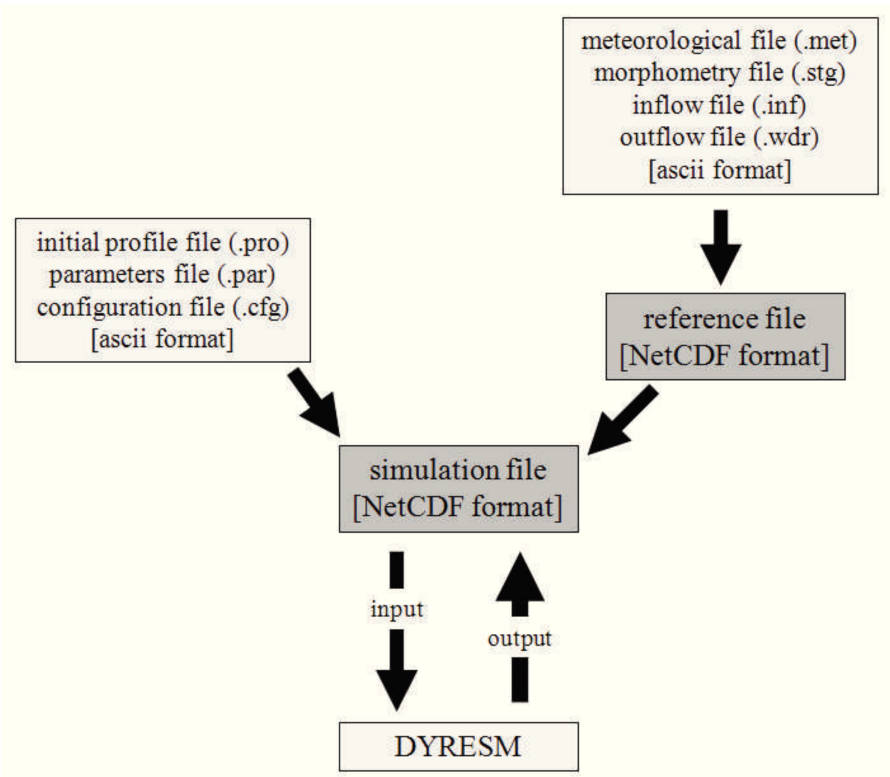

Abbildung 2: Modellierungsprozess des eindimensionalen hydrodynamischen Modells DYRESM (Antenucci and Imerito, 2003).

Der Sättigungsdampfdruck wurde auf Basis der Lufttemperatur und Luftfeuchte an der DWD-Messstation Raisting-Wielenbach mit der sogenannten Magnus-Formel berechnet (Zmarsky et al., 2007).

Die morphometrische Eingangsdatei (.stg) beinhaltet neben der Bathymetrie des Sees, genauer gesagt den Volumina (m³) der einzelnen horizontalen Schichten, außerdem Informationen zur geographischen Lage des Gewässers sowie zu relevanten Zu- und Abflüssen. Die täglichen Durchflussmengen dieser Fließgewässer sind in der hydrologischen

Zufluss- (.inf) und Abfluss- (.wdr) Datei organisiert. Darüber hinaus stellt man in der Zufluss-Datei tägliche Mittelwerte zu Wassertemperatur (°C) und Salinität des Zuflusses (PSS) bereit. Die hydrologischen Daten am Ammersee wurden vom Bayerischen Landesamt für Umwelt (LfU) erhoben. Die Durchflusswerte der Ammer wurden am Pegel Fischen gemessen, die Durchflusswerte der Amper am Pegel Stegen. Allerdings war es notwendig, eine Wasserhaushaltsanalyse durchzuführen (Baumgartner und Liebscher 1996). Dabei wurde im Durchschnitt ein tägliches Defizit von 20.180 m³ im Zeitraum 1975-2007 ermittelt und auf die täglichen Durchflusswerte der Ammer summiert. Erst durch diese Korrektur konnte ein stabiler Modellierungsprozess gewährleistet werden, da der See ansonsten in der Simulation über- oder ausläuft und DYRESM die Simulation abbricht.
In der Initialprofil-Datei (.pro) werden, wie bereits oben erwähnt, Temperatur und Salinität in verschiedenen Tiefen der Wassersäule zum Zeitpunkt des Starts der Simulation eingegeben. Im Rahmen der vorliegenden Modellierungsstudie am Ammersee wurde dies für 16 verschiedene Tiefen realisiert, um die thermischen Verhältnisse gut abzubilden. Die Wassersäule an der tiefsten Stelle des Gewässers steht in eindimensionalen Modellierungsansätzen repräsentativ für den gesamten See. Die Daten zur Erstellung des vertikalen Initialprofils wurden von der Bayerischen Wasserwirtschaftsverwaltung (WWV) und vorübergehend von einer projekteigenen Messstation an der tiefsten Stelle des Sees bereitgestellt.
Neben den zur Modellierung notwendigen Eingangsvariablen werden zur hydrodynamischen Simulation mit DYRESM grundlegende spezifische Modellparameter benötigt. Diese werden in der Parameterdatei (.par) und der Konfigurationsdatei (.cfg) definiert. In der Konfigurationsdatei des Modells werden neben Startdatum, Dauer und Output-Intervall der Modellierung auch spezielle Konfigurationsparameter festgelegt. Diese umfassen zum Beispiel die Tiefe (m) sämtlicher Ober- und Untergrenzen der vom Anwender zu definierenden, horizontalen Schichten sowie den „light extinction coefficient (m^{-1})“, welcher bestimmt, in welcher Weise die Sonnenstrahlung vom Wasser des Sees absorbiert und in thermische Energie umgewandelt wird und somit die Wassertemperatur des Epilimnions direkt beeinflusst (Imberger and Patterson, 1981). In der Parameterdatei befinden sich Parameter, die einen direkten Einfluss auf limno-physikalische Modellprozesse, wie etwa vertikale Durchmischung oder Wärmeflüsse im See, haben. Dazu zählen beispielsweise die „mean albedo of water“, welche beeinflusst, wie viel kurzwellige Strahlung direkt in den Wasserkörper eintritt, und der „critical wind speed (m/s)“, bei dessen Überschreitung der Modellalgorithmus zur Durchmischung aktiviert wird. Eine Beschreibung sämtlicher spezifischer Modellparameter sowie die Darstellung der Parameter- und Konfigurationsdateien von DYRESM ist dem im Rahmen dieser Kumulativpromotion erstellten Fachartikel von Weinberger and Vetter (2012) (Publikation I) zu entnehmen. Eine ausführliche Erläuterung zusammen mit den zugrunde liegenden mathematischen Formeln des Modells DYRESM findet sich im technischen Paper von Imerito (2007). Einzelne Modellparameter werden später im Kapitel zur Kalibrierung und Validierung des hydrodynamischen Modells am Ammersee aufgegriffen (Kapitel 1.3).

1.2.2 Regionales Klimamodell REMO

Zur Modellierung der möglichen zukünftigen vertikalen Temperaturverteilung im Gewässer sowie zur Ableitung klimawandelbedingter, limno-physikalischer Veränderungen wurden in dieser Studie, vergleichbar zu früheren Dissertationen an der LMU München (Marke, 2008; Brey, 2013), simulierte, meteorologische Eingangsdaten aus dem regionalen Klimamodell REMO (Jacob et al., 2007; Teichmann et al., 2013) verwendet. Dieses wurde am Max-Planck-Institut für Meteorologie (MPI-M) entwickelt und ist auf Grund seiner Auflösung von 10 x 10 km besonders gut für derartige Impact-Studien geeignet. Das numerische Klimamodell stellt simulierte Daten zu kurzwelliger Sonneneinstrahlung, Lufttemperatur, Niederschlag, Wind-

geschwindigkeit, Sättigungsdampfdruck, Wolkenbedeckung und relativer Luftfeuchte auf Basis verschiedener IPCC Emissionsszenarien zur Verfügung. Diese Daten werden vom globalen, gekoppelten Atmosphäre-Ozean-Zirkulationsmodell ECHAM5/MPI-OM abgeleitet. Somit sind sämtliche meteorologische Eingangsvariablen zur Modellierung zukünftiger limno-physikalischer Verhältnisse mit DYRESM vorhanden.
Da REMO verschiedene meteorologische Variablen im Untersuchungsgebiet über- bzw. unterschätzt (Jacob et al., 2008), ist es notwendig, vor Nutzung regionaler Klimamodelldaten zur Seemodellierung eine sogenannte Bias-Korrektur durchzuführen (Helfer et al., 2012; Sahoo et al., 2013). Diese wurde in Weinberger and Vetter (2012) (Publikation I) am Ammersee realisiert, indem Messdaten der vorher genannten Messstationen (Kapitel 1.2.1) aus dem Zeitraum 1990 bis 2006 mit simulierten REMO-Daten des Zeitraumes 2001 bis 2017 verglichen wurden. Auf Basis der Monatsmittelwerte bzw. Monatssummen konnte somit ein Bias-Wert ermittelt werden, der anschließend zur linearen Korrektur auf die täglichen Mittelwerte bzw. Tagessummen der meteorologischen Variablen des REMO-Modells angewendet wurde (Piani et al., 2009; Mudelsee et al., 2010; Terink et al., 2010).

1.3 Kalibrierung und Validierung des hydrodynamischen Modells

Zur manuellen Kalibrierung des hydrodynamischen Modells DYRESM am Ammersee wurde, wie beispielsweise auch in einer früheren Studie mit DYRESM angewandt (Perroud et al., 2009), die sogenannte „root mean square error minimization method“ gewählt. Diese basiert auf der Gegenüberstellung simulierter sowie gemessener Daten der Wassertemperatur als Key-Variablen sowie auf der Ermittlung der Gütemaße „mean absolute error“ (MAE) und „root mean square error“ (RMSE) in verschiedenen Wassertiefen (Legates and McCabe, 1999). Die statistischen Kriterien können zum Vergleich der Kalibrierung und späteren Validierung mit anderen Modellstudien herangezogen werden. Zu diesem Zweck wurde auch eine Regressionsanalyse durchgeführt. Sämtliche hier aufgeführten statistischen Qualitätskriterien wurden aufgrund ihrer erfolgreichen Anwendung in früheren hydrodynamischen Modellierungsstudien ausgewählt, wie zum Beispiel in Chao et al. (2007), Trolle et al. (2008) und Wang and Xu (2008). Die Vergleichs-Messdaten zur Wassertemperatur in verschiedenen Tiefen stammen wiederum von der Bayerischen WWV.
Die Modellkalibrierung im Rahmen dieser Dissertation am Ammersee umfasst die Periode 2004-2007. Aufgrund der Erfahrung von Rinke et al. (2010) mit DYRESM am Bodensee wurden zur Kalibrierung die Modellparameter „layer thickness“, „wind stirring efficiency“ und „light extinction coefficient“ verwendet. Deren Ausgangswerte stimmten mit denen der australischen Modellentwickler überein (Imerito, 2007) und wurden anschließend einzeln und schrittweise verändert. Die getesteten Wertebereiche der Parameter sowie die endgültigen, am Ammersee verwendeten Werte können dem im Rahmen dieser Promotion erstellten Artikel von Weinberger and Vetter (2012) (Publikation I) entnommen werden.
Die Modellvalidierung erfolgte für den Zeitraum 1993-1999 ebenfalls auf Basis des Vergleichs gemessener und modellierter Wassertemperaturen. Um die gute Qualität von Kalibrierung und Validierung des Modells DYRESM am Ammersee aufzuzeigen, wird in Abbildung 3 für beide Perioden der Vergleich gemessener und modellierter Wassertemperaturen in unterschiedlichen Gewässerschichten dargestellt. Im Epilimnion, welches in dieser Studie den Bereich zwischen 0 und 10 Metern Wassertiefe umfasst, wurde in beiden Zeiträumen eine sehr gute Übereinstimmung der Wassertemperaturen zwischen Modell und Realität erreicht. Eine Regressionsanalyse unter Verwendung von 29 Wassertemperaturwerten ergab während der Kalibrierung (2004-2007) Bestimmtheitsmaße (R^2) von 0,94 bis 0,96 (mit Ausnahme der Wassertiefe von 8 Metern: 0,9). Im Metalimnion, zwischen 10 und 20 Metern, unterschätzt das Modell die gemessenen Wassertemperaturen sowohl während der Kalibrierung als auch während der Validierung. Der saisonale Trend der Temperaturwerte

wird vom Modell aber gut reproduziert. Im Hypolimnion, unterhalb von 20 Metern, kommt es ebenfalls zu einer Unterschätzung der realen Temperaturwerte durch das Modell. Das Bestimmtheitsmaß liegt in Meta- und Hypolimnion zwischen 0,71 und 0,87. Die oben erwähnten statistischen Fehlerwerte, MAE und RMSE, liegen sowohl bezüglich der Kalibrierung (2004-2007) als auch der Validierung (1993-1999) am Ammersee im Bereich der Modellfehler vergleichbarer Studien mit DYRESM (Weinberger and Vetter, 2012).
Die zufriedenstellende Übereinstimmung von gemessenen und modellierten Wassertemperaturen in den oberen 10 Metern des vertikalen Profils wurde beispielsweise auch in den Studien von Gal et al. (2003) und Trolle et al. (2008) aufgezeigt. Ebenso wurde die Unterschätzung der Wassertemperaturen durch das Modell im Metalimnion und Hypolimnion bereits in früheren Untersuchungen entdeckt, zum Beispiel in der Untersuchung von Perroud et al. (2009). Diese betrachteten die Funktionalität von vier eindimensionalen hydrodynamischen Seemodellen am Genfer See und stellten fest, dass die eben angesprochene Unterschätzung der Wassertemperaturen auf unzureichender Abbildung der Durchmischungsvorgänge in den Wasserschichten im Modell DYRESM basiert.

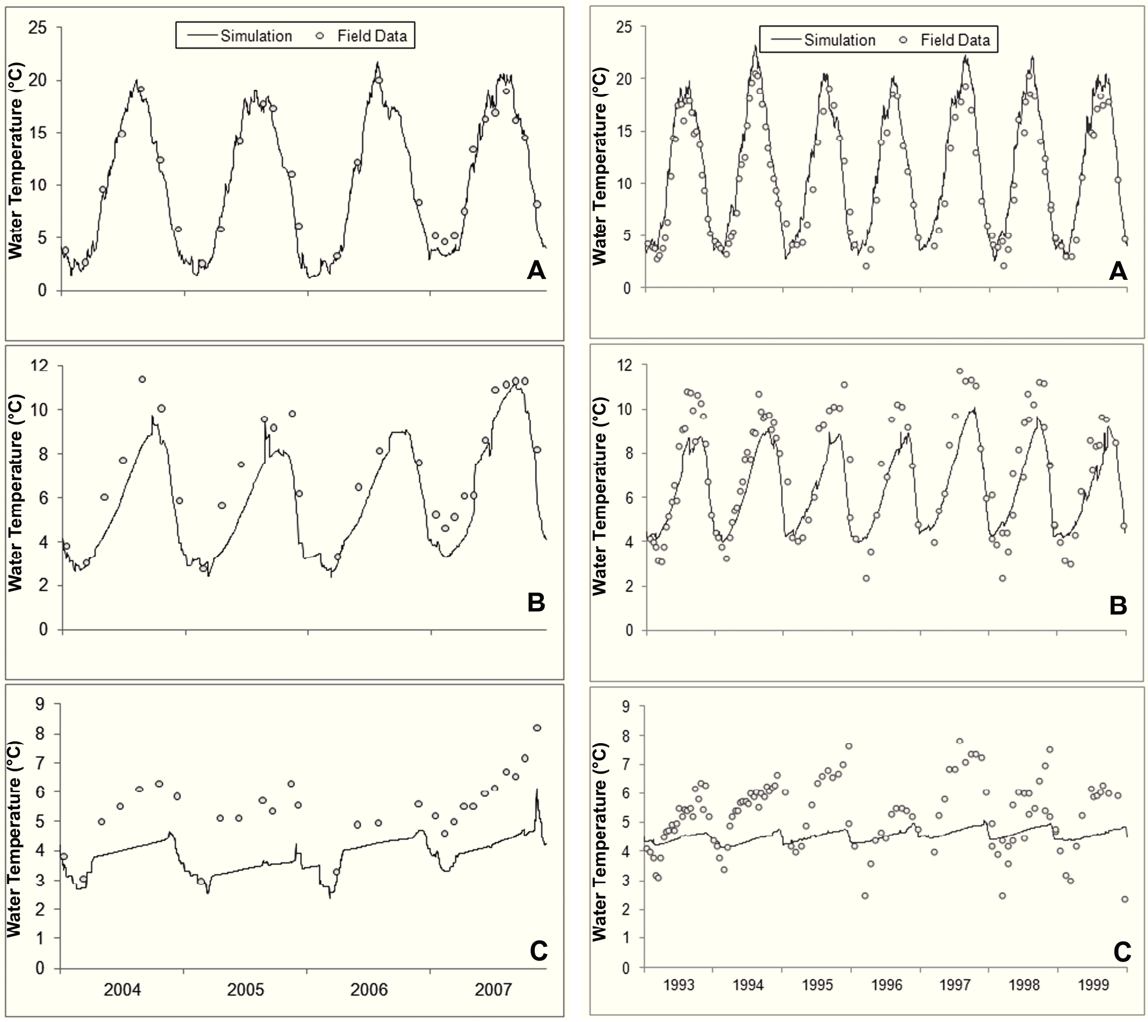

Abbildung 3: Simulierte Wassertemperaturen mit dem Modell DYRESM und Messwerte in Epilimnion (A), Metalimnion (B) und Hypolimnion (C), links für die Kalibrierungsperiode 2004-2007, rechts für die Validierung von 1993-1999 (Weinberger and Vetter, 2012).

Dennoch kamen sie zu dem Ergebnis, dass das Modell DYRESM im Vergleich zu anderen eindimensionalen Seemodellen die Variabilität der Wassertemperatur-Profile und die saisonale Thermokline gut reproduziert.

1.4 Anwendung von DYRESM und REMO zur Zukunftsmodellierung

Zur Modellierung möglicher künftiger Veränderungen im Gewässer wurden die im Kapitel 1.2.2 genannten meteorologischen Eingangsdaten des regionalen Klimamodells REMO verwendet. Dabei wurde das Emissionsszenario A1B ausgewählt, da es von einer ausgeglichenen Nutzung aller verfügbaren Energiequellen ausgeht (Nakicenovic et al., 2000; Solomon et al., 2007). Dieses Szenario simuliert einen Anstieg der globalen Jahresmitteltemperatur um ca. 3 Kelvin von 1990 bis ins Jahr 2100. In Weinberger and Vetter (2012) (Publikation I) wird die Basis zur Abschätzung zukünftiger limno-physikalischer Verhältnisse im Ammersee vorgestellt, wobei nach der erfolgreichen Kalibrierung und Validierung von DYRESM und einer Bias-Korrektur der REMO-Daten die vertikale Temperaturverteilung für die Periode 2041-2050 modelliert wurde. Abbildung 4 vergleicht die für diesen zukünftigen Zeitraum simulierten Werte der monatlichen Wassermitteltemperatur im Epilimnion mit den aus Messwerten berechneten monatlichen Mitteln des Kalibrierungszeitraums 2004-2007. Mit Ausnahme der Monate Januar, Juli, November und Dezember (siehe Abbildung 4) zeigt die Simulation einen Anstieg der mittleren Wassertemperaturen an der Oberfläche des Ammersees auf, wobei die maximalen Werte für den Monat August modelliert wurden. In den Wintermonaten kam es, ähnlich der oben erwähnten Modellierung des Hypolimnions, während der Kalibrierung und der Validierung zu einer Unterschätzung der Wassertemperaturen.

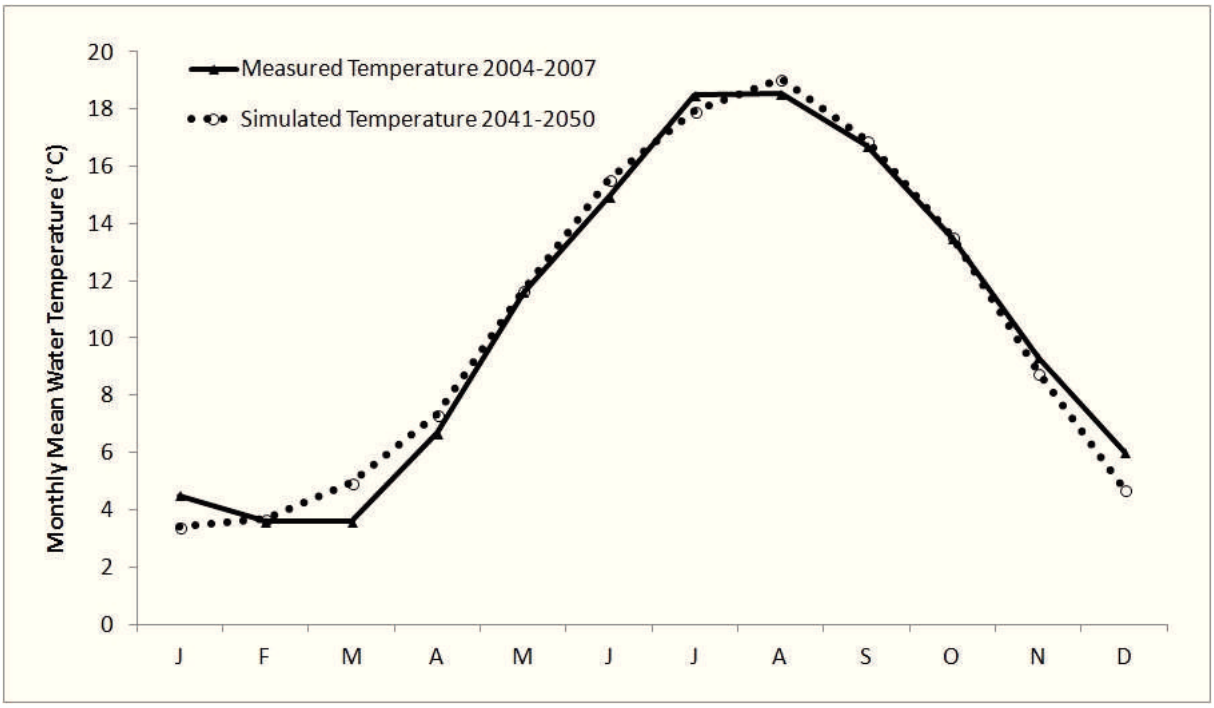

Abbildung 4: Monatliche Wassermitteltemperaturen im Epilimnion, gemessen in der Kalibrierungsperiode (2004-2007) und simuliert mit DYRESM für die Zukunft (2041-2050).

1.5 Ableitung limno-physikalischer Veränderungen

In Weinberger and Vetter (2014) (Publikation II) erfolgte dann die Ableitung möglicher limno-physikalischer Veränderungen im Gewässer. Im Genauen wurden aus den auf Basis der REMO-Daten (A1B-Szenario) simulierten Wassertemperaturen der Wärmeinhalt sowie die thermische Stabilität der Wassersäule für die Periode 2041-2050 berechnet. Anschließend erfolgte ein Vergleich dieser Ergebnisse mit den limno-physikalischen Eigenschaften des Ammersees in der Vergangenheit. Desweiteren wurden mögliche Veränderungen bezüglich der Dauer der sommerlichen Stagnation, der Tiefe der Thermokline sowie der Mächtigkeit des Metalimnions im See untersucht.

Zum einen wurde in den oberen 3 Metern des Epilimnions ein zukünftiger Anstieg des Wärmeinhalts für die Monate März bis Mitte November modelliert, verglichen mit dem errechneten Wärmeinhalt der Periode 1997-2007 (Abbildung 5a). Diese zukünftige Erhöhung der oberflächlichen Wassertemperaturen wird auch von anderen limnologischen Studien, welche sich mit Auswirkungen des Klimawandels auf Seen beschäftigen, konstatiert (Adrian et al., 2009; Ludovisi and Gaino, 2010; Schneider and Hook, 2010; Rimmer et al., 2011; Vetter and Sousa, 2012). Für die gesamte Wassersäule aber wurde gegensätzliches deutlich; hier ergab die Simulation in allen Monaten eine Abnahme des Gesamtwärmeinhalts bis zum Zeitraum 2041-2050 (Abbildung 5d). Dieses Ergebnis kommt Annahmen von früheren Arbeiten nahe (Robertson and Ragotzkie, 1990; Hondzo and Stefan, 1993; Livingstone, 2003), die ebenfalls eine zukünftige Abnahme oder ein Gleichbleiben der hypolimnischen Temperaturen im Sommer prognostizieren. In der Community wird diese Entwicklung kontrovers diskutiert.

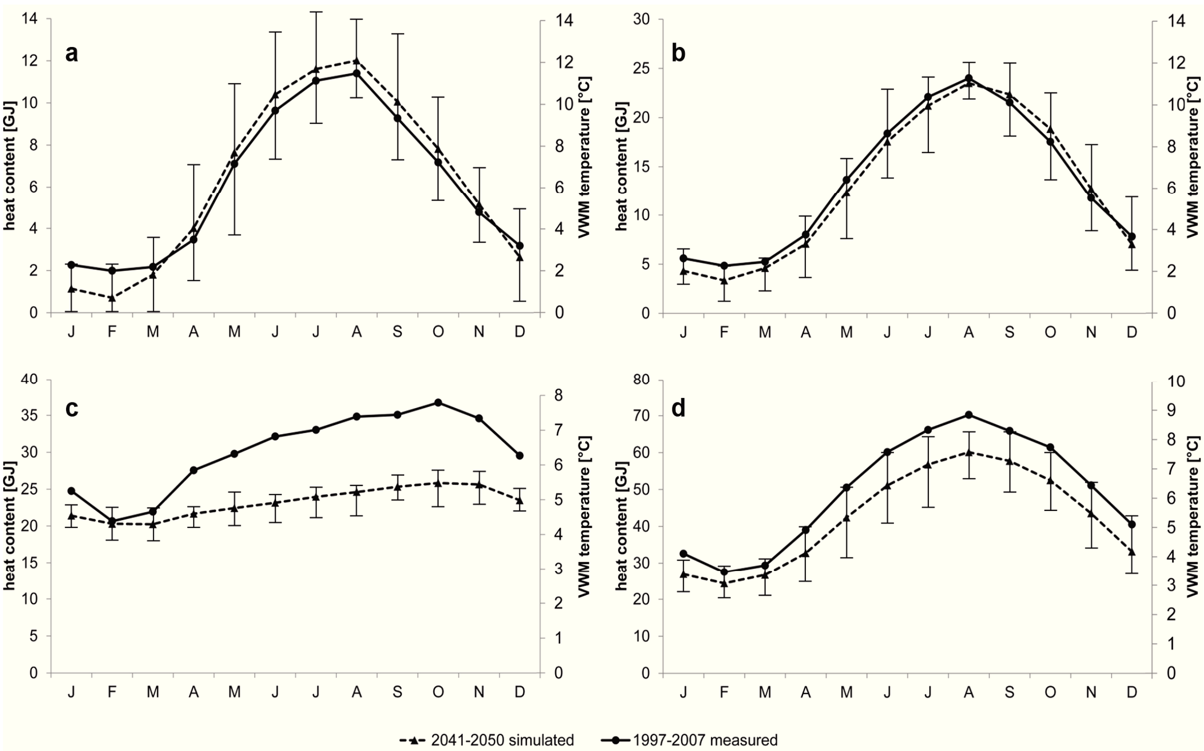

Abbildung 5: Monatlicher mittlerer Wärmeinhalt und entsprechende volumengewichtete Mitteltemperatur (VWM) in der Tiefe von 0-3m (a), 3-10m (b), unter 10m (c) und für den gesamten See (d), berechnet für den Ammersee aus gemessenen (1997-2007) und simulierten Daten (2041-2050, A1B-Szenario). Die Fehlerbalken zeigen Maxima und Minima der simulierten Werte, aus welchen die jeweiligen Monatsmittel errechnet wurden (Weinberger and Vetter 2014).

Die mathematische Formel zur Errechnung des Wärmeinhalts wurde dem Werk von Schwoerbel und Brendelberger (2005) entnommen und wird im Rahmen des Methodenteils in Weinberger and Vetter (2014) (Publikation II) ausführlich dargestellt.
Bezüglich der thermischen Stabilität der Wassersäule im Sommer, welche die sogenannte Schmidt Stabilität nach Idso (1973) repräsentiert, wird bis zur Periode 2041-2050 ein hoch signifikanter (nach Welch two-sample t-test, genaue Werte siehe Publikation II) Anstieg gegenüber Vergleichsdaten von 1985-2007 simuliert. Dabei fallen nicht nur die Schmidt Stabilitäts-Werte der Zukunft höher aus als die der Vergangenheit, sondern auch Ausreißer im Sommer oberhalb des 95%-Quantils treten häufiger auf (Abbildung 6). Mit der starken Erhöhung des Temperaturgradienten zwischen Oberfläche und Tiefenwasser und der einhergehenden Erhöhung der thermischen Stabilität der Wassersäule ist die oben aufgeführte Entwicklung des Gesamtwärmeinhalts im Ammersee somit sehr gut zu erklären.

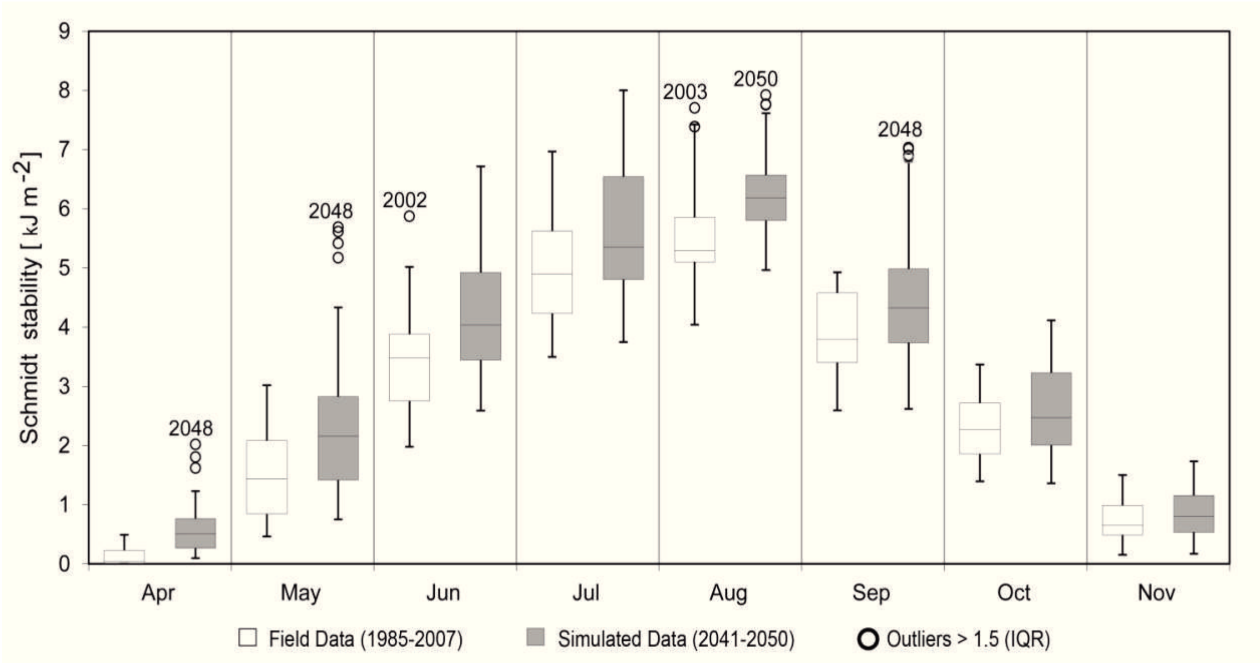

Abbildung 6: Boxplot-Diagramm zum Vergleich der berechneten Schmidt Stabilität aus gemessenen (1985-2007) und simulierten (2041-2050, Basis A1B Emissionsszenario) Daten (Weinberger and Vetter, 2014).

Bei der Ableitung der Dauer der sommerlichen Stagnation im See ist ersichtlich, dass die sommerliche Schichtung im Mittel in der Zukunft sowohl früher beginnen als auch später enden wird. Der Beginn der Schichtung war in der Vergangenheit (1985-2007) im Mittel der 15. Mai eines Modell-Jahres, das Ende der 10. Oktober, womit bei Betrachtung der folgenden Abbildung 7 die prognostizierten Veränderungen für die Periode 2041-2050 klar zu erkennen sind.

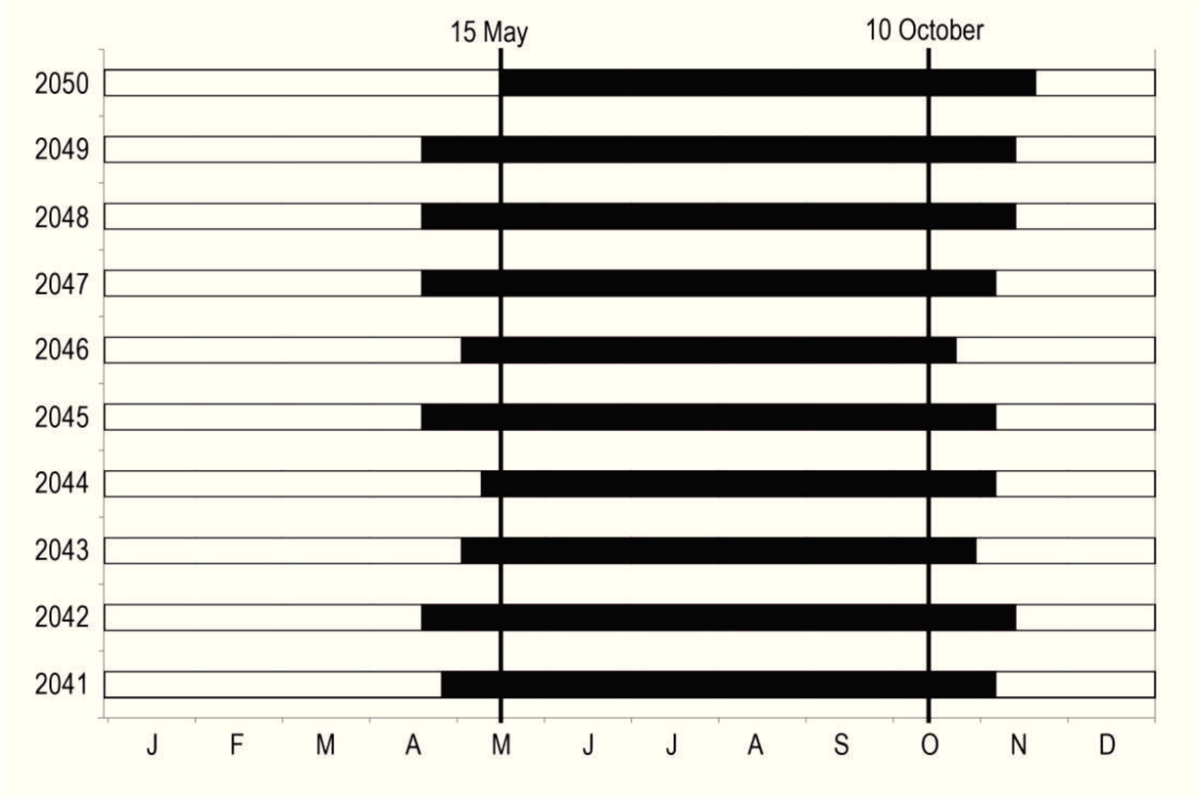

Abbildung 7: Prognostizierte Dauer der sommerlichen Stagnation für die Periode 2041-2050, abgeleitet aus simulierten Wassertemperaturdaten des Modells DYRESM (A1B Szenario); eingezeichnet auch der von 1985-2007 beobachtete mittlere Beginn und das mittlere Ende der Schichtung (Weinberger and Vetter, 2014).

Während der Periode von 1985-2007 lag die kürzeste beobachtete Schichtungsdauer bei 127 und die längste bei 169 Tagen. Dem gegenüber steht ein signifikanter Anstieg (nach Welch two-sample t-test, $p = 0.0011$) dieser Dauer bis zur Periode 2041-2050, mit mindestens 162 Tagen und einem Maximum von 204 Tagen. Der klare Anstieg der Schichtungsdauer und die gleichzeitige Verkürzung der zur Durchmischung des Sees verfügbaren Zeit wurde auch in anderen Studien behandelt (Austin and Colman, 2008; MacKay et al., 2009; Rempfer et al., 2010). Zur Ableitung der Schichtungsdauer wurde die Vorgehensweise von Birge (1897) angewandt, welcher die Thermokline als die Region im vertikalen Temperaturprofil definierte, in der die Temperatur um 1 K pro Meter Tiefe abnimmt. Tritt also solch eine Differenz auf, wird eine Schichtung angenommen.

Ebenso konnten Veränderungen in der Mächtigkeit des Metalimnions sowie in der Tiefe der Thermokline nach Hutchinson (1957) festgestellt werden, welcher die Thermokline als Ebene in der Tiefe der Wassersäule definierte, in welcher die größte relative Temperaturänderung zwischen zwei Layern auftritt. Die zukünftige Tiefe (2041-2050) der Thermokline nimmt laut Modell von Mai bis Juni im Mittel ab und von Anfang August bis Oktober zu. Darüber hinaus zeichnet sich eine Zunahme der Dicke des Metalimnions von Mai bis Oktober bis zur Periode 2041-2050 ab. Dies geht mit einer Abnahme der sommerlichen Dicke des Epilimnions einher, worin auch Gaiser et al. (2009) und Rimmer et al. (2011) übereinstimmen. Die hier vorgestellten Ergebnisse bezüglich der abgeleiteten limno-physikalischen Parameter werden in Weinberger and Vetter (2014) ausführlich diskutiert und mit weiteren Grafiken verdeutlicht (Publikation II).

1.6 Entwicklung automatisierter IT-Tools

In der hydrodynamischen Modellierer-Community besteht aktuell ein hoher Bedarf an speziellen und automatisierten IT-Lösungen, die dazu dienen sollen, „das Rad nicht in jedem Untersuchungsgebiet neu erfinden zu müssen“ (Mooij et al., 2010; Trolle et al., 2012), sondern bestehende Methoden weiterzuverwenden und Erfahrungen in der Community auszutauschen. Daher wird die vorliegende Dissertation in Weinberger et al. (submitted) (Publikation III) dadurch ergänzt, die bisher verwendeten IT-Methoden zur limnologischen Modellierung, vom Antrieb durch ein regionales Klimamodell bis hin zur Simulation zukünftiger limnologischer Zustände im Gewässer, zu einem Workflow zusammenzufassen (Abbildung 8). Somit werden sowohl der gesamte Modellierungsprozess als auch der Vergleich von Modell-Studien aus verschiedenen Regionen der Erde untereinander vereinfacht. Außerdem kann so im Umgang mit großen Datenmengen, sowohl mit Eingangsdaten als auch Ergebnisdatensätzen in hoher zeitlicher und räumlicher Auflösung, wertvolle Arbeitszeit eingespart werden, die in Modellierungsprojekten häufig einen limitierenden Faktor darstellt. Dadurch ist es möglich, zusätzliche Läufe zur Modellkalibrierung und Validierung durchzuführen und die Qualität der Studie weiter zu verbessern.

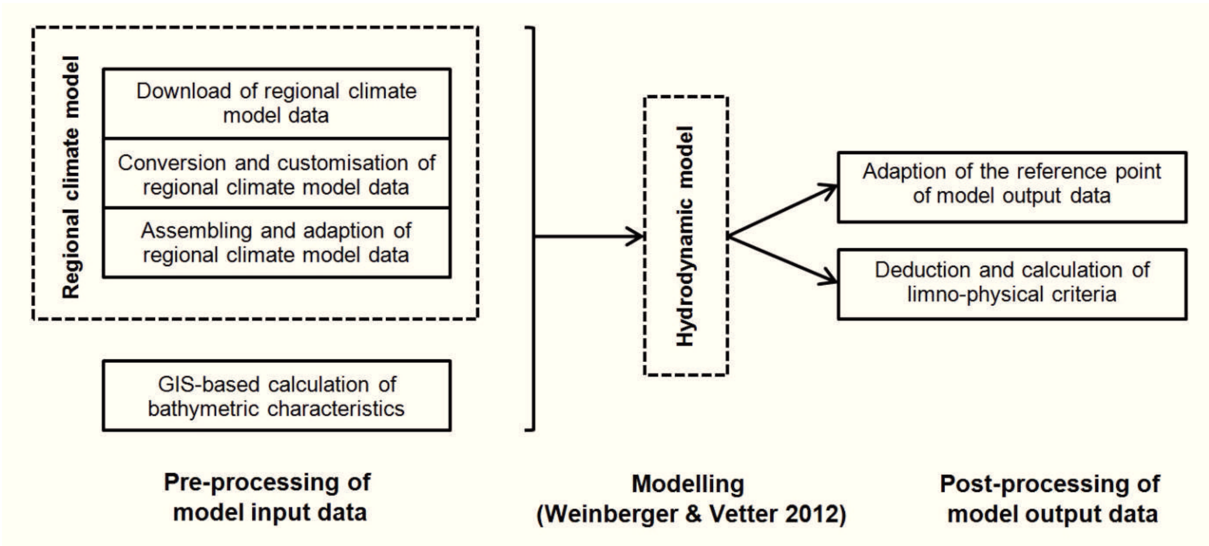

Abbildung 8: Automatisierte IT-Tools vom Output eines regionalen Klimamodells bis zur hydrodynamischen Modellierung zukünftiger limno-physikalischer Verhältnisse (Weinberger et al., submitted).

Im Folgenden werden nun ausgewählte automatisierte IT-Werkzeuge kurz dargestellt. Ein wichtiger Bestandteil des Workflows ist ein im Linux- Betriebssystem entwickeltes Shell Script. Mit Hilfe dieses Makros werden die meteorologischen Daten des regionalen Klimamodells REMO nach dem Download auf dem Desktop automatisch konvertiert, räumlich und zeitlich zugeschnitten und für die weitere Verarbeitung vorbereitet (Abbildung 9). Dabei kommen auch Software und Befehle der Open Source Lösung Climate Data Operators (CDOs) zum Einsatz (Schulzweida et al., 2012).

Nach eben beschriebener Konvertierung und Begrenzung werden die meteorologischen REMO-Daten weiterverarbeitet, um mit dem notwendigen Format der meteorologischen Eingangsdatei für das hydrodynamische Modell DYRESM übereinzustimmen. Hierzu wurde im Rahmen dieser Studie am Ammersee ein nutzerfreundliches Microsoft (MS) VBA-Makro entwickelt.

Des Weiteren ist im beschriebenen Workflow ein GIS-Makro eingebunden, mit Hilfe dessen eine automatisierte Berechnung der zur hydrodynamischen Modellierung nötigen Volumen der horizontalen Schichten im See möglich ist. Dies geschieht auf Basis bathymetrischer Daten zum Wasserkörper. Das Makro wurde in Esri ArcGIS unter Verwendung der Erweiterungen Spatial Analyst, 3D Analyst sowie dem Programmierwerkzeug ModelBuilder erstellt.

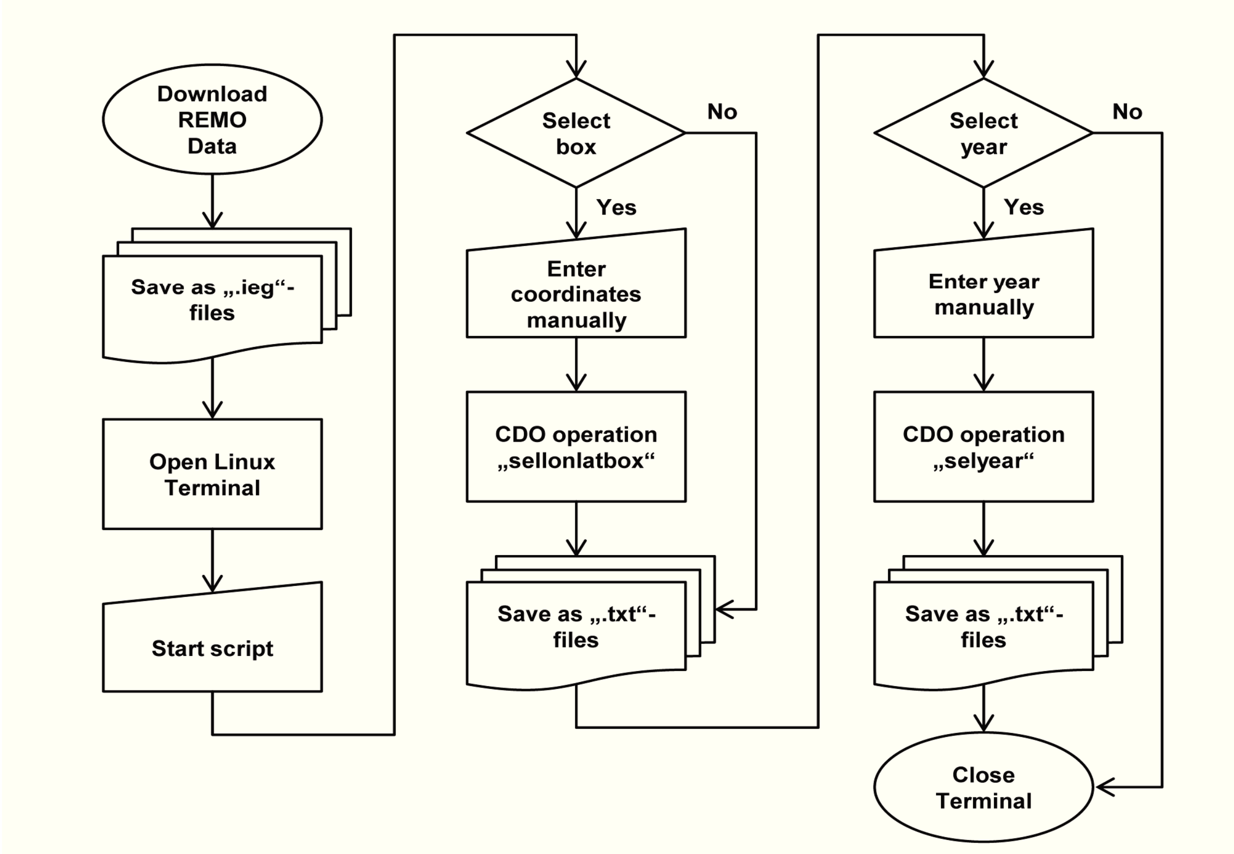

Abbildung 9: Flussdiagramm des Linux Shell Scripts zur automatisierten Konvertierung sowie zum räumlichen sowie zeitlichen Zuschneiden von Daten aus dem regionalen Klimamodell REMO (Weinberger et al., submitted).

Weitere IT-Tools und Programmcodes zur Ableitung und Berechnung limno-physikalischer Zustände im Gewässer sowie zugehörige Abbildungen wurden in Weinberger et al. (submitted) zur Veröffentlichung eingereicht und können im Anhang Publikation III eingesehen werden. Dort finden sich auch eine genaue Beschreibung der System-voraussetzungen sowie eine Diskussion, in wie fern ein gemischter Workflow aus Open Source Lösungen und Formaten, sowie weit verbreiteter kommerzieller Software, die Bedürfnisse der aquatischen Modellierer-Communtiy decken kann. Ebenso wird aufgeführt, wie Umweltmodellierer im Allgemeinen mit großen Datenmengen bis hin zu Big Data umgehen und welche Entwicklungen in Zukunft darüber hinaus wünschenswert wären.

1.7 Fazit und Ausblick

Im Rahmen dieser Dissertation wurde am Beispiel des Ammersees nachgewiesen, dass das hydrodynamische Modell DYRESM, nach sorgfältiger Kalibrierung und Validierung, die thermischen Eigenschaften und den Wärmehaushalt von Seen gut abbildet. Das Modell ist in der Lage, unter Verwendung von Eingangsdaten regionaler Klimamodelle (z.B. REMO), die zukünftigen limno-physikalischen Eigenschaften des Ammersees abzuschätzen. Die zu er-

wartenden Veränderungen im See, wie etwa ein starkes Ansteigen der oberflächlichen Wassertemperaturen sowie eine erhöhte Schichtungsstabilität, können weitreichende Auswirkungen auf die Wasserqualität und das Ökosystem des Gewässers haben, wie bereits in anderen Studien festgestellt wurde (Quayle et al., 2002; Adrian et al., 2009; Vetter and Sousa, 2012; Riverson et al., 2013). Dies gilt es an Hand weiterer Modellierungen und einer Kopplung des hydrodynamischen Modells mit einem seeökologischen Modell auch für den Ammersee aufzuzeigen. Für derartige Studien stellt die vorliegende Dissertation einen klaren Mehrwert dar und kann direkt als Basis verwendet werden. Auch wurde der gesamte Modellierungsprozess durch die im Rahmen der vorliegenden Arbeit entwickelten, automatisierten IT-Tools deutlich beschleunigt und vereinfacht. Durch die Verwendung flexibler Programm-Codes in Verbindung mit Open Source Lösungen sowie gängiger Software zur Datenverarbeitung ist es möglich, sämtliche Makros innerhalb der Modellierer-Community zu verbreiten und somit zukünftige hydrodynamische Studien an Seen und Reservoiren zu vereinfachen. Besonders wünschenswert wäre auch der Transfer des entwickelten Know-hows in Entwicklungsländer, deren Oberflächengewässer häufig zur flächendeckenden Trinkwasserversorgung genutzt werden.
Alles in allem ist es so möglich, weitere noch bestehende Lücken in der Modellierung des Klimawandel-Einflusses auf aquatische Ökosysteme zu schließen und zu einem zukünftigen nachhaltigen Wassermanagement beizutragen.

2. Publikationen im Rahmen dieser Promotion

2.1 Zusammenhang der Publikationen

Wie der vorangegangenen, erweiterten Zusammenfassung zu entnehmen ist, wurden im Rahmen dieser kumulativen Dissertation drei Publikationen zur Veröffentlichung in internationalen Peer-Review Journals erstellt (in Erstautorenschaft). Diese stellen ausführlich die Gesamtleistung der Arbeit dar, beinhalten wissenschaftliche Abhandlungen zu Untersuchungsgebiet, Methodik, Ergebnissen, Diskussion und besonderem Mehrwert der vorliegenden Promotion und bauen direkt aufeinander auf. Der rote Faden, welcher sich durch das Dissertations-Vorhaben zieht, wird nochmals durch Abbildung 10 verdeutlicht.
Publikation I beschreibt die ersten Schritte dieser Arbeit. Diese umfassen die sorgfältige Kalibrierung und Validierung des hydrodynamischen Modells DYRESM am Ammersee sowie die Nutzung simulierter meteorologischer Eingangsvariablen aus dem regionalen Klimamodell REMO zur Modellierung der möglichen zukünftigen, vertikalen Temperaturverteilung im Gewässer. Auch wird die ökologische Bedeutung eventueller Klimawandeleinflüsse diskutiert.
In Publikation II wird die darauf aufbauende Ableitung limno-physikalischer Zustände für Vergangenheit und Zukunft zur Identifikation möglicher klimawandelbedingter Veränderungen behandelt. Dabei werden umfangreiche Vergleiche zum bisherigen Stand der Forschung gezogen.
Publikation III ist letztendlich etwas methodischer ausgerichtet und stellt die Ergebnisse bezüglich der Entwicklung automatisierter IT-Tools dar. Durch die im Beitrag neu entwickelten Skripte und Makros wird der Modellierungsprozess deutlich beschleunigt und vereinfacht. Die Qualität der Modellierung wird durch das Möglichwerden weiterer Kalibrierungsläufe und Sensitivitätsanalysen auf Basis der eingesparten Zeit deutlich verbessert und es kann darüber hinaus eine größere Anzahl an Modell-Parametern kalibriert werden. Die Software-Tools können innerhalb der aquatischen Modellierungs-Community auch zur zukünftigen Modellierung anderer Gewässer verwendet werden.

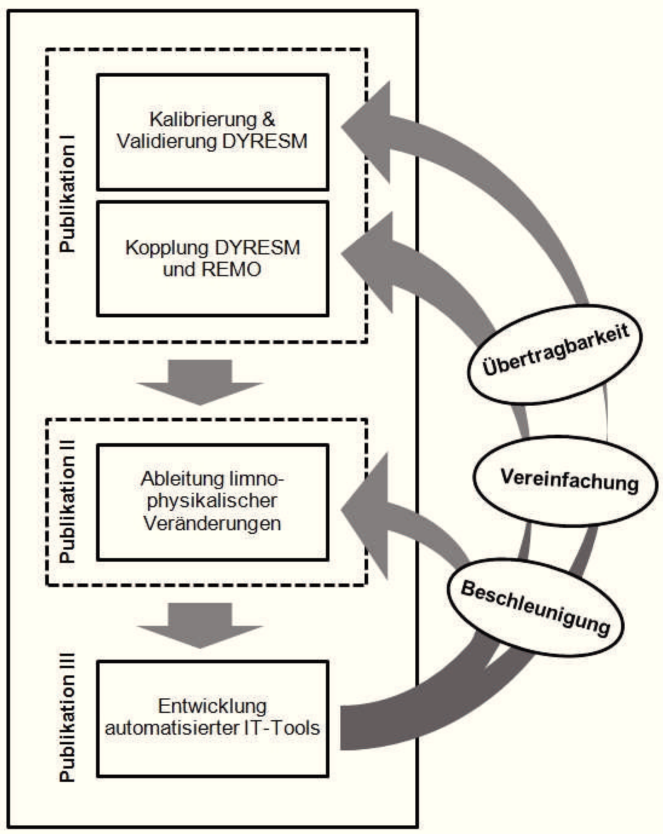

Abbildung 10: Zusammenhang der im Rahmen der vorliegenden kumulativen Promotion erstellten Publikationen.

2.2 Überblick über die Publikationen

2.2.1 Publikation I

Using the hydrodynamic model DYRESM based on results of a regional climate model to estimate water temperature changes at Lake Ammersee

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Ecological Modelling, published 2012, DOI:10.1016/j.ecolmodel.2012.06.016

Abstract:
In order to enhance our research work on the impact of climate change on bodies of water, it is necessary to establish coupled hydrodynamic and ecosystem models that take into account simulated data of climate models. We assume that the coupled hydrodynamic models, along with the regional climate models, can serve to gain further knowledge on the future climatic impact upon lake ecosystems. For this purpose we use the one-dimensional hydrodynamic model DYRESM and the regional climate model REMO and apply them to the pre-Alpine, 83-m-deep, currently dimictic Lake Ammersee. The objectives of this study are to calibrate and validate the model DYRESM in order to simulate the vertical thermal distribution in Lake Ammersee and to prepare bias-corrected meteorological data from the model REMO (IPCC

A1B scenario) to establish a first hydrodynamic simulation run for the period 2040-2050. The IPCC A1B emission scenario, which assumes a balanced use of all available energy sources in the world, predicts the global mean temperature to increase by about 3 Kelvin from 1990 to the year 2100. To calibrate and validate the model DYRESM carefully, we used date from 2004–2007 and 1993–1999. When comparing simulated and measured water temperatures regarding the calibration period, we observed small mean absolute errors (0.96 K–1.61 K) and root mean square errors (1.42 K–1.96 K), as well as high coefficients of determination (0.71–0.96) at all depths. We conclude that the hydrodynamic model can be used to identify potential drawbacks of climate change (e.g. extended duration of stratification, higher thermal stability, lack of mixing) on the lake ecosystem by higher water temperatures. In addition this modelling provides the basis for coupled aquatic ecological model.

2.2.2 Publikation II

Lake heat content and stability variation due to climate change: coupled regional climate model (REMO) – lake model (DYRESM) analysis

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Journal of Limnology, published 2014, DOI: *10.4081/jlimnol.2014.668*
(Open Access Journal)

Abstract:
Climate change-derived higher air temperatures and the resulting increase in lake surface temperatures are known to influence the physical, biological and chemical processes of water bodies. By using hydrodynamic lake models coupled with regional climate models the potential future impact of a changing climate can be investigated. The present study hence elucidates limno-physical changes at the peri-Alpine, 83-m deep, currently dimictic Ammersee in southeastern Germany, both to underline the role of lakes as sentinels of climate change and provide a sound basis for further limnological investigations. This was realised by using water temperatures simulated with the hydrodynamic model DYRESM for the period 2041-2050, based on the results of the regional climate model REMO (IPCC A1B emission scenario). Modelling of future heat content resulted in a projected increase in the upper 3 m of the epilimnion from end of March to mid-November, whereas a decrease in future total heat content (January-December) of the entire water column was simulated compared to that observed in 1997-2007. Lake thermal stability is projected to be higher in the period 2041-2050 than in 1985-2007. Stratification is expected to occur earlier and to last longer in the future than the pattern observed in the years 1985-2007. The future mean May-June depth of the thermocline is simulated to be situated above its past average vertical position, whereas a decline in mean thermocline depth is projected for the beginning of August to October. Furthermore, the mean May-October thickness of the metalimnion is simulated to increase. Additionally we investigated the sensitivity of these limno-physical results to changes in the model parameter light extinction coefficient (LEC), which determines how the solar radiation is absorbed by the lake water. The elucidation of physical changes at Ammersee by means of a regional climate model provides a sound basis on which to face the new challenges of lake modelling.

2.2.3 Publikation III

Automated tools for lake-related climate change impact modelling

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Computers and Geosciences, submitted 2014

Abstract:
To improve the simulation of limnological conditions in the future and facilitate the use of results of the regional climate model REMO as input data for hydrodynamic lake models, we show a workflow, supported by information technology (IT). We created an application (Linux Shell script) to convert and customise REMO data automatically and provide a macro in Visual Basic for Applications (VBA) to assemble and pre-process meteorological input data for the hydrodynamic model DYRESM. An automated, geographic information system (GIS)-based analysis was included to calculate the volumes of different horizontal layers on the basis of bathymetric lake data, using the Esri GIS ArcMap together with the 3D Analyst and Spatial Analyst extensions and the visual coding language ModelBuilder. To compare water temperatures in the vertical water column independent from changing water levels, we automatically adapted the reference point of the DYRESM output data from the lake bottom to the surface (VBA script). The automated deduction of limno-physical criteria of a lake was done by additional auxiliary routines in VBA. All the presented tools as well as the program codes are flexible and can be imitated when adapting different hydrodynamic models. In our case, we applied the routines to investigate the impact of climate change on the limno-physical conditions of Lake Ammersee in Middle Europe. In doing so, it is possible to save valuable time when dealing with big data in numerical lake modelling and to achieve substantial progress in the field of specialised, automated IT-solutions, enabling modellers to conduct more comprehensive and accurate calibration and validation runs.

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Anhang A

Im Folgenden sind die drei im Rahmen dieser Dissertation erstellten Peer-Review Publikationen im Original aufgeführt.

Publikation I

Weinberger, S., Vetter, M., 2012. Using the hydrodynamic model DYRESM based on results of a regional climate model to estimate water temperature changes at Lake Ammersee. Ecological Modelling 244, 38-48.

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Using the hydrodynamic model DYRESM based on results of a regional climate model to estimate water temperature changes at Lake Ammersee

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Water management

ABSTRACT

In order to enhance our research work on the impact of climate change on bodies of water, it is necessary to establish coupled hydrodynamic and ecosystem models that take into account simulated data of climate models. We assume that the coupled hydrodynamic models, along with the regional climate models, can serve to gain further knowledge on the future climatic impact upon lake ecosystems. For this purpose we use the one-dimensional hydrodynamic model DYRESM and the regional climate model REMO and apply them to the pre-Alpine, 83-m deep, currently dimictic Lake Ammersee. The objectives of this study are to calibrate and validate the model DYRESM in order to simulate the vertical thermal distribution in Lake Ammersee and to prepare bias-corrected meteorological data from the model REMO (IPCC A1B scenario) to establish a first hydrodynamic simulation run for the period 2040–2050. The IPCC A1B emission scenario, which assumes a balanced use of all available energy sources in the world, predicts the global mean temperature to increase by about 3 K from 1990 to the year 2100. To calibrate and validate the model DYRESM carefully, we used date from 2004–2007 and 1993–1999. When comparing simulated and measured water temperatures regarding the calibration period, we observed small mean absolute errors (0.96–1.61 K) and root mean square errors (1.42–1.96 K), as well as high coefficients of determination (0.71–0.96) at all depths. We conclude that the hydrodynamic model can be used to identify potential drawbacks of climate change (e.g. extended duration of stratification, higher thermal stability, lack of mixing) on the lake ecosystem by higher water temperatures. In addition this modelling provides the basis for coupled aquatic ecological models.

1. Introduction

Various studies have demonstrated that climate change has a strong impact on water temperatures (Edinger et al., 1968; Quayle et al., 2002; Leon et al., 2005; Thompson et al., 2005; Coats et al., 2006; Dokulil et al., 2006; Salmaso et al., 2007; Schneider et al., 2009; Schneider and Hook, 2010) and lake ecosystems (Verburg and Hecky, 2009; Guilizzoni et al., 2012). Thereby biological variables also depend on water temperatures. For example, Wagner and Adrian (2008) explained that shifts in the climate regime of lakes caused substantial trophic- and species-dependent changes within ecosystems. Lakes play a role as sentinels, integrators and regulators of the climate change (Danis et al., 2004; Schindler, 2009; Williamson et al., 2009a). In addition, the regional influence of humans by land-use activities should be considered (Alvarez Cobelas, 2007; Williamson et al., 2008), because the impact of climate change on the ecosystem of lakes is often superposed by impacts due to anthropogenic activity in the catchment area (Vetter and Sousa, 2012). Several information gaps exist in modelling impacts on aquatic ecosystems (MacKay et al., 2009). Often insufficient observational data is available, and a general need exists to improve our knowledge of climate change impacts on hydrology and lake ecosystems. Studies using data and information from regional climate models as input for aquatic ecosystem models are almost entirely non-existent (Bates et al., 2008).

In general modelling the thermal structure and heat content of lakes is becoming more important for ecological lake models in order to account for the effects of climate change. Therefore, for further investigation of these future climate change effects, it is advisable to use well-calibrated and validated hydrodynamic and ecosystem models that take into account the aforementioned data from existing regional climate models, e.g. REMO (Jacob et al., 2007, 2008) on the basis of different IPCC emission scenarios (Nakićenović et al., 2000; Solomon et al., 2007). These climate models are the only available tool to satisfactorily estimate different future rates of climate change (Samuelsson, 2010), and the hydrodynamic models are able to simulate future water quality accounting for a changing climate (Perroud et al., 2009).

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In this study, we want to show that the one-dimensional hydrodynamic model DYRESM (Imberger and Patterson, 1981; Imerito, 2007), which was established successfully in different investigation areas around the world (Han et al., 2000; Gal et al., 2003; Romero et al., 2004; Trolle et al., 2008; Perroud et al., 2009; Rinke et al., 2010), is suitable to investigate the supposed climate change impacts on Lake Ammersee. It was essential to carefully calibrate and validate this hydrodynamic model.

So far Lake Ammersee, which is representative of all dimictic lakes affected by anthropogenic and climate impacts in the Northern Foothills of the Alps, is known to have undergone a recent re-oligotrophication (Ernst et al., 2009), but whether this trend will continue under climate change conditions is not clear (Vetter and Sousa, 2012). In general different estimations of specific outcomes exist that climate change could cause. For example, Danis et al. (2004) expected Lake Ammersee to undergo a dramatic and persistent lack of mixing starting around the year 2020. The resulting lack of oxygenation would irreversibly destroy the deepwater fauna. Because of these risks, it is important to check prior estimations using new modelling approaches to investigate the lake's ecological future.

The objectives of this study were (1) to carefully calibrate and validate the one-dimensional model DYRESM in order to simulate the vertical thermal distribution in Lake Ammersee and (2) to prepare meteorological data from the regional climate model REMO as input data for the hydrodynamic model. After these tasks were accomplished, DYRESM was then suitable (3) to carry out first simulation results regarding the vertical thermal distribution in Lake Ammersee for 2041–2050, using the abovementioned REMO data on the basis of the IPCC emission scenario A1B. Finally, for further investigation, we use this study to elucidate additional prospective physical changes (e.g. stratification and mixing changes) in the lake and to couple the hydrodynamic model with an aquatic ecological model to support future water quality management (Hakanson et al., 2003; Rinke et al., 2010). Such a comprehensive calibration and validation of a hydrodynamic model has not been achieved in any other lake in the southeast of Germany.

2. Material and methods

2.1. Study area

As our study area, we selected the pre-Alpine, 83-m deep, currently dimictic Lake Ammersee, which is located 30 km south west of Munich and shown in Fig. 1. This lake was chosen because, in our opinion, it is representative of many other lakes in the northern foothills of the Alps based on their similarities in geogenic, climate geographic and limnologic characteristics. With an expanse of 46.6 km^2 and a water volume of 1.75e + 009 m^3, Lake Ammersee is the third largest lake in Bavaria and has a glacial morphologic origin. The lake has one basic tributary called the Ammer, three smaller inflows called the Windach, Rott and Kienbach, and one main outflow called the Amper. Lake Ammersee is close to the Munich metropolitan area and is very important for regional tourism and fisheries. Naturally, the trophic conditions of the lake would be oligotrophic, but due to intensive land use in the catchment area starting around the year 1950, the lake became mesotrophic. On the other hand, in the last 20 years, after special sewerage arrangements, Lake Ammersee has undergone a re-oligotrophication (Ernst et al., 2009). Recent studies of the lake are investigating how climate change could influence this trend (Vetter and Sousa, 2012).

2.2. Model DYRESM

For this study, we used the one-dimensional hydrodynamic model DYRESM (v4.0.0-b2), which was developed by the Centre for Water Research at the University of Western Australia, to predict the vertical distribution of temperature, salinity and density in lakes and reservoirs (Imberger and Patterson, 1981). It is a process-based model with a Lagrangian layer scheme, which means that the horizontal layers are adjusted to stay within user-defined limits (Imberger and Patterson, 1981; Antenucci and Horn, 2002). The layer mixing appears when the turbulent kinetic energy in the topmost horizontal layer exceeds a potential energy threshold. The kinetic energy is produced by convective overturn, wind stirring and shearing (Perroud et al., 2009). DYRESM was applied to different study areas, as mentioned in Section 1 and is particularly suitable for the simulation of longer periods. In comparison with other one-dimensional lake models, DYRESM reproduced the variability of the water temperature profiles and seasonal thermocline satisfactorily (Perroud et al., 2009). DYRESM can be run either in isolation for hydrodynamic studies, or coupled to an aquatic ecological model, e.g. CAEDYM, for the investigation of biological and chemical processes (Imerito, 2007).

2.3. Meteorological model input variables

The meteorological conditions directly affect the thermodynamic processes of a lake, e.g. the water temperature profile. To simulate thermal conditions, the hydrodynamic model DYRESM requires 6 meteorological variables assembled in the meteorological input file (.met-file). These variables must be available throughout the whole simulation period and include shortwave radiation [$W(m^2)^{-1}$], cloud cover (okta), air temperature (°C), vapour pressure (hPa), wind speed at a height of 2 m ($m\,s^{-1}$) and precipitation (m). To calibrate and validate the model DYRESM at Lake Ammersee, the meteorological data was provided by the German Weather Service (DWD) and one private station. Data from this private station was checked for plausibility by a correlation analysis using measured data from the DWD stations, and we confirmed that it could be used for our study. For example, the correlation coefficient for the variable shortwave radiation amounted to 0.76 in July (lowest) and 0.95 (highest) in May. All meteorological variables are entered into the model as daily means or daily totals, dependent on the availability of measured data and in accordance with the analogous proceeding in other studies with the model DYRESM. The input time step of the hydrodynamic model could be minimised to 10 min. Furthermore, the meteorological input file contains information about the temporal resolution, the calculation method of the long wave radiation taking into account cloud cover fraction, sensor type and altitude of the measuring station.

The short wave radiation data for the calibration of the hydrodynamic model was provided at 5-min intervals by the private meteorological station Diessen-Obermühlhausen, which is located near the waterside of Lake Ammersee. In our study, we calculated a daily mean value of 129 $W(m^2)^{-1}$ for 2004–2007. For the best results when calibrating the model, we reduced daily solar radiation by 15%. A similar adaptation of radiation data was implemented by Gal et al. (2003), who reduced the long wave radiation at Lake Kinneret (Israel) by 12.5%. The cloud cover fraction in our study area was observed by eye at the Raisting–Wielenbach DWD measuring station. These observations are essential for estimating the long wave radiation from atmospheric conditions, which is included in the program code of DYRESM (Imerito, 2007). Values for air temperature, precipitation and wind speed were provided by the same DWD station at 1-h intervals. To use the onshore wind speed data for investigations on the lake, it was necessary to calculate a multiplication factor depending on exposition,

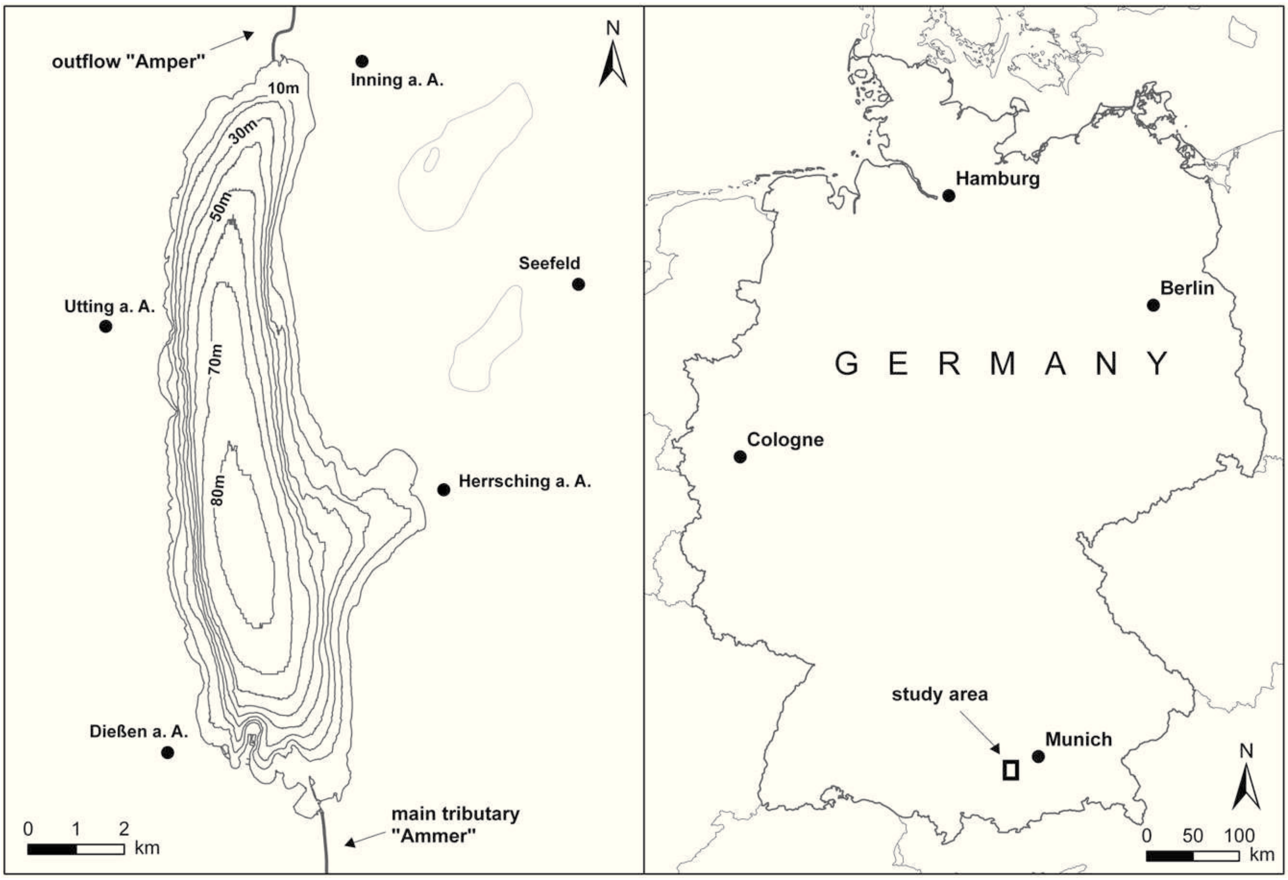

Fig. 1. Bathymetry and study area at Lake Ammersee southwest of Munich.

distance between the measuring station and the lake, surrounding vegetation, and regional climatic conditions. For that reason at the beginning of our calibration runs we determined a wind multiplication factor of 1.3, which was also used by a study group investigating Lake Constance and resulted in the lowest deviations during their calibration process (Rinke et al., 2010). Within the scope of our calibration of the hydrodynamic model, we found that, for Lake Ammersee, a multiplication factor of 1.2 leads to realistic wind speed values and to the lowest deviation between measured and simulated water temperatures in the water column. The vapour pressure (Ew) was calculated with respect to the air temperature (t) and humidity correlation at the Raisting–Wielenbach weather station using the Magnus formula (Zmarsky et al., 2007):

$$\mathrm{Ew} = 6.1\,\mathrm{hPa} \times 10^{7.5t/t+237.2\,^{\circ}\mathrm{C}}$$

2.4. Hydrologic variables and other parameters

The hydrodynamic model DYRESM provides the opportunity to account for any number of surface or sub-terrestrial inflows and outflows. Values of inflow ($\mathrm{m^3\,d^{-1}}$) are organised in the model's inflow (.inf) and withdrawal (.wdr) files using a daily input time step. The inflow file also contains the daily mean water temperatures (°C) and salinity values (PSS) of each tributary. Lake Ammersee has one basic tributary called the Ammer and the three smaller inflows called the Windach, the Rott and the Kienbach. From 1975–2007, the averaged inflow volume of the Ammer River was $17.01\,\mathrm{m^3\,s^{-1}}$; the Windach was $1.46\,\mathrm{m^3\,s^{-1}}$; the Rott was $0.92\,\mathrm{m^3\,s^{-1}}$; and the Kienbach was $0.13\,\mathrm{m^3\,s^{-1}}$. In our modelling approach, we added the inflow volumes from the smaller tributaries to the amount from the Ammer. The outflow river of Lake Ammersee called the Amper has a mean runoff of $20.75\,\mathrm{m^3\,s^{-1}}$ for the same period (1975–2007). All runoff data was provided by the Bavarian Environmental Agency. However, the gauging stations are not able to measure the entire inflow because it is assumed that some of the water reaches the lake subterraneous (Melzer et al., 1988). To compensate for the resulting water deficit and to ensure a balanced water budget, which is necessary for the model to run, we implemented a water balance analysis for 1975–2007 (Baumgartner and Liebscher, 1996). A detected daily deficit of $20{,}180\,\mathrm{m^3}$ was added to each daily inflow value for the Ammer tributary. After this correction, the water level in the model remained almost constant over the whole calibration and validation period.

The vertical profile of water temperature and salinity at the beginning of the simulation is defined by the initial profile file (.pro), as DYRESM calculates each of the horizontal water layers separately. The thickness and properties of these horizontal layers were calculated for each simulation day (Imerito, 2007). In our study, we defined the water temperatures at 16 different depths, as presented in Table 1, using the height above the lake zero height elevation. Water temperature and conductivity values were provided by the Bavarian Environmental Agency and our own project measuring system on the lake. The salinity was calculated using the relation of temperature, density and water pressure in the water column (Unesco, 1981).

Specific simulation data is entered into the model with the configuration file (.cfg), which also contains starting time, duration and output time step of the model. The smaller the chosen output time step, the higher the calculated temporal resolution. To simulate longer periods, it is advisable to use a daily time step with respect to the elapsed calculation time of the model. The specific data of the configuration file includes the layer thickness, the light

Table 1
Initial DYRESM profile at the beginning of our calibration period (1 January 2004).

Height (m)	T (°C)	S (pss)
0	3.8	0.276
2	3.8	0.223
4	3.8	0.223
6	3.8	0.223
8	3.8	0.223
10	3.8	0.223
13	3.8	0.222
16	3.8	0.223
20	3.8	0.222
30	3.8	0.223
40	3.8	0.222
50	3.8	0.222
60	4.2	0.222
70	4.2	0.222
80	4.2	0.222
83.72	4.2	0.222

Table 2
DYRESM configuration file as used for the calibration period (2004–2007).

Setting	Description
2004001	Simulation start day
1439	Simulation length (in days)
.FALSE.	Run CAEDYM
1	Output interval (in days)
0.25	Light extinction coefficient (m^{-1})
0.25	Min layer thickness (m)
3	Max layer thickness (m)
3600	Time steps (s)
3	Number of output selections
Salinity temperature density	List of output selections
.FALSE.	Activate bubbler
.TRUE.	Activate non-neutral atmos. stability

extinction coefficient and the possibility of activating a non-neutral atmospheric stability. By adapting the layer thickness, the user can define the limits of the layers based on the Lagrangian layer scheme of the model DYRESM. The light extinction coefficient determines how the solar radiation is absorbed by the lake water and directly influences the heating of the epilimnion (Imberger and Patterson, 1981) and the atmospheric stability in our case describes how a volume of air above the lake reacts to a vertical shifting. Table 2 shows the configuration file with the values used in our simulation approach.

Most of the variable parameters are defined in the parameters file (.par) of DYRESM, which is provided in Table 3. This file was accurately adapted to the study area. In the following the most relevant parameters are mentioned. The bulk aerodynamic transport coefficient simulates the impact of wind on the water surface. The mean albedo of water is necessary to calculate the effective short wave radiation that enters the body of water. Using the emissivity of a water surface, the model estimates long wave emission and reflection. When the critical wind speed is exceeded, the model algorithm of mixing is activated. The time of day for output includes the date when visualisation data should be collected, while the shear production efficiency has a strong impact on kinetic energy, which is discharged by the movement of different water layers and is partially used for mixing. The potential energy mixing efficiency describes the transformation of potential energy to turbulent kinetic energy and is delivered when the stratification of the water column becomes unstable due to vertical convective movements in a body of water. The wind stirring efficiency indicates the potency of wind in mixing the water and its effect on the hypolimnetic layers. The benthic boundary layer (BBL) detrainment diffusivity influences the efficiency of heat conduction in the benthic zone. All values for the configuration and the parameter files are described by Imberger and Patterson (1981).

Table 3
DYRESM parameters file as used for the calibration period (2004–2007).

Setting	Description
1.3E−3	Bulk aerodynamic mmt. transport coefficient
0.08	Mean albedo of water
0.96	Emissivity of a water surface
3.0	Critical wind speed ($m\,s^{-1}$)
64,800	Time of day for output (s from midnight)
0.02	Bubbler entrainment coefficient
0.083	Buoyant plume entrainment coefficient
0.08	Shear production efficiency
0.2	Potential energy mixing efficiency
0.4	Wind stirring efficiency
1.0E+7	Effective surface area coefficient (m^2)
1.4E−5	BBL detrainment diffusivity
200	Vertical mixing coefficient

The original version of the model DYRESM is not able to proceed the modelling process when water temperatures decrease below 0 °C. Therefore, a simulation at Lake Ammersee with this version would not be possible. The Centre for Water Research at the University of Western Australia provided a modified version for the simulation of pre-Alpine lakes with freezing avoidance, where negative values of water temperature were set back to 0 °C to allow a continuous and stable simulation. Although this modification violates the energy conservation assumption, the introduced error is small for large pre-Alpine lakes as they rarely freeze and the cooling-down is not very intense (Danis et al., 2004). Moreover, the effect of freezing avoidance diminishes throughout the season when surface temperatures are approaching a value corresponding to the equilibrium energy exchange between the lake and the atmosphere.

The geographical position of the lake, its height above sea level and the number of inflows and outlets is specified in the morphometry file (.stg). This file also contains the geometry of the riverbed and the important bathymetry information of the lake.

2.5. Field data

For both calibration and validation, including the initial profile of the hydrodynamic model, it is necessary to use field data. At Lake Ammersee, a series of water temperature and conductivity measurements have been collected since 1976, with regular measurements carried out since 1984. These data were collected at the deepest point of the lake by the Bavarian Environmental Agency. In the epilimnion, the measurements were arranged every 2 m, in the metalimnion, every 3 m, and in the hypolimnion, every 10 m. The time step of data collection varied, but in general, the measurements were taken at least every month.

2.6. Model calibration and validation

In our study, calibration of the model DYRESM was performed between 2004 and 2007 utilising parameter values provided by the model developers (Imerito, 2007) and using Rinke et al. (2010) as a basis. The calibration was implemented manually by using the root mean square error minimisation method (Perroud et al., 2009), considering the simulated and measured water temperatures as key variables. Our objective was to rate the sensitivity of different input parameters, to set the model for further studies and to understand the model evaluation process (Edward, 1996). At Lake Ammersee, the hydrodynamic model was calibrated with respect to the parameters layer thickness, wind stirring efficiency and light extinction coefficient, which were changed one by one. The performed calibration range of each value is included in Section 3. The model validation of Lake Ammersee that took into consideration water temperatures covered the period 1993–1999 using field data of the

Bavarian Environmental Agency as described before. The purpose of the validation process is a test based on comparison of simulated data with the observed data, which should be included whenever possible (Edward, 1996).

Several different statistical methods exist to investigate the quality of model's calibration and validation results. In our study, we compared modelled and observed data by using a regression analysis and the quality criteria mean absolute error (MAE) and root mean square error (RMSE) (Legates and McCabe, 1999). Hence, the calibration and validation results can be easily compared to other model studies and are specified in Section 3. The relevant statistical quality criteria were selected due to their frequent usage in other ecological modelling studies, e.g. in Chao et al. (2007), Trolle et al. (2008), Wang and Xu (2008), and Perroud et al. (2009).

2.7. Future simulation

Our primary objective was to ensure that the model DYRESM at Lake Ammersee was suitable to estimate future trends in the development of the lake's thermal characteristics, which have a significant influence on future ecological conditions (Adrian et al., 2009; Williamson et al., 2009b; George, 2010). From these trends, further limno-physical parameters can be deduced for the future, e.g. Schmidt-stability, the position of the metalimnion, and the occurrence of circulation and stagnation events, as well as the corresponding stagnation and circulation periods.

We implemented a future simulation on the basis of the IPCC A1B emission scenario for the period 2041–2050. The A1B emission scenario was selected due to the fact that it assumes a balanced use of all available energy sources (Nakićenović et al., 2000; Solomon et al., 2007). The climate change conditions in the future are derived from the regional climate model REMO (Jacob et al., 2007, 2008), which was selected because of the suitable cell size in the area of study. It performs calculations for cells of 10 km × 10 km. For the cell of the study area, the REMO simulation provides parameters including short-wave radiation, air temperature, precipitation, wind speed, vapour pressure, total cloud cover and relative humidity, which are all values that have strong influence on the heat budget of a lake. The long-wave radiation for the simulation is estimated from atmospheric conditions using cloud cover fraction (Imerito, 2007).

When using the REMO data, it is necessary to implement a BIAS-correction. This was realised by comparing previously measured meteorological data from the study area (period 1990–2006) with the data simulated by the regional climate model (period 2001–2017). Based on these comparisons, statistical relationships for every month can be discovered that are relevant for the correction of calculated future climatic conditions. For example, when correcting the air temperature values derived from the REMO model, an absolute correction value was adapted to the daily mean air temperatures, while the correction of daily precipitation sums was implemented relatively by using a multiplication factor (Mudelsee et al., 2010; Piani et al., 2010; Terink et al., 2010). All the correction values used in this study, sorted by month, are shown in Table 4.

As an example for potential limno-physical changes, we deduced the duration of thermal stratification in the lake for the simulated period 2041–2050 and compared it to the observed duration of stratification in the past. Thereby we proceeded like Birge (1897), who defined the thermocline as the region in the vertical profile of a lake, where the temperature decreases by 1 K m^{-1} of depth. If such a difference in temperature is measured or simulated, the lake is stratified at that time.

Table 4
BIAS correction values for air temperature and precipitation for every month, calculated by using measured (1990–2006) and simulated (2001–2017) data.

Month	Temperature (absolute in °C)	Precipitation (relative)
January	0.81	0.39
February	1.79	0.52
March	2.90	1.00
April	3.77	0.95
May	1.64	1.18
June	2.54	0.73
July	2.31	0.65
August	1.65	0.80
September	3.98	0.76
October	2.91	0.48
November	3.47	0.54
December	2.60	0.55

3. Results

At the beginning of this section, we want to present the results of the calibration process. Afterwards the quality of the calibration and validation will be compared. Also, we show the meteorological data from the regional climate model REMO taking into account a BIAS correction that is necessary to estimate the lake's ecological future. We also wanted to compare mean water temperatures using the periods of calibration (2004–2007) and future simulation (2041–2050) to estimate possible changes. To show potential limno-physical variations in the lake we derived the duration of thermal stratification for the simulated years 2041–2050 and compared it to stratification periods in the past.

The numerous calibration runs showed a high sensitivity of the model to the maximum layer thickness, wind stirring efficiency and light extinction coefficient parameters. When analysing the maximum layer thickness in our calibration period (2004–2007) with a range of 2.0–7.0 m, a value of 3.0 m produced the lowest discrepancies between simulated and measured water temperatures in all depths. For the wind stirring efficiency parameter, we tried a range of 0.4–0.8 and reached the best simulation results using the value 0.4. The light extinction coefficient parameter fell in a range of 0.2–0.37 m^{-1}. At the end of the calibration process, we set this parameter to 0.25 m^{-1}. The wind stirring efficiency and light extinction coefficient values that we used matched the values originally used by the model's developers (Imberger and Patterson, 1981; Imerito, 2007). All parameter values used in our DYRESM model approach were already shown in Tables 2 and 3.

To verify the quality of the calibration and validation process, in Figs. 2 and 3, we compare the modelled and field data for 2004–2007 and 1993–1999. Simulated and measured water temperatures in the epilimnion, which in our study covers depths from 0–10 m, showed good compliance in calibration as well as in validation. In the metalimnion, which in our study covers depths between 10 and 20 m, the hydrodynamic model generally underestimates the measured water temperature values in both periods. However, the seasonal trend of the measured data is readily cognisable. The graphs of simulated data in the hypolimnion, in our study below 20 m, run in a straight line every calendar year, even though the field data show a slight seasonal increase of water temperatures. At the end of the year, this trend is interrupted. Also the simulated water temperature values in the hypolimnion in the most cases are lower than the measured values. This fact can be seen in Fig. 4 as well. When looking at Figs. 2 and 3, it should be considered, that we used different scales due to naturally given variations in water temperature measurements. As a consequence, the pictured deviation between simulated and measured water temperature values in the metalimnion and hypolimnion seems higher than the real deviation.

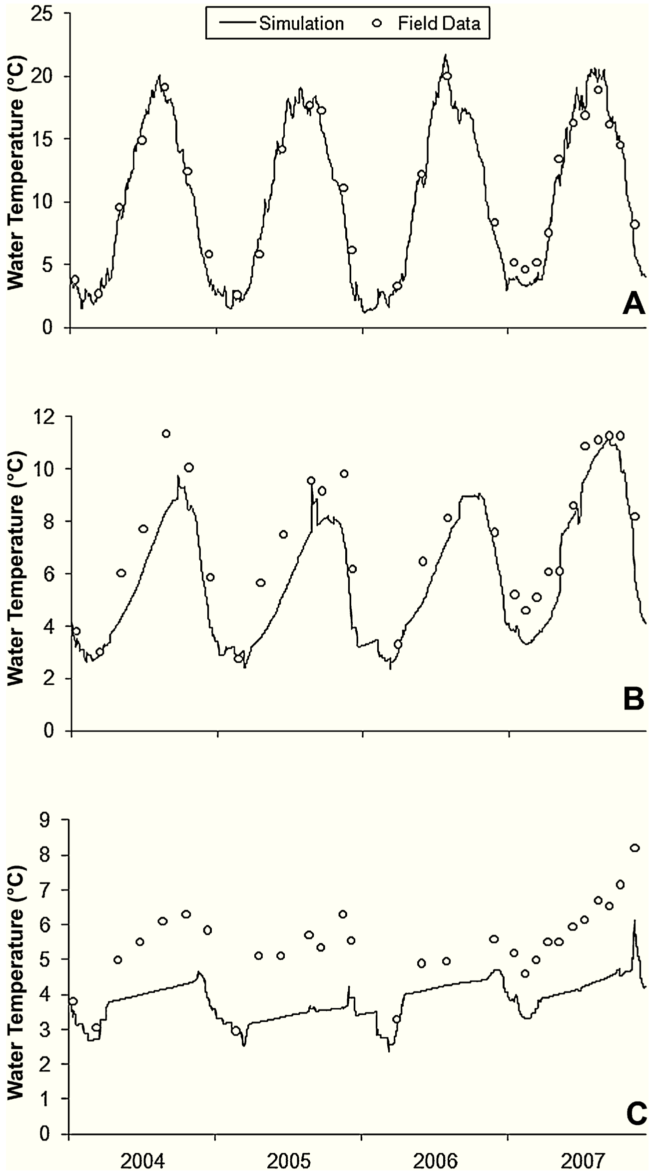

Fig. 2. DYRESM-simulated water temperatures and measured temperatures in epilimnion (A), metalimnion (B) and hypolimnion (C) in the calibration period January 2004–December 2007.

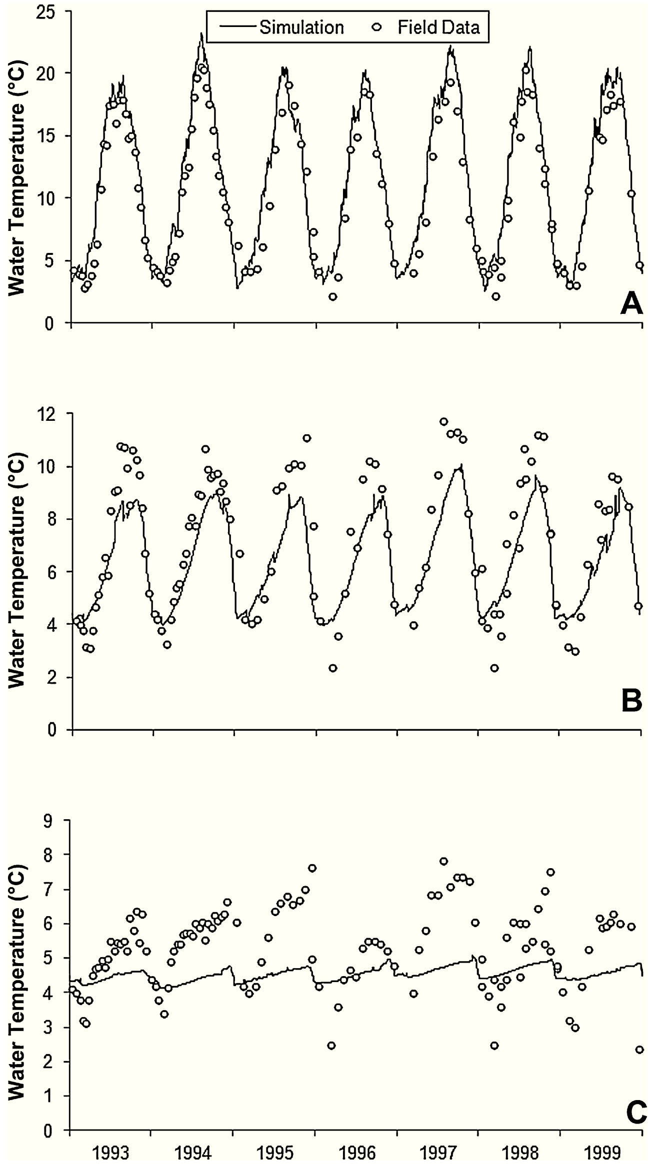

Fig. 3. DYRESM-simulated water temperatures and measured temperatures in epilimnion (A), metalimnion (B) and hypolimnion (C) in the validation period January 1993–December 1999.

Fig. 4 shows the regression analysis and coefficient of determination for the calibration period (2004–2007) at different depths. The size of the sample was 29 values per graph. In the epilimnion, except at a depth of 8 m, the graphic shows a very high coefficient of determination between 0.94 and 0.96. In the observed depths of the metalimnion and the upper hypolimnion, the deviation is higher with a coefficient of determination between 0.71 and 0.87. Like already mentioned before, the simulated water temperature values in the hypolimnion in the most cases are lower than the measured values.

Vertical temperature profiles are very significant in elucidating possible impacts on the ecology of a lake. The thermocline shift, the changes in the thickness of the epilimnion and in the vertical temperature gradient are readily recognisable potential effects. Fig. 5 shows one daily vertical temperature profile of simulated and field data for every season of the year 2007. In winter a homothermic profile is visible, while the simulation underestimates the water temperatures by at least 1 K. In spring a slight stratification is observable in the epilimnion, and below 3 m, the water temperatures are underestimated by the model. In summer the typical summer stratification is visible, while the epilimnion is reproduced very well by the model, and in the hypolimnion, the water temperatures are slightly underestimated, with a deviation in the region of 1 K for the whole water column. In autumn, before the initiation of the typical mixing, there is a stable stratification in the modelled as well as in the measured temperature profile visible.

As quality criteria for calibration and validation of the hydrodynamic model DYRESM, we calculated the mean absolute error (MAE) and root mean square error (RMSE) in different depths, and they are listed in Table 5. In the upper 13 m of Lake Ammersee, the MAE and RMSE, with the exception of depths of 8 and 10 m, were lower during the calibration period (2004–2007) than during the validation period (1993–1999). Below depths of 13 m, we observed that the validation produces lower MAE and RMSE than the calibration. Our RMSE maximum of 2.83 K occurred at the water surface during the validation period.

When using data from the regional climate model REMO, it became apparent that the temperature and precipitation values for

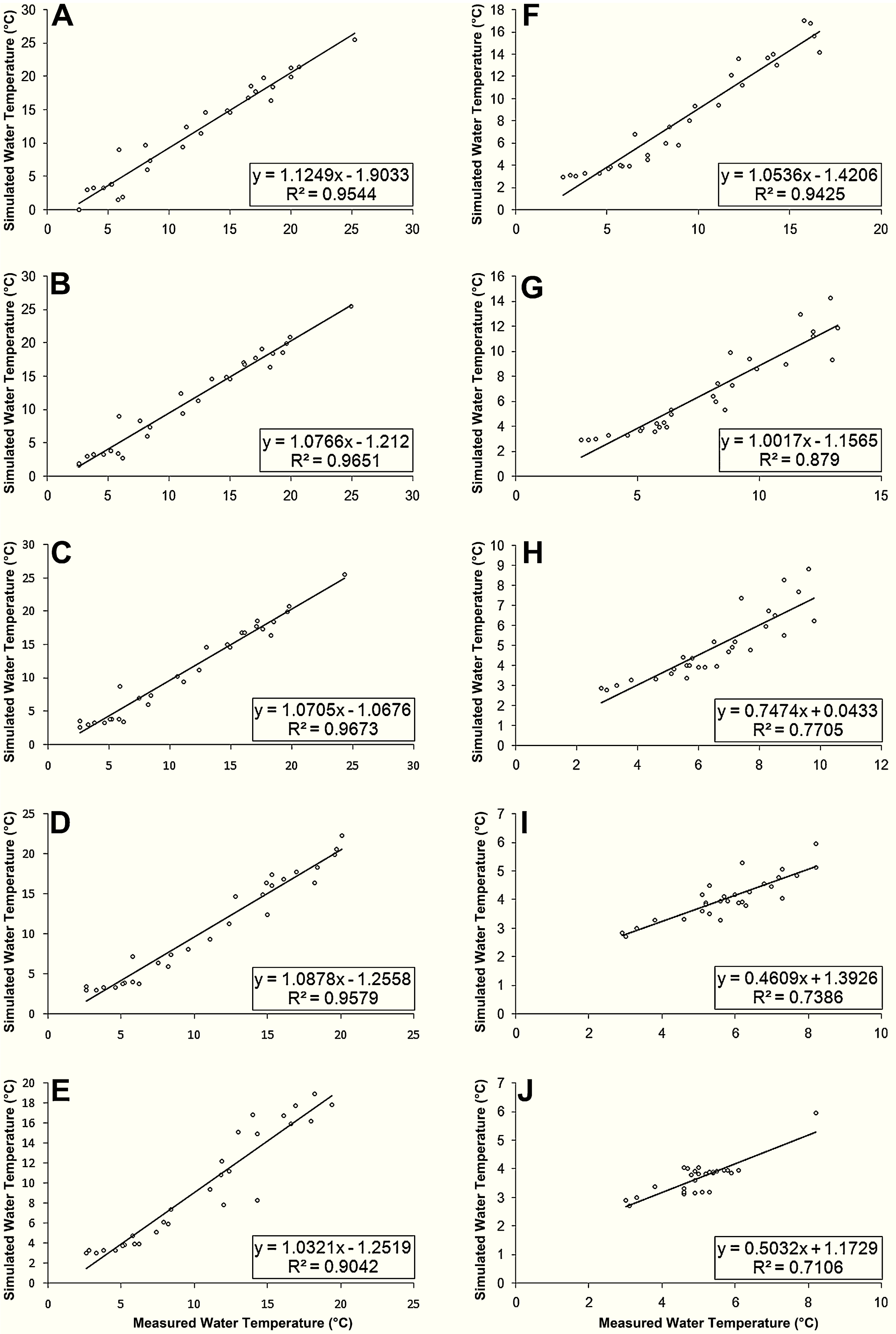

Fig. 4. Regression analysis and coefficient of determination (R^2) between simulated and measured water temperatures in depth of 0 m (A), 2 m (B), 4 m (C), 6 m (D), 8 m (E), 10 m (F), 13 m (G), 16 m (H), 20 m (I) and 30 m (J) in the calibration period January 2004–December 2007.

the future are overestimated, by what a BIAS correction gets necessary (Mudelsee et al., 2010; Piani et al., 2010; Terink et al., 2010). Fig. 6 shows monthly mean temperatures and precipitation sums measured by the German Weather Service (DWD) for 1990–2006, the original simulated data by the REMO model from 2041–2050 and the bias-corrected values for the same period. After these corrections, no unexpected changes were visible from January to March. In contrast the simulated and corrected precipitation

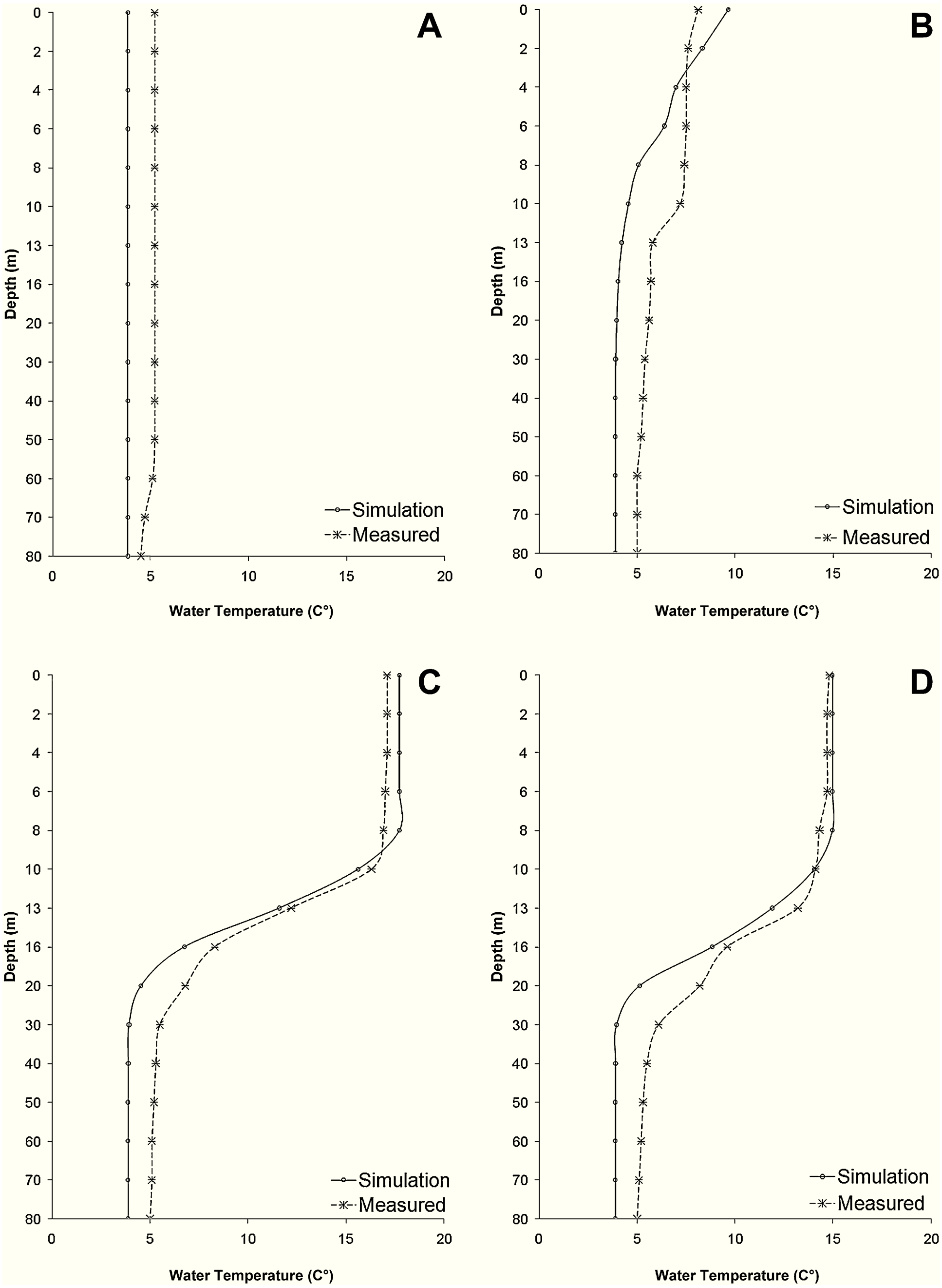

Fig. 5. Vertical water temperature profiles of Lake Ammersee on 15 January 2007 (A), 10 April 2007 (B), 11 July 2007 (C) and 10 October 2007 (D), comparison of simulated and measured values.

Table 5
MAE and RMSE values for calibration (Cal) and validation (Val) at different depth.

Depth (m)	MAE (K)		RMSE (K)	
	Cal	Val	Cal	Val
0	1.27	2.61	1.79	2.83
2	1.05	2.02	1.42	2.26
4	0.96	2.02	1.34	2.34
6	1.13	1.53	1.43	1.84
8	1.41	1.35	1.96	1.64
10	1.11	1.12	1.48	1.38
13	1.30	1.41	1.64	1.38
16	1.48	1.35	1.85	1.71
20	1.61	1.33	1.92	1.60
30	1.20	0.88	1.44	1.14

values for the future in April, May, July and August were much higher and in June were lower than the measured DWD values in the past. In September the REMO data was twice as high as the measured data, and from October to December, the precipitation in the future increased slightly. The bias-corrected monthly mean air temperature rose, especially in winter. In our future period (2041–2050) an obvious increase in mean air temperatures occurred in August.

As we mentioned in Section 2, after careful calibration and validation, we implemented a future simulation run at Lake Ammersee (2041–2050). Fig. 7 emphasises again the high quality of the model calibration, by showing graphs for simulated and measured mean water temperatures in the epilimnion during the calibration period (2004–2007). Also Fig. 7 presents the simulated,

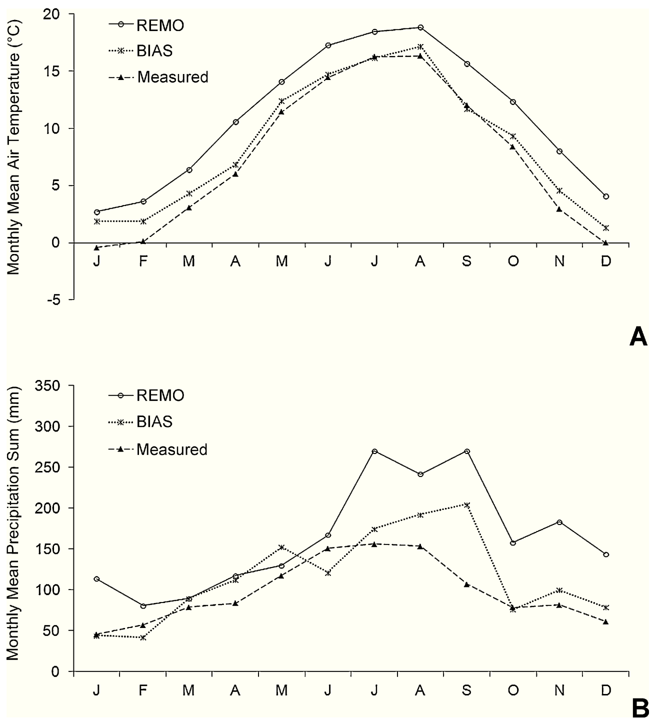

Fig. 6. Monthly mean air temperature (A) and monthly mean precipitation sum (B) simulated for the future by the model REMO (2041–2050), BIAS-corrected (2041–2050) and measured by the DWD (1990–2006).

expected mean water temperature changes in the epilimnion, by comparing the measured mean water temperatures during calibration (2004–2007) and the simulated mean water temperatures in the future period (2041–2050). Except for the months of January, July, November and December, the mean water temperatures in the future were expected to increase in comparison to the simulated mean water temperatures from 2004–2007. The water temperature maximum was modelled in August.

To elucidate potential limno-physical changes in consequence of aforementioned increasing water temperatures, we deduced the stratification behaviour of Lake Ammersee for the simulated period 2041–2050 and compared it to the observed duration of stratification in the period 1985–2011. In the past, the average date in the year that the stratification was observed to occur was 15 May, while the average end of stratification was 10 October. Against this in the future the beginning of stratification is simulated to appear averagely on 27 April and the average end of stratification is modelled to be 08 November. In sum the simulated stratification in the future is expected to occur earlier and to last longer than the observed stratification in the past. In Table 6 we give a summary of the stratification behaviour of the lake.

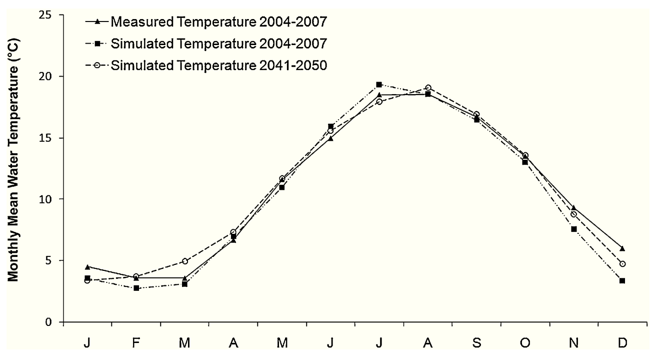

Fig. 7. Monthly mean water temperatures in the epilimnion, measured and simulated for the calibration period (2004–2007) and simulated for the future (2041–2050).

Table 6
Average derived beginning, end and duration of thermal stratification for the past period 1985–2011 (observed) and the future period 2041–2050 (simulated).

	Period 1985–2011	Period 2041–2050
Beginning (date)	15 May	27 April
End (date)	10 October	08 November
Duration (number of days)	149	196

4. Discussion

During calibration of the 1D-DYRESM model at Lake Ammersee, we observed variations in the modelled water column caused by changes in the calibrated parameters. In general the thermocline became diffuse when the maximum layer thickness was defined too broadly. Also the temperature gradient within the hypolimnion increased when high values of this parameter were used, resulting in an unsatisfactory representation of reality. Changes of the wind stirring efficiency parameter in our case study mainly influenced the water temperatures in depths between 5 and 35 m, and by changing the light extinction coefficient parameter we observed clear variations in the water temperature in all depths. A further reduction in the light extinction coefficient led to a decrease in surface water temperatures in summer and an increase in surface temperatures in winter. Other variables have also been analysed regarding their lower sensitivity on the model process and could be excluded during the calibration process.

The high quality of the calibration and validation is demonstrated in Figs. 2 and 3 by comparing modelled and measured water temperatures for 2004–2007 and 1993–1999. The satisfying accordance of simulated and field data in the upper 10 m of the lake was also demonstrated by Gal et al. (2003) and Trolle et al. (2008). The underestimation of measured water temperatures by the model in the metalimnion and hypolimnion, as well as the slight annual variations in the simulated hypolimnetic water temperatures, has been described in previous studies with the model DYRESM. Perroud et al. (2009) compared the ability of four one-dimensional lake models to simulate the water temperature profiles of Lake Geneva. They also observed that this underestimation of the model DYRESM in the metalimnion and the hypolimnion was due to insufficient heat diffusion from above and that there is no variation in the simulated water temperatures below a depth of 50 m. Nevertheless, Perroud et al. (2009) found that DYRESM is one of the best one-dimensional models to reproduce the variability of the water temperature profiles satisfactorily. In another study by Copetti et al. (2006), the model DYRESM was also capable of simulating the surface temperature seasonal trend and the thermal gradient accurately with an underestimation of the bottom water temperatures during summer stratification. The investigation by Gal et al. (2003) showed that the metalimnion was the part of the water column in which the largest variation between simulated and measured water temperatures occurred all year round.

When calculating the MAE and RMSE in different depths (Table 5), in the upper 13 m, with the exception of depths of 8 and 10 m, we observed lower MAE and RMSE values in the calibration period (2004–2007) than in the validation period (1993–1999). This finding could be due to a higher variability in measured water temperatures during the longer validation period and the fact that the model parameters were adapted especially for the years used for calibration. The fact that the validation produces lower MAE and RMSE below 13 m than the calibration does seem surprising but was readily detected by Trolle et al. (2008). In general the error values in our study are similar to the MAE and RMSE values in other DYRESM investigations. Our RMSE maximum of 2.83 K was observed during validation (1993–1999) at the water surface, while Perroud et al. (2009), for example, calculated a RMSE maximum of 3.00 K at a depth of 5–15 m. With respect to the MAE and RMSE results, which show good compliance between simulated and measured water temperatures, it can be assumed that DYRESM is suitable for modelling future thermal characteristics for Lake Ammersee. Therefore, it is necessary to use the input data from regional climate models to simulate future meteorological conditions. However, when using a regional climate model, it is advisable to consider difficulties, e.g. different orography of the study areas and different model cell sizes (Jacob et al., 2007, 2008). Afterwards, the models can provide all the necessary meteorological input data to simulate the heat content and the ecosystem of a lake.

For that purpose, we noticed that initially it is necessary to correct this climate input data with a bias value (Table 4). Furthermore, the necessity of a bias correction when using data from the regional REMO model was also addressed in detail by former studies (Mudelsee et al., 2010; Piani et al., 2010; Terink et al., 2010). In our investigation, we observed (Fig. 6) that the bias-corrected monthly mean air temperature from 2041–2050 rose, especially in winter. This finding matches the predicted trend for the entire northern hemisphere (Solomon et al., 2007). We also observed an obvious increase of mean air temperatures in August. These future increases in summer air temperatures will in turn cause a water warming (Ambrosetti and Barbanti, 1999; Livingstone, 2003; Thompson et al., 2005; Schneider and Hook, 2010) and consequently important ecological changes in the lake (Quayle et al., 2002; Adrian et al., 2009).

In our simulation results at Lake Ammersee for the period 2041–2050 (Fig. 7), we modelled the water temperature maximum in August. Our predictions were in accordance with the estimated increase in mean air temperatures in August derived from the REMO regional climate model; the air temperature values are shown in Fig. 6. Also the predicted increase in mean air temperatures in winter is reproduced by increasing simulated water temperatures in November, December, February and March and is reflected in the earlier occurrence and longer lasting duration of thermal stratification (Table 6). All these results emphasise the impact of meteorological conditions on the water column (Livingstone, 2003; Schneider and Hook, 2010).

5. Conclusion

In our case study on Lake Ammersee, we showed that the hydrodynamic model DYRESM, after careful calibration and validation, is suitable to simulate the current and future heat content of lakes. The model DYRESM underestimated water temperatures in the metalimnion and parts of the upper hypolimnion even after our calibration process. Our investigation also demonstrated that the use of regional climate models such as REMO for hydrodynamic model studies after the obligatory bias-correction is a practicable way to estimate future impacts of climate warming on lake ecosystems in the Northern Foothills of the Alps.

It can be assumed by this investigation, in accordance with previous studies (Quayle et al., 2002; Livingstone, 2003; Salmaso et al., 2007; Adrian et al., 2009; Schneider and Hook, 2010), that higher energy input from the atmosphere has a strong impact, which in turn leads to higher water temperatures, especially at the surface of a lake. The predicted impact on the water temperatures directly affects the stratification characteristics and the mixing processes of a body of water, e.g. the depth of the thermocline, duration of inter-annual stratification and mixing, and the thickness of the metalimnion. Furthermore, a shift in the dates of mixing events (spring and autumn turnover) during the year can be derived from the thermal simulation results (Livingstone, 2003). The depth reached by convective mixing has gradually been reduced in recent decades, and in the future a greater quantity of energy derived from external forces will be required to initialise complete mixing (Ambrosetti et al., 2010). In some deep, temperate lakes, climate warming in the future will likely inhibit complete mixing, even during intense wind storms (Rempfer et al., 2010).

These physical changes in general are a crucial point for the ecosystem of the lake (Quayle et al., 2002; Adrian et al., 2009). In future studies, possible drawbacks on the ecosystem should be investigated, e.g. how it can also produce an eutrophication-like signal in Lake Ammersee (Trolle et al., 2011; Guilizzoni et al., 2012), or how global warming and eutrophication could act together with self-stabilising positive feedback (Rinke et al., 2010). Furthermore, at our study site, ecological processes, such as rates of growth and respiration, could be accelerated, and nutrient cycling in the lake will be intensified due to increasing water temperatures. Also, the stronger stratification could induce changes in the phytoplankton community (Rinke et al., 2010). An increased development of warm-water cyanobacteria will also have impacts on the lake ecosystem, e.g. species such as *Daphnia magna* could be eliminated from surface waters (Bednarska et al., 2011; Gallina et al., 2011).

In conclusion, the limno-physical outcome of the hydrodynamic model DYRESM is suitable as a sound basis for further ecological and limnological studies. Hence, to investigate the possible future ecological consequences on a lake mentioned before, the limno-physical model output has to be coupled with an ecological model of the lake, like realized at other study sites (Burger et al., 2008; Gal et al., 2009; Rinke et al., 2010; Trolle et al., 2011). This finally can contribute to improving our knowledge (Bates et al., 2008; Huber et al., 2008; Fang and Stefan, 2009; MacKay et al., 2009) about modelling the impact of climate change on ecosystems.

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ORIGINAL ARTICLE

Lake heat content and stability variation due to climate change: coupled regional climate model (REMO)-lake model (DYRESM) analysis

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ABSTRACT

Climate change-derived higher air temperatures and the resulting increase in lake surface temperatures are known to influence the physical, biological and chemical processes of water bodies. By using hydrodynamic lake models coupled with regional climate models the potential future impact of a changing climate can be investigated. The present study hence elucidates limno-physical changes at the peri-Alpine, 83-m deep, currently dimictic Ammersee in southeastern Germany, both to underline the role of lakes as sentinels of climate change and provide a sound basis for further limnological investigations. This was realised by using water temperatures simulated with the hydrodynamic model DYRESM for the period 2041-2050, based on the results of the regional climate model REMO (IPCC A1B emission scenario). Modelling of future heat content resulted in a projected increase in the upper 3 m of the epilimnion from end of March to mid-November, whereas a decrease in future total heat content (January-December) of the entire water column was simulated compared to that observed in 1997-2007. Lake thermal stability is projected to be higher in the period 2041-2050 than in 1985-2007. Stratification is expected to occur earlier and to last longer in the future than the pattern observed in 1985-2007. The future mean May-June depth of the thermocline is simulated to be situated above its past average vertical position, whereas an increase of mean thermocline depth is projected for the beginning of August to October. Furthermore, the mean May-October thickness of the metalimnion is simulated to increase. Additionally, we investigated the sensitivity of these limno-physical results to changes in the model parameter light extinction coefficient which determines how the solar radiation is absorbed by the lake water. The elucidation of physical changes at Ammersee by means of a regional climate model provides a sound basis on which to face the new challenges of lake modelling.

Key words: DYRESM, lake Ammersee, regional climate model REMO, aquatic ecosystem, stratification, water management.

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INTRODUCTION

The impact of climate change-driven increases in air temperature on lake water temperatures has been the subject of numerous studies in recent years (Livingstone, 2003; Adrian *et al.,* 2009; Fang and Stefan, 2009; Williamson *et al.,* 2009a; Ludovisi and Gaino, 2010; Schneider and Hook, 2010; Weinberger and Vetter, 2012). The resulting heating of the vertical water column in turn leads to substantial changes in the physical properties of the lake (Gaiser *et al.,* 2009; Ambrosetti *et al.,* 2010; Braig *et al.* 2010; Rempfer *et al.,* 2010), more precisely in terms of mixing processes, stratification characteristics (Danis *et al.,* 2004; Ambrosetti and Barbanti, 2005; Austin and Colman, 2008; MacIntyre *et al.,* 2009; MacKay *et al.,* 2009; Rimmer *et al.,* 2011) and heat content (Hondzo and Stefan, 1993; Dokulil *et al.,* 2006; Vetter and Sousa, 2012). Investigations dealing with these limno-physical changes are crucial, as the latter directly influence nearly all biological and chemical processes. For example, substantial trophic- and species-dependent changes are caused by shifts in the climate regime of lakes (Kirilova *et al.,* 2009; Wagner and Adrian, 2009; Rinke *et al.,* 2010; Gallina *et al.,* 2011), while the distribution of nutrients and oxygen is also affected (Braig *et al.,* 2010; Rempfer *et al.,* 2010; Vetter and Sousa, 2012).

In order to improve our understanding of the aforementioned physical, biological and chemical processes, it is necessary to use hydrodynamic and ecological lake models (Huber *et al.,* 2008; Fang and Stefan, 2009; Ambrosetti *et al.,* 2010) in addition to field studies and statistical analysis of historical lake data (Peeters *et al.*, 2002). These mathematical models are able to simulate the future impact of a changing climate on lake ecosystem and water quality (Perroud *et al.,* 2009). Even though others have already made this point, there remains a need for substantial studies investigating these environmental consequences. Such investigations should utilise data and information derived from regional climate models, *e.g.* REMO (Jacob *et al.,* 2007), which represent the only tools able to satisfactorily estimate future rates of climate change (Samuelsson, 2010). The simulations produced by these climate models are based on different IPCC emission scenarios (Nakicenovic *et al.,* 2000; Solomon *et al.,* 2007). However, information gaps remain in modelling impacts on limnological ecosystems (MacKay *et al.,* 2009); studies using regional climate model data were largely unavailable in the past (Bates *et al.,* 2008).

As a result of the above-mentioned issues, in Weinberger and Vetter (2012) a first hydrodynamic simulation approach was implemented using the hydrodynamic model DYRESM (Imberger and Patterson, 1981; Imerito, 2007), based on the results of the regional climate model REMO for Ammersee. Initially the one-dimensional model DYRESM was calibrated and validated to simulate lake vertical thermal distribution, with meteorological data from the regional climate model REMO (IPCC A1B emission scenario) then employed as input data for DYRESM and a simulation run carried out for the period 2041-2050. The produced results regarding potential future water temperature changes thus provide the basis of the present study, making it possible to address the limno-physical impacts of climate change in particular.

The study site, Ammersee, is a peri-Alpine, 83-m deep, currently dimictic lake located 30 km southwest of the Munich metropolitan area. The third largest lake in Bavaria and very important for regional tourism and fisheries, Ammersee has a surface area of 46.6 km^2, a water volume of 1.75×10^9 m^3 and a glacial morphologic origin. Ammersee was selected as the study site because of its geogenic, climatic, geographic and limnological characteristics, which are representative of many other lakes in the northern foothills of the Alps. The lake freezes over in winter in some years (Danis *et al*., 2004). It has one main inflow called the Ammer, three smaller inflows known as the Windach, Rott and Kienbach, and one main outflow called the Amper. The Ammersee would naturally be oligotrophic (Kucklentz, 2001; Vetter and Sousa, 2012), but due to intensive land use in the catchment area from around 1950, the lake became mesotrophic. In the last 20 years Ammersee has undergone re-oligotrophication after the establishment of specialised sewerage (Ernst *et al,*. 2009), but whether this trend will continue under projected climate change conditions is not clear (Vetter and Sousa, 2012). Different estimations have been postulated regarding future limno-physical and ecological development as a consequence of anthropogenic and climatic impacts. Danis *et al.* (2004), for example, projected Ammersee to undergo a dramatic and persistent lack of mixing, starting in around 2020; the resulting lack of oxygenation would irreversibly destroy the lake's deep-water fauna. Joehnk and Umlauf (2001) mentioned the importance of modelling oxygen conditions in Ammersee. These environmental risks, as well as the desire to improve the existing level of knowledge regarding the impact of climate change on limnological systems and their catchment area (Niedda and Pirastru, 2013), demonstrate the necessity of new modelling studies using well-prepared regional climate model data (Mooij *et al.* 2010; Trolle *et al.,* 2011). In doing so it is then possible to estimate the lake's ecological future and support subsequent water quality management. Studies employing DYRESM have been able to effectively simulate future Ammersee water temperature changes (Weinberger and Vetter, 2012; Bueche and Vetter, 2013), with the model now established as a sound basis for the deduction of prospective limno-physical variations.

The objective of the present study was to therefore use the predicted water temperatures simulated by the hydrodynamic model DYRESM, based on the results of the regional climate model REMO (IPCC A1B emission scenario), to calculate i) the heat content of Ammersee for the years 2041-2050; and ii) the thermal stability of the lake water column for the same period. These results were then assessed and compared to past limno-physical properties of Ammersee. In addition iii), changes in the duration of thermal stratification were investigated, while iv) the depth of the thermocline as well as the depth of the upper and lower metalimnion were also deduced. Finally, v) the sensitivity of the limno-physical results to the model parameter light extinction coefficient was analysed. To underline the motivation for this study it should be said, that the elucidation of physical changes by means of a regional climate model at Ammersee can provide further important knowledge with which to estimate the potential impact of climate change on water bodies in the northern foothills of the Alps.

METHODS

The present study used the one-dimensional hydrodynamic model DYRESM (v4.0.0-b2), developed by the Centre for Water Research at the University of Western Australia. Able to predict the vertical distribution of temperature, salinity and density in lakes and reservoirs (Imberger and Patterson, 1981), DYRESM is a process-based model with a Lagrangian layer scheme, which means that the horizontal layers are adjusted to stay within user-defined limits (Imberger and Patterson, 1981; Antenucci and Horn, 2002). Layer mixing appears when the turbulent kinetic energy in the topmost horizontal layer, produced via convective overturn, wind stirring and shearing (Perroud *et al.,* 2009), exceeds a potential energy threshold. DYRESM has been applied to different study areas around the world (Han *et al.,* 2000; Gal *et al.,* 2003; Romero *et al.,* 2004; Trolle *et al.,* 2008; Perroud *et al.,* 2009; Rinke *et al.,* 2010) and is particularly suitable for the simulation of longer periods. In comparison to other one-dimensional lake models, DYRESM is able to satisfactorily reproduce the variability of both water temperature profiles and seasonal thermoclines (Perroud *et al.,* 2009). DYRESM can also be run either in isolation for hydrodynamic studies, or coupled to an aquatic ecological model, *e.g.* CAEDYM, for the investigation of biological and chemical processes (Imerito, 2007). For the analysis of Ammersee, DYRESM was carefully calibrated (for the period 2004-2007) and validated (1993-1999) taking into account simulated and measured water temperatures. Furthermore, to determine the quality of the calibration and validation process, modelled and observed data were compared via the use of regression analysis and the quality criteria mean absolute error (MAE) and root mean square error (RMSE) (Legates and McCabe, 1999). As small mean absolute errors (0.96-1.61 K) and root mean square errors (1.42-1.96 K) were observed, as well as high coefficients of determination (0.71-0.96) at all depths, the selected hydrodynamic model was considered able to identify the potential drawbacks of climate change on the lake and thus provide the basis for subsequent coupled aquatic ecological modelling.

Nevertheless, it has to be said that DYRESM is originally not able to continue the simulation process when water temperatures decrease below 0°C. Hence, at Ammersee, we used a modified version with freezing avoidance, which means that negative values of water temperature were set back to 0 °C to ensure a continuous and stable simulation. Although, because of this, ice cover is not included in the model directly, the introduced error is small for large peri-Alpine lakes as they rarely freeze and the cooling-down is not very intense. Full ice cover was observed at Ammersee in 15 years from 1934 to 1971 (Danis *et al.,* 2004). For the period from 1971 to 2012 there are no publications dealing with ice cover available, but according to own observations and analyses the lake has frozen over in 5 years. Moreover, the effect of freezing avoidance diminishes throughout the season when surface temperatures are approaching a value corresponding to the equilibrium energy exchange between the lake and the atmosphere (Weinberger and Vetter, 2012). More details regarding the comprehensive calibration and validation of DYRESM for Ammersee can be also found in Bueche and Vetter (2013).

When estimating the impact of climate change on lakes, it is generally advisable to use meteorological input data produced by regional climate models. The climate data employed in the present study were acquired from the regional climate model REMO (Jacob *et al.,* 2007), which was selected because its cell calculation size of 10x10 km was considered suitable for analysis of the Ammersee area. The REMO simulation provides variables including short-wave radiation, air temperature, precipitation, wind speed, vapour pressure, total cloud cover and relative humidity, all of which have a strong influence on the heat budget of a lake. Long-wave radiation was estimated from atmospheric conditions using cloud cover fraction (Imerito, 2007). Use of REMO data also requires the implementation of bias correction; this process had already been carried out in an earlier study by comparing previously-measured meteorological data from the study area (covering the period 1990-2006) with those simulated by the regional climate model (2001-2017) (Weinberger and Vetter, 2012). Based on these comparisons, statistical relationships for each month could then be determined that were relevant to the correction of calculated future climatic conditions. For example, when correcting the air temperature values derived from the REMO model, an absolute correction value was adapted to the daily mean air temperatures, whereas the correction of daily precipitation sums was implemented relatively via the use of a multiplication factor (Piani *et al.,* 2009; Mudelsee *et al.,* 2010; Terink *et al.,* 2010). Our investigations demonstrate that the use of regional climate models such as REMO in hydrodynamic model studies (after obligatory bias correction) is a practicable way of estimating future impacts of climatic warming on lake ecosystems in the northern foothills of the Alps.

The research presented in Weinberger and Vetter (2012) and taken as basis for this study, includes such a simulation for Ammersee, based on the IPCC A1B emission scenario for the period 2041-2050. The A1B emission scenario was selected due to the fact that it assumes balanced use of all available energy sources (Nakicenovic *et al.,* 2000; Solomon *et al.,* 2007). In this scenario, the global mean air temperature is predicted to increase by about 3 K between 1990 and 2100. Future climate change conditions in the present study were also derived from the aforementioned regional climate model REMO; the vertical thermal distribution in Ammersee was then simulated for the period 2041-2050 using bias-corrected REMO meteorological data as input values for the hydrodynamic model DYRESM. This simulation method is, as mentioned previously, now established as a sound basis on which to both deduce potential future physical changes, such as those mentioned in the Introduction, and to provide further important knowledge which can be used to estimate the potential impact of climate change.

To clarify which are the main drivers for changes in limno-physical conditions in the future we investigated sensible, latent and radiative heat fluxes. At Ammersee, the sensitivity of the hydrodynamic model DYRESM to changes in meteorological input variables and to changes in water temperatures of the inflow was analysed. Thereby the greatest influences on the heat budget and on the dynamics of the lake were detected for modifications of air temperature and wind speed (Bueche and Vetter, 2013). The variable wind speed is known to influence mixing and the exchange of both latent and sensible heat at the water surface (Livingstone, 2003). The fact that the variable air temperature has the greatest ramifications was also detected by Trolle *et al*. (2011), who included only a simple air temperature offset in representing future meteorological conditions in their lake modelling study. All the changes in monthly mean air temperatures simulated by the model REMO (A1B scenario) until the period 2041-2050 at Ammersee can be seen in Tab. 1. To elucidate that there are also existing more pessimistic emission scenarios than A1B, in Tab. 1 we additionally show bias-corrected air temperatures based on the emission scenario A2. This scenario assumes that the global mean air temperature will increase by about 3.5 K between 1990 and 2100 due to regionally oriented economic development and a continuously increasing world population (Nakicenovic *et al.,* 2000). For further limno-physical research at Ammersee, as mentioned before, in this study we take the scenario A1B as basis, which is based on assumptions that are more realistic.

Nevertheless, the potential effects of other meteorological variables and processes should not be neglected. For example cloud cover can affect both long-wave and short-wave radiation, while relative humidity influences the exchange of latent heat (Livingstone 2003, Trolle *et al.* 2011). Hence these variables, provided by the regional climate model REMO, were also taken into account in our study at Ammersee. To compare the simulated hydrodynamic results with data obtained in the field, a series of water temperature and conductivity measurements were used which have been collected at Ammersee since 1976, with regular readings carried out since 1985. These data are collected at the deepest point of the lake by the Bavarian Environmental Agency. Measurements within the epilimnion are taken every 2 m, in the metalimnion every 3 m and in the hypolimnion every 10 m. The time step of data collection has varied, but in general measurements have been carried out at least every month. This field data both provided a sound basis for the calibration and validation of the hydrodynamic model DYRESM employed in Weinberger and Vetter (2012), and was also used to calculate past values of limno-physical variables for the present study. Total lake heat content (W) can be calculated by summing the heat content of single layers (from lake surface to lake bottom) based on their mean water temperatures (Schwoerbel and Brendelberger, 2005):

$$\mathbf{W = \int_0^{Z_{max}} T(z) c_p(z) \rho(z) A(z) d(z)} \quad \text{(eq. 1)}$$

where T(z) is the mean water temperature (°C) at depth z, $c_p(z)$ is the specific heat capacity (kJ kg^{-1} K^{-1}) at depth z, ρ(z) is the density of water (kg m^{-3}) at depth z, A(z) is the isobath plane (m^2) at depth z and d(z) is the depth interval. In addition to mean total lake heat content, heat content was also calculated for the layers from 0-3, 3-10 and below 10 m. To make it easier to compare the results for Ammersee with results of similar studies, the heat content is additionally given in terms of volume-weighted mean (VWM) temperatures.

To derive the thermal stability of the water column, values of Schmidt stability were determined according the following equation:

$$S = g A_0^{-1} \int_0^{Z_{max}} (z - z^*)(\rho(z) - \rho^*) A(z) d(z) \quad \text{(eq. 2)}$$

where A_0 is lake surface area (m^2), A(z) is lake area (m^2) at depth z, ρ(z) is density (kg m^{-3}) calculated from temperature at depth z, ρ* is the volume-weighted mean density of the water column (kg m^{-3}), z* is the depth (m) at which mean density occurs, d(z) is the depth interval (m) and g is acceleration due to gravity (m s^{-2}). Representing the work that would be required to transform a thermally stratified lake into a lake characterised by isothermal conditions, the Schmidt stability value has been used to account for the intensity of summer stratification in a number of lake studies (Ambrosetti and Barbanti, 2005; Gaiser *et al.,* 2009; Braig *et al.,* 2010). Other climate change impact studies that have used Schmidt stability as a measure of lake stratification include Livingstone (2003), Coats *et al*. (2006), Jankowski *et al*. (2006) and Rempfer *et al.* (2010). Calculation of Schmidt stability requires the determination of lake water density and conductivity. For Ammersee, the density at different depths was calculated according to Chen and Millero (1986), while conductivity was determined using the relationship between temperature, density and water pressure in the water column (UNESCO 1987).

Also deduced was the duration of lake thermal stratification for the simulated period 2041-2050; again this was then compared to the observed duration of stratification in the past (1985-2007). The present study follows the work of Birge (1897), who defined the thermocline as the region in the vertical profile of a lake, where the temperature decreases by 1 K per metre of depth. If such a difference in temperature is measured or simulated, the

Tab. 1. Monthly mean air temperature (°C) at lake Ammersee measured in the past and simulated for the future by the model REMO.

Month	1990-2006	2041-2050 A1B	2041-2050 A2
January	-0.4	1.9	1.8
February	0.1	1.9	1.2
March	3.1	4.4	4.7
April	6.0	6.8	8.2
May	11.5	12.4	13.1
June	14.5	14.8	15.7
July	16.3	16.2	17.2
August	16.4	17.2	16.6
September	12.0	11.7	13.9
October	8.4	9.4	9.2
November	2.9	4.6	4.5
December	0.0	1.3	1.1

Values are bias-corrected and based on emission scenarios A1B and A2.

lake is considered stratified at that time. As per Hutchinson (1957), the thermocline was also considered as the depth plane at which the largest relative change in water temperature occurs. Using observed past water temperatures and simulated water profiles for the period 2041-2050, it was possible to detect changes in the depth of the thermocline potentially due to climate change. Definition of the upper and lower borders of the metalimnion was carried out in the same manner as the deduction of the duration of thermal stratification, *i.e.* following Birge (1897). Accordingly, the metalimnion was considered to be the region in the vertical profile of a lake within which the temperature decreases by 1 K per metre of depth.

To assess whether the differences between the estimated changes for the future, deduced from the hydrodynamic model, and the measured historical data are statistically significant, we conducted Welch two-sample *t*-tests for the variables duration of thermal stratification, depth of thermocline and Schmidt stability. After calculation of limno-physical variables for the future, we also investigated the sensitivity of these results to changes in the parameter light extinction coefficient (LEC) of the water, which has to be set in the input files of the hydrodynamic model DYRESM. This parameter determines how the solar radiation is absorbed by the lake water and directly influences the heating of the epilimnion (Imberger and Patterson 1981). Hence the LEC was already used for the calibration of the model DYRESM at Ammersee and at the end set to 0.25 m^{-1} (Weinberger and Vetter, 2012). For our sensitivity analysis in the recent study we first reduced the LEC by 10% to a value of 0.225 m^{-1} and afterwards raised the LEC by 10% to a value of 0.275 m^{-1}.

RESULTS

Heat content

Lake heat content was calculated for the layers from 0-3, 3-10, below 10 m and for the whole lake. This was achieved using both simulated (future) and measured (past) data. Fig. 1 presents a comparison of the resulting mean heat content for each month for the periods 2041-2050 and 1997-2007.

Analysis of graph a in Fig. 1 reveals that the heat content of the upper 3 m of the epilimnion is predicted to be higher in the future from end of March to mid-November. The highest increase is expected during June to October, with the maximum heat content simulated at 12 GJ or

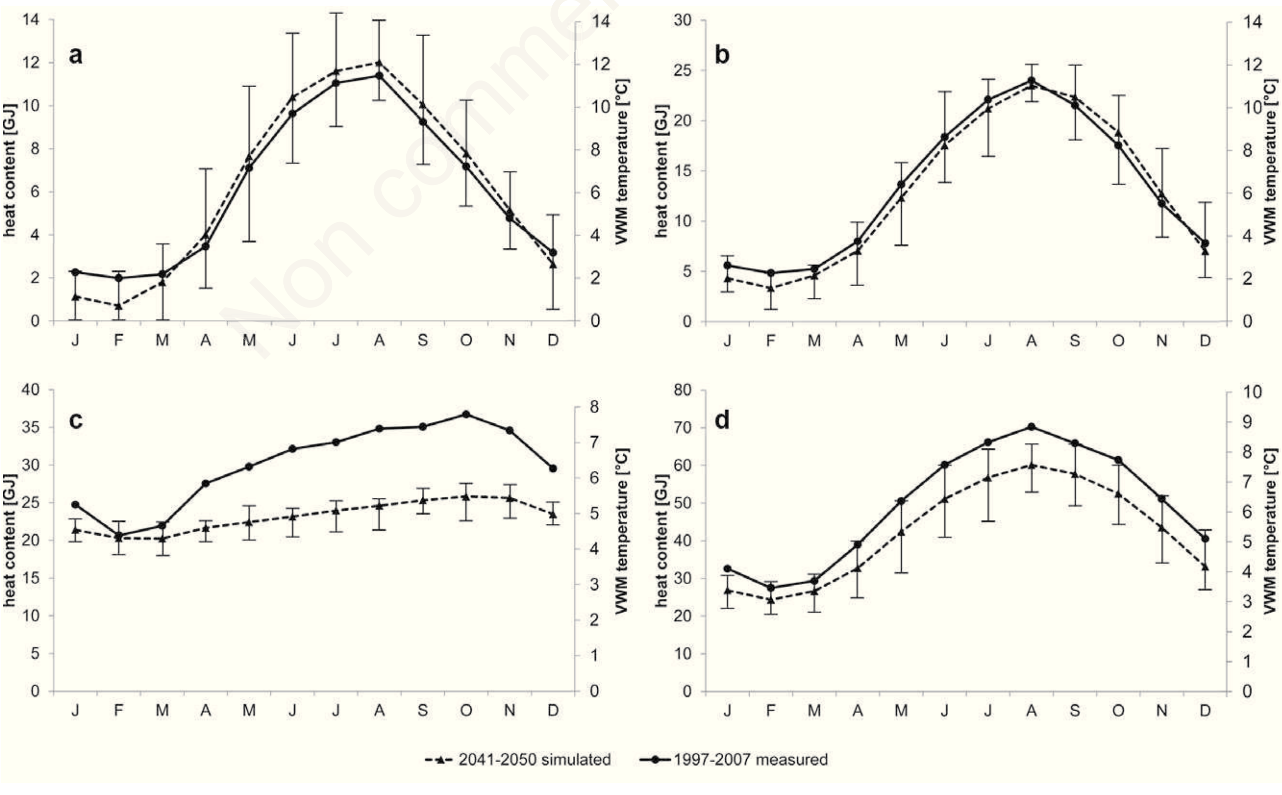

Fig. 1. Monthly mean heat content and respective volume-weighted mean (VWM) temperature at a depth of 0-3 (a), 3-10 (b), below 10 m (c) and for the whole lake (d), calculated for Ammersee from measured (1997-2007) and simulated data (2041-2050, A1B emission scenario). The error bars show the maximum and the minimum of the simulated values used to calculate the simulated monthly mean.

12°C (volume-weighted mean (VWM) temperature) in August. The measured maximum was also observed in August, at 11.5 GJ (VWM temperature: 11.5°C). Winter values are projected to be lower than in the past. Between 3 and 10 m depth (Fig. 1b), an increase in heat content is predicted only for September, October and November; an obvious decrease is estimated for January and February, while in the remaining months a merely slight decrease is visible from the past to the period 2041-2050. Below 10 m depth (Fig. 1c), a clear decrease in January as well as from April to December lake heat content is simulated, with a maximum decrease of around 10 GJ (VWM temperature: around 2°C) projected for October. February lake heat content is expected to remain nearly constant, whereas March values are predicted to decrease only slightly in the future. Analysis of total lake heat content (Fig. 1d) reveals decreasing values for the whole year. Maximum total heat content for Ammersee was observed in August for both measured and simulated values, at 70 GJ (VWM temperature: 9°C) and 60 GJ (VWM temperature: 7.5°C), respectively.

When calculating the heat content, the process of freezing avoidance during the simulation run, as mentioned in the *Methods*, should be considered. Thereby negative values of water temperature are set back to 0°C to ensure a continuous and stable simulation. During eleven years of calibration and validation (2004-2007 and 1993-1999) at Ammersee (Weinberger and Vetter, 2012), water temperatures were set back to 0°C by the model DYRESM on 49 days, whereas during the 10 years-model run from 2041 to 2050 the freezing avoidance was set up on 63 days.

Thermal stability

Fig. 2 presents a comparison of box-and-whisker plots for observed (past: 1985-2007) and simulated (2041-2050) Schmidt stability data for each month relevant to thermal stratification. The boxes in Fig. 2 consist of median and upper and lower quartile (25th and 75th percentile), with upper and lower whiskers and some outliers also illustrated. The end of the upper whisker in the present case study was set at the 97.5th percentile, and the end of the lower whisker at the 2.5th percentile of the data. Outliers were defined as only those values lying beyond the threshold of 1.5 times the interquartile range (IQR) above the 75th percentile.

It is apparent from analysis of Fig. 2 that lake thermal stability is expected to increase in the future for each month from April to November, with the simulated 25th percentile, median and 75th percentile lying above the respective observed field data values. Indeed, in April and August the projected 25th percentiles are nearly as high as the measured 75th percentiles for the same months. Furthermore, all upper and lower whiskers, with the exception of those for October and November, are projected to be higher in the future. Also included were the minimum and maximum Schmidt stabilities, as well as the upper outliers (Tab. 2).

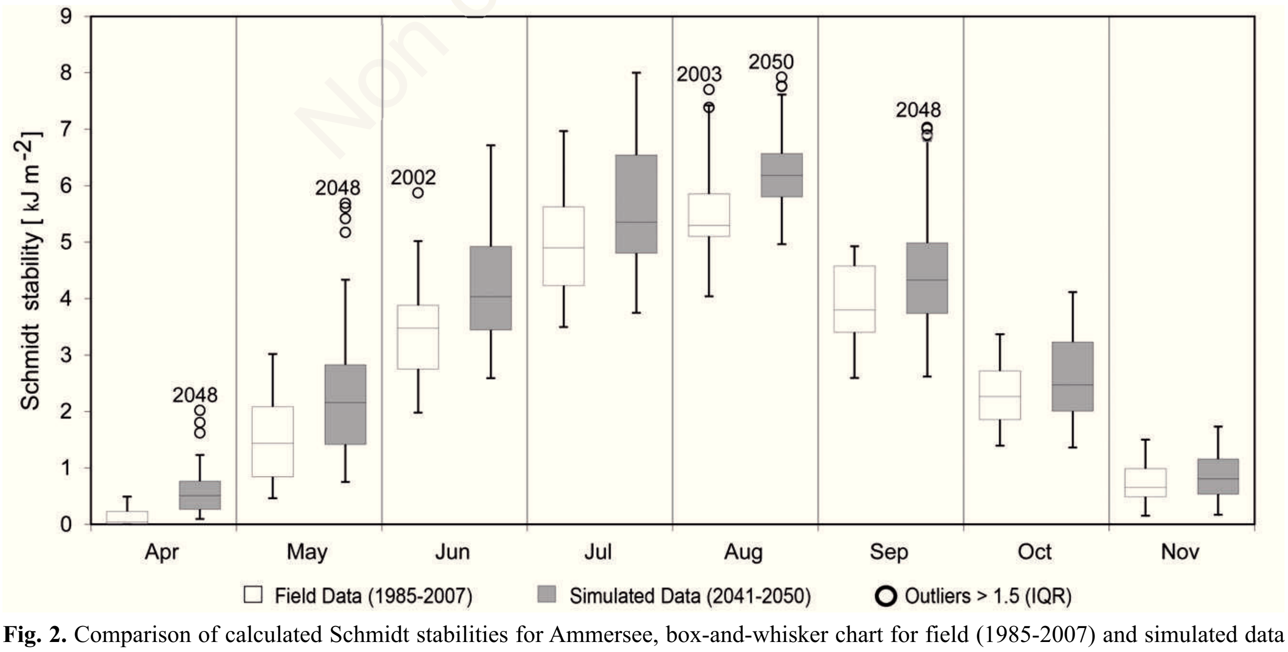

Fig. 2. Comparison of calculated Schmidt stabilities for Ammersee, box-and-whisker chart for field (1985-2007) and simulated data (2041-2050, A1B emission scenario) with outliers for different months. Maximum outliers are specifically marked by year number.

The number of upper outliers as defined in the boxplot chart is also predicted to increase in the future (2041-2050), with 3 occurring in April, 4 in May, 3 in August and 5 in September. During the period 1985 to 2007, only 1 outlier was observed in June (5.87 kJm^{-2} in 2002) and 2 outliers in August (maximum outlier 7.70 kJm^{-2} in 2003). All upper outliers as well as the year number corresponding to the maximum outliers are also shown in Fig. 2. While minimum Schmidt stabilities are simulated to remain similar to those observed in the past, monthly maximum values are expected to increase clearly, with the exception of those in August and November. In May and September the increase in maximum thermal stability is expected to be higher than 2 kJm^{-2}, while the maximum predicted monthly value of 8.59 kJm^{-2} is projected to occur in July (Tab. 2).

To assess whether these changes in Schmidt stability are statistically significant, we conducted a Welch two-sample *t*-test (Tab. 3). Thereby it becomes obvious that the increase in thermal stability is highly significant from April to October.

Duration, onset and end of thermal stratification

Another aspect of possible limno-physical change resulting from increasing water temperatures is the duration and timing of onset of thermal stratification. The simulated stratification behaviour of Ammersee for the period 2041-2050 was thus compared with observed stratification data for the period 1985-2007. During the former, thermal stratification is modelled to commence on average on the 27th of April and end on the 8th of November, with the earliest date of onset the 16th of April and the latest end the 19th of November. The average date of observed stratification according to field data was the 15th of May, with the average end of stratification date the 10th of October. The earliest historic onset was observed on the 7th of May, and the latest end on the 22nd of October. The longest period of stratification during the years 1985-2007 was 169 days, whereas the shortest lasted for only 127 days. The duration of thermal stratification at Ammersee is simulated to increase significantly in the future (Welch two-sample *t*-test, P=0.0011*)*, with a maximum of 204 days and a minimum of 162 days. A summary of the obtained data is provided in Tab. 4.

Fig. 3 displays the duration of simulated thermal stratification for each year during the period 2041-2050; the vertical black lines represent the observed average beginning and end dates of stratification recorded between 1985 and 2007. Analysis of Fig. 3 and Tab. 4 reveals not only a projected increase in the duration of thermal stratification, but also that the shortest period of stratification in the future is estimated to be nearly equal to the longest period measured in the past. In summary, thermal stratification of Ammersee is expected to occur earlier and to last longer than previously recorded.

When looking at Fig. 3 and Tab. 4, it is very important to consider that it is not possible to predict dates of onset and end of thermal stratification exactly. We are only able to deduce these dates directly from the simulated water temperatures using a daily model time step. Thereby we follow Birge (1897), as mentioned above and take into account mean dates during each period.

Depth of thermocline and metalimnion

Any changes in the position of the thermocline are expected to be very important for the ecology of water bodies. In the present study two methods of analysis were

Tab. 2. Number of upper outliers, maximum and minimum values (kJ m^{-2}) of Schmidt stability for the past and the future.

Month	Past (1985-2007)			Future (2041-2050)		
	Outliers	Max	Min	Outliers	Max	Min
April	0	0.51	0	3	2.02	0.03
May	0	3.37	0.14	4	5.69	0.58
June	1	5.87	1.96	0	7.06	2.35
July	0	7.22	3.50	0	8.59	3.17
August	2	7.70	3.80	3	7.92	4.51
September	0	4.96	2.56	5	7.03	2.31
October	0	3.64	1.28	0	4.56	1.03
November	0	1.51	0.13	0	1.87	0

Tab. 3. Comparison of simulated Schmidt stability and depth of thermocline (2041-2050) *vs* measured values of field data, using a Welch two-sample *t*-test.

	Schmidt stability (*t*/df/P)	Depth of thermocline (*t*/df/P)
April	11.0/54/<0.0001	
May	4.4/46/<0.0001	13.6/45/<0.0001
June	5.2/42/<0.0001	8.9/42/<0.0001
July	3.4/49/=0.0015	0.3/58/=0.7762
August	5.3/40/<0.0001	2.4/55/=0.0176
September	4.1/51/=0.0002	8.3/56/<0.0001
October	2.9/43/=0.0058	10.2/48/<0.0001
November	1.2/44/=0.2303	

df, degree of freedom.

Tab. 4. Dates and onset of thermal stratification for the past (1985-2007, observed) and derived directly from the model DYRESM for the future (2041-2050).

	1985-2007	2041-2050
Earliest beginning (date)	7 May	16 April
Latest end (date)	22 October	19 November
Longest period (days)	169	204
Shortest period (days)	127	162

carried out: the first comparing the mean depth of the thermocline as defined by Hutchinson (1957) using recorded (1985-2007) and simulated data (2041-2050) for each month from mid-May to mid-October, and the second contrasting the mean depth and mean thickness of the metalimnion as per Birge (1897) for the same periods. The results can be seen in Fig. 4.

The position of the thermocline relocates towards the lake bottom between May and October in both recorded and simulated data. The minimum mean depth of the thermocline in the past was measured in May at around 6 m, while the projected depth during the same month is around 4 m. The maximum mean recorded depth was observed at around 12 m and the modelled value for 2041-2050 at around 13 m. Between May and June the mean depth of the thermocline is projected to lie above its historically-recorded position, although in July the vertical position of the thermocline is modelled to remain in a similar range to its previous depth. However, for the period from the beginning of August to October, an increase of the mean depth of thermocline is predicted. Using a Welch two-sample t-test, we investigated that the changes in depth of thermocline are highly significant with the exception of July (Tab. 3). The mean thickness of the metalimnion is simulated to increase for the whole period between May and October, with the largest expanse of 8 m occurring at the end of August. In contrast, the largest thickness of 6 m during the period 1985 to 2007 was observed in July.

The mean depth of the upper and lower delineation of the metalimnion increases between May and October in both recorded and simulated data. The recorded and pro-

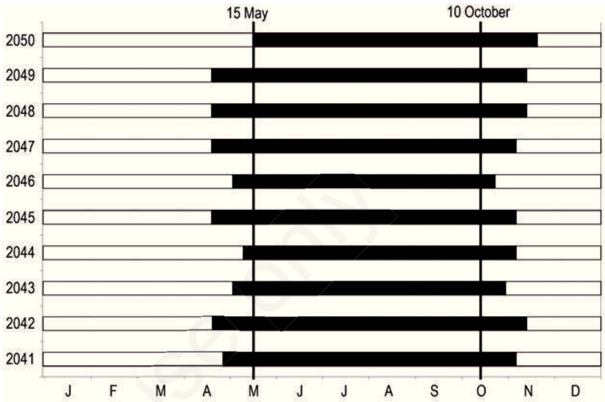

Fig. 3. Expected duration of lake thermal stratification deduced from simulated DYRESM data (2041-2050, A1B emission scenario), together with an illustration of the observed average start and end of stratification (1985-2007).

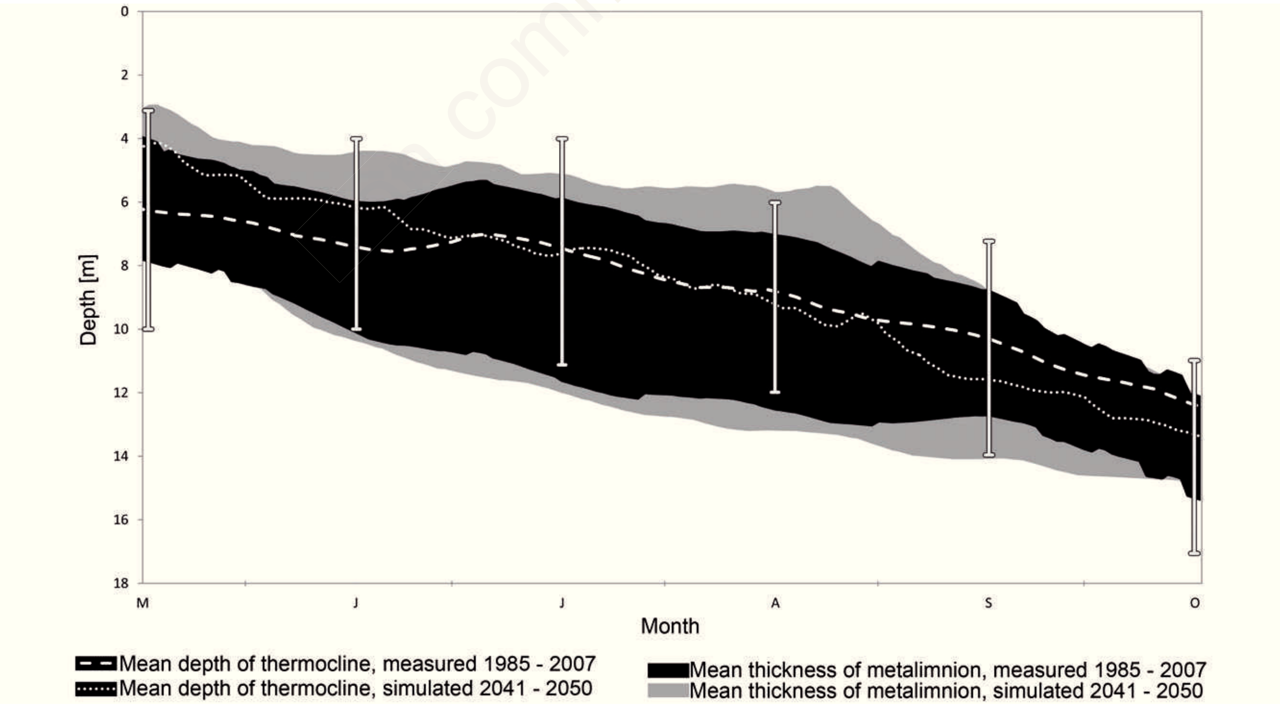

Fig. 4. Mean depth of thermocline and mean thickness of metalimnion deduced from field (1985-2007) and simulated data (2041-2050, A1B emission scenario). The error bars show the maximum and the minimum of the simulated values used to calculate the monthly mean of thermocline depth.

jected minimum mean depth of the upper border of the metalimnion was observed at 4 m and 3 m, respectively, with the maximum mean depth at around 12 m in both periods. The minimum mean depth of the lower border of the metalimnion was around 8 m for both past and predicted data, with the maximum mean depth between 15 and 16 m for 1985-2007 and between 14 and 15 m for 2041-2050.

Sensitivity to light extinction coefficient

The water temperatures simulated by the model DYRESM and the calculated limno-physical variables for the future are sensitive to the parameter light extinction coefficient (LEC) of the water, which has to be set in the input files of the hydrodynamic model DYRESM. For our sensitivity analysis we first reduced the LEC by 10% to a value of 0.225 m^{-1}. This resulted in a slight decrease of modelled surface water temperatures in spring and summer as well as increasing water temperatures in the metalimnion and hypolimnion (below 10m) and a higher heat content of the whole lake (Fig. 5). This in turn resulted in lower stratification and in the following more heat was able to reach the deeper layers. Afterwards we raised the LEC by 10% to a value of 0.275 m^{-1}. As a consequence, we were able to observe just the opposite. This implies that the modelled surface water temperatures in spring and summer slightly increased and decreasing water temperatures were observed in the metalimnion and hypolimnion (below 10m), which resulted in a lower heat content of the whole lake (Fig. 5) and in stronger stratification of the water column.

DISCUSSION

The following section discusses the results of the present study regarding possible physical and ecological consequences, comparing them to the outcomes of similar limnological investigations. When looking at the results of our one-dimensional hydrodynamic modelling study at Ammersee, it should be considered, that the hydrodynamic processes in the lake are obviously simplified (Bayer *et al.,* 2013). Subsequently the model DYRESM for example underestimates water temperatures in the metalimnion and hypolimnion, as investigated during our calibration and validation period at Ammersee (Weinberger and Vetter, 2012). Also the meteorological data provided by the regional climate model REMO, which is derived from a global circulation model, may contain uncertainties in the estimation of the local climate. However these uncertainties can be minimised by a bias correction, as mentioned above. Additionally, even the measured meteorological data may contain measurement errors, which in turn could have an influence on the quality of the calibration process due to the model's strong sensitivity to these climatic input variables (Bueche and Vetter, 2013). Nevertheless, at Ammersee we showed that the models DYRESM and REMO can be used to identify potential drawbacks of climate change on the lake ecosystem (Weinberger and Vetter, 2012).

For the period between end of March and mid-November, an increase in lake heat content is projected (2041-2050) to occur in the upper 3 m of the epilimnion with respect to recorded values (1997-2007) (Fig. 1a). A similar rise in surface water temperatures has also been predicted by other limnological studies investigating the role of lakes as sentinels of climate change (Livingstone, 2003; Adrian *et al.,* 2009; Ludovisi and Gaino, 2010; Schneider and Hook, 2010; Rimmer *et al.,* 2011; Vetter and Sousa, 2012). The highest increase in Ammersee heat content was predicted, as expected, for the months of June to October. Both recorded and simulated maximum heat contents occur in August, which matches the findings of Livingstone (2003) for lake Zurich. The fact, that winter water temperatures are expected to be lower in the period 2041-2050, is likely due to an underestimation of water temperatures by DYRESM (Weinberger and Vetter, 2012). However, this underestimation is of little importance to lake ecological development and thus will not be discussed further here. Whereas only minor changes in heat content between 3 and 10 m depth were projected to take place in future summer months (Fig. 1b), below 10 m (Fig. 1c), *i.e.* in the metalimnion and hypolimnion, a clear decrease was projected occurring from April to January. Only in February is heat content expected to remain nearly constant, with March the only month in which a merely slight decrease was simulated. The simulated development of total lake heat content (Fig. 1d) is expected to be similar, but with decreasing lev-

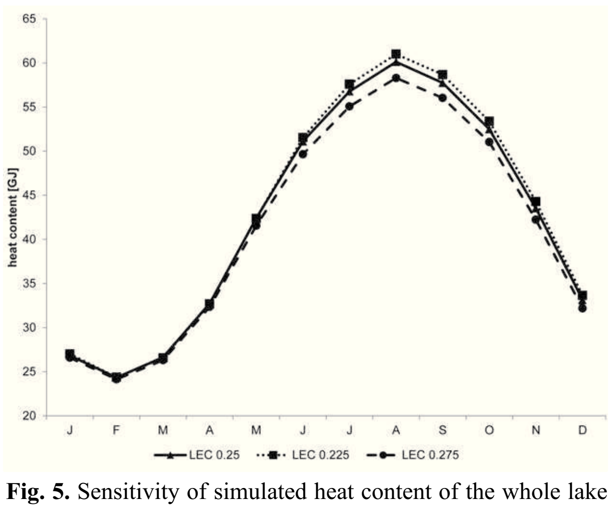

Fig. 5. Sensitivity of simulated heat content of the whole lake (2041-2050) to 10% changes in DYRESM input parameter light extinction coefficient (LEC) (m^{-1}).

els for the whole year until the period 2041-2050. These model results may at first seem surprising; in previous studies, the heat has been observed going beyond the barrier of the thermocline in recent years, suggesting that increasing heat content (even in the metalimnion and hypolimnion) could be a consequence of climate change (Dokulil *et al.,* 2006; Ambrosetti *et al.,* 2010). Therefore it was decided to divide the lake into different horizontal layers for further interpretation, making it possible to investigate the varying response of the water column to higher air temperatures, as well as the resulting heat content at different depths in the future. The predicted decrease in metalimnetic, hypolimnetic and total heat content in the present study could be the result of earlier establishment of a stable water column at higher epilimnetic and lower hypolimnetic temperatures (Livingstone, 2003). Hondzo and Stefan (1993) simulated that after climate change, hypolimnetic temperatures in seasonally-stratified dimictic lakes will be largely unchanged or even lower than at present, in agreement with our results. They also found their modelled data surprising, with the main reason suggested for the predicted values being a more rapid onset of stratification in early spring due to an increased net rate of surface heating after climate change; colder hypolimnetic water is thereby more quickly and effectively shielded from surface heating. Other authors with similar findings include Robertson and Ragotzkie (1990), who expected midsummer hypolimnion temperatures to change very little or increase only slightly in response to climatic warming.

Nevertheless, when calculating the heat content by means of the model DYRESM, the uncertainty based on the use of the modified version for freezing avoidance during the hydrodynamic simulation should be considered. The model DYRESM set back negative water temperatures to 0°C on 49 days during calibration and validation (2004-2007 and 1993-1999) and on 63 days during the future modelling period (2041-2050). Hence we assume that negative water temperatures will still appear in the period 2041 to 2050 and the ice-cover periods will be corresponding to those mentioned by Danis *et al.* (2004), who observed the duration of full ice-cover at Ammersee to be generally less than one month. Anyhow, it should be an objective for future studies at Ammersee, to investigate if the lake will still freeze over in the future and if there will be changes in frequency and duration of ice cover. These changes could have a strong influence on the mixing characteristics and hypolimnetic temperatures of the lake. For example, if the ice-cover disappears completely, there would be a potential for heat carry-over from one year to the next (Peeters *et al.,* 2002) and for changes in the mixing regime of the lake from dimictic to monomictic. One explanation given earlier for the projected decrease in heat content at Ammersee was the potentially higher thermal stability of the water column, which would act as a barrier to heat entering the lake. This theory was verified after calculating Schmidt stability from field (1985 to 2007) and simulated (2041 to 2050) data, with thermal stability expected to be higher in the future for each month from April to November and the number of outliers (as defined in the boxplot chart) also increasing (Fig. 2, Tab. 2). Furthermore, the maximum value of lake thermal stability, which currently stands at the 7.70 kJm^{-2} observed during the outstanding warm year of 2003, is simulated to be exceeded in the period 2041-2050.

The influence of changes in water temperature on lake density gradients and the resulting increase in water column thermal stability has been examined in a number of studies (MacIntyre *et al.* 2009; Williamson *et al.* 2009b; Rimmer *et al.* 2011). The main reason for increased thermal stability is typically a rise in surface water temperatures and a concomitant decrease or constancy in hypolimnetic temperatures, known as the vertical temperature gradient (Livingstone, 2003). Significantly, long-term changes in lake thermal structure may in the future be responsible for a shift in mixing regimes, changing nutrient and oxygen concentrations and thus also the vertical distribution and composition of lake biota (Adrian *et al.,* 2009; Braig *et al.,* 2010; Rempfer *et al.,* 2010). Jankowski *et al.* (2006), for example, detected strong hypolimnetic oxygen depletion associated with an extremely high degree of thermal stability. As a result of increasing thermal stability, a greater quantity of energy derived from external forces will then be required to initialise complete mixing (Ambrosetti *et al.,* 2010). Ammersee is predicted to be affected by a combination of lower heat content in the deeper layers and changes to the timing and duration of thermal stratification. According to a comparison of the projected stratification behaviour of the lake for the simulated period 2041-2050 with observed duration data recorded in 1985-2007, stratification is expected to occur earlier in spring and to last longer through autumn (Tab. 4, Fig. 3). A similar increase in the duration of stratification and reduced duration of winter mixing has also been detected elsewhere (Austin and Colman, 2008; Gaiser *et al.,* 2009; MacKay *et al.,* 2009; Rempfer *et al.,* 2010). Although the simulated maximum duration of stratification at Ammersee was 204 days, no persistent lack of mixing was projected for the period 2041 to 2050. Thus, the lake is estimated to remain dimictic, with complete mixing in autumn and spring and the occurrence of an inverse stratification in winter. Hence, no long-term increase in hypolimnetic water temperatures is visible. This result is different to that of Danis *et al.* (2004), who predicted an absence of mixing at Ammersee, which would irreversibly destroy deepwater fauna, occurring from the year 2020. The increase in stratification duration simulated in the present study approximately matches that of Livingstone (2003), who calculated an extension of 2 to 3 weeks.

Other studies have also predicted long-term variation in thermocline depth as a result of changes in the water column density gradient, *e.g.* Adrian *et al.* (2009). Since the hydrodynamic model DYRESM satisfactorily reproduces the variability of water temperature profiles and seasonal thermocline, and also successfully models the metalimnion boundary (Perroud *et al.,* 2009), it was decided in the present study to determine the extent of possible changes in thermocline and metalimnion depth (Fig. 4). The predicted future reduction in summer epilimnion thickness by Gaiser *et al.* (2009) and Rimmer *et al.* (2011) is in agreement with the modelling results presented here, simulating a decrease in the depth of the upper border of the metalimnion from May to September. In addition, our model results show a deepening of the thermocline from May to October. The limno-physical reasons for that are convective cooling and stronger vertical mixing, which are caused by increased wind speed. More precisely, the surface water temperatures and the thermal stability in autumn decrease and there is sufficient wind to initialise a vertical mixing of the water column. This was also detected by Livingstone (2003), who observed the deepest annual position of the thermocline in autumn. The mean thickness of the metalimnion in the present study was simulated to increase for the entire May to October period in the future (2041-2050), a pattern which contrasts with the findings of Rimmer *et al.* (2011) who observed a decrease in metalimnion thickness between 1969 and 2008. The mean depth of the thermocline at Ammersee could in the future be situated above its historically-recorded vertical May-June position. This change could be due to increased heat input into the lake, as previously mentioned by Tanentzap *et al.* (2007) and as predicted in a number of regional climate models. However, the vertical position of the thermocline in July is projected to remain constant, a result similar to that of Robertson and Ragotzkie (1990), who simulated both no change in thermocline depth during midsummer and a shallower position in autumn. This latter prediction was also determined in the present study, with mean thermocline depth projected to increase between the beginnings of August to October with respect to observed data (1985-2007).

In this paper, it was also possible to show that the modelled physical properties of the lake are sensitive to a 10% change in light extinction coefficient (LEC) of the water. Our findings, that higher LEC results in increasing modelled surface water temperatures in spring and summer as well as in decreasing water temperatures in the metalimnion and hypolimnion (below 10 m) for the same period, are in line with the results of previous studies. In general it can be said that the LEC is known to affect the vertical distribution of heat in the water column (Tanentzap *et al.,* 2008; Rinke *et al.,* 2010). Also the lower heat content of the whole lake (Fig. 5) and the stronger stratification of the water column with increasing LEC were already detected in aforementioned studies. Since LEC describes water transparency, which is subject to ecological conditions in the lake, the physical properties of lakes are not only the basis to simulate ecological conditions, but also are affected by changes in the trophic state of the water body.

CONCLUSIONS

The coupling of regional climate and hydrodynamic models enables forward-looking statements to be made regarding the limnological impact of climate change. Although the results obtained via this method are of course just estimations, such coupling remains yet the only available tool with which to assess the aforementioned effects. In the present study, it was possible to elucidate a wide range of limno-physical consequences that can be investigated by the use of these models, with a concrete examination made of an important mid-European, comparatively large fresh water body. Evaluation of the relevant literature reveals that the impact of a changing climate on the lake's hypolimnetic heat content is particularly contested and should thus be explored further using new modelling techniques. In our opinion and according to the presented simulation results, the hypolimnetic heat content of Ammersee will experience a clear decrease in the future due to higher thermal stability in the water column. Anyhow, we estimate that the mixing type of Ammersee will remain dimictic. Additionally, it is essential that further limnological research is conducted to assess the impact of changes in ice cover as well as to allow a coupling of the hydrodynamic model with an ecological model of the lake. It is therefore also advisable to conduct and assess carefully calibrated and validated limno-physical modelling. The present study represents a sound basis for such modelling, with the employed methods recommendable for other members of the lake ecosystem modelling community (Mooij *et al.,* 2010).

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Title: "Automated tools for lake-related climate change impact modelling"

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Abstract

To improve the simulation of limnological conditions in the future and facilitate the use of results of the regional climate model REMO as input data for hydrodynamic lake models, we show a workflow, supported by information technology (IT). We created an application (Linux Shell script) to convert and customise REMO data automatically and provide a macro in Visual Basic for Applications (VBA) to assemble and pre-process meteorological input data for the hydrodynamic model DYRESM. An automated, geographic information system (GIS)-based analysis was included to calculate the volumes of different horizontal layers on the basis of bathymetric lake data, using the ESRI GIS ArcMap together with the 3D Analyst and Spatial Analyst extensions and the visual coding language ModelBuilder. To compare water temperatures in the vertical water column independent from changing water levels, we automatically adapted the reference point of the DYRESM output data from the lake bottom to the surface (VBA script). The automated deduction of limno-physical criteria of a lake was done by additional

auxiliary routines in VBA. All the presented tools as well as the program codes are flexible and can be imitated when adapting different hydrodynamic models. In our case, we applied the routines to investigate the impact of climate change on the limno-physical conditions of Lake Ammersee in Middle Europe. In doing so, it is possible to save valuable time when dealing with big data in numerical lake modelling and to achieve substantial progress in the field of specialised, automated IT-solutions, enabling modellers to conduct more comprehensive and accurate calibration and validation runs.

Keywords: Aquatic ecosystem, hydrodynamic modelling, regional climate model, automated processes, GIS analysis

1. Introduction

Recently, there has been an urgent need for specialised solutions to estimate the impacts of climatic and environmental changes on aquatic systems more precisely and resource-efficient. Important investigations in this field, which could profit by the tools presented in this paper, deal with, for example: changes in water temperatures (Livingstone, 2003; Adrian et al., 2009; Schneider and Hook, 2010; Dokulil, 2013); physical properties of lakes (Gaiser et al., 2009; Ambrosetti et al., 2010; Hadley et al., 2013; Sahoo et al., 2013); trophic- and species-dependent changes (Kirilova et al., 2009; Wagner and Adrian, 2009; Rinke et al., 2010; Guilizzoni et al., 2012); and the distribution of nutrients and oxygen (Braig et al., 2010; Rempfer et al., 2010; Vetter and Sousa, 2012; Riverson et al., 2013). A major step forward in the aquatic modelling community was the development of hydrodynamic and ecosystem models, which help to improve our understanding of these topics (Huber et al., 2008; Fang and Stefan, 2009; Trolle et al., 2012). They have been applied to different study areas around the world (Joehnk and Umlauf, 2001; Gal et al., 2003; Weinberger and Vetter, 2012; Bayer et al., 2013).

In order to compare impacts on different aquatic systems and to continue applying existing hydrodynamic models to different study sites, the procedure of gaining knowledge in that subject area should be simplified and automated by IT-methods, addressing lake-specific model runs. Also, processes of model coupling and the interoperability between complex Earth system models in general should be improved (Laniak et al., 2013). This could be done by integrated modelling frameworks and systems, which are an environment for coupling model components and data through a common calling interface (Turuncoglu et al., 2013), using tools and technologies from computer science and software engineering (Argent, 2004; Viviroli et al., 2009), for example programming and geoprocessing (Haidong, 2013), which should be wholly transparent and provide a user-friendly interface (Covelli et al., 2002). When considering the future development and integrated use of hydrological models for sustainable management of water resources in general, it is important to keep in mind that tools should always be flexible, particularly in view of the fact that scientists use different software and modelling systems for the same purpose (Kralisch et al., 2005) and time is often limited. In the lake modelling community this fact was taken up by Mooij et al. (2010) and Trolle et al. (2012), who recommend the use of existing hydrodynamic models, and improving communication between and transparency of these models instead of 're-inventing the wheel'.

Hence to face these challenges, we show automated processes from the output of the regional climate model REMO (Jacob et al., 2012; Teichmann et al., 2013) to future simulation and assessment of limno-physical conditions, with the hydrodynamic model DYRESM (Dynamic Reservoir Simulation Model) (Imberger and Patterson, 1981). In the same way, such tools can be created for community-based open-source models, such as GLM (General Lake Model) and FABM (Framework for Aquatic Biogeochemical Models), which are currently developed and used for example in the Aquatic Ecosystem Modelling Network (AEMON) (Trolle et al., 2012).

The objectives of this study are to describe how: (1) to create a Shell script to convert and customise meteorological data automatically from the regional climate model REMO, using commands of the Climate Data Operators (CDO) software; (2) to write a macro in VBA program language, which is able to assemble and pre-process the meteorological input data for the hydrodynamic model DYRESM. This includes an automatic calculation of vapour pressure, as well as overall precipitation; (3) to implement an automated, GIS-based calculation of the volumes of the different horizontal layers of the lake; (4) to adapt the reference point of the DYRESM output data from the lake bottom to the surface automatically by a VBA program code, in order to compare water temperatures in the vertical water column independent from changing water levels; (5) to generate auxiliary routines in VBA, to compute the density and thermal stability in the water column from temperature and conductivity data, as well as the heat content in different layers of the lake.

The presented automated tools and the program codes are flexible and can be applied to investigations of different lakes or reservoirs, like those listed above.

2. Models and methods

2.1. Hydrodynamic modelling

For our investigations at Lake Ammersee (Weinberger and Vetter, 2012; Bueche and Vetter, 2013) we used the one-dimensional hydrodynamic model DYRESM (v4.0.0-b2). This process-based model was developed by the Centre for Water Research at the University of Western Australia, and is able to predict the vertical distribution of temperature, salinity and density in lakes and reservoirs. DYRESM uses a Lagrangian layer scheme, which means that the horizontal layers are adjusted to stay within user-defined limits (Imberger and Patterson, 1981; Antenucci and Horn, 2002). The layer mixing appears when the turbulent kinetic energy in the topmost horizontal layer exceeds a potential energy threshold. The kinetic energy is produced by convective overturn, wind stirring and shearing (Perroud et al., 2009). The hydrodynamic model was applied to different study areas around the world, and is particularly suitable to simulate longer periods. Compared to other one-dimensional lake models developed in recent years, DYRESM reproduced the variability of the water temperature profiles and seasonal thermocline satisfactorily (Perroud et al., 2009). The model can be run either in isolation for hydrodynamic studies, or coupled with an aquatic ecological model, e.g. CAEDYM (Computational Aquatic Ecosystem Dynamics Model), for the investigation of biological and chemical processes (Hipsey et al., 2007; Imerito, 2007).

In the future, to support an increasing transparency of model structure, assumptions and techniques (Trolle et al., 2012), and to make collaboration within the aquatic modelling community easier (Mooij et al., 2010), it is advisable to use also open-source models and frameworks, among widely used commercial software like e.g. ESRI ArcGIS. One example for collaboration of modellers from different countries, to develop such community-based techniques, is the Aquatic Ecosystem Modelling Network (AEMON) and its GLM and FABM models (Trolle et al., 2012). Hence, to meet the requirements of these new hydrodynamic models, which are currently under development, we decided to organise our processes in a user-friendly, transparent and customisable manner as possible. In this way, our workflow can be imitated when using new hydrodynamic model approaches in the future.

2.2. Regional climate model

To estimate the impact of climate change on lakes, it is advisable to use meteorological input data produced by regional climate models. For example, one regional climate model, which was used for hydrodynamic studies at Lake Ammersee and which provides the meteorological input data at the beginning of our workflow, is called REMO (Jacob et al., 2012). This climate model was selected because of its suitable cell calculation size of 10x10 km, and because it provides all the values that have a strong influence on the heat budget of lakes. These parameters include short-wave radiation, air temperature, precipitation, wind speed, vapour pressure, total cloud cover and relative humidity. Long-wave radiation values, which are also needed for hydrodynamic studies, were estimated from atmospheric conditions using cloud cover fraction (Imerito, 2007). When using REMO data, it is essential to implement a BIAS-correction. This process had already been carried out in an earlier study, comparing previously-measured meteorological data from the study area with those simulated by the regional climate model (Weinberger and Vetter, 2012). After BIAS-correction, the use of the regional climate model REMO is a practical way to estimate future impacts of climatic warming on lake ecosystems.

2.3. System requirements and software

The system requirements and computational demands to develop and apply the tools and processes covered by this manuscript are quite modest. We utilised PC platforms under Windows and Linux Ubuntu operating systems, and frequently used software packages Microsoft (MS) Excel 2007 and ESRI ArcGIS 10, with their embedded functions MS VBA Editor, ESRI 3D Analyst, ESRI Spatial Analyst and ESRI ModelBuilder. To convert and process the data of the regional climate model REMO, provided by the Max Planck Institute for Meteorology (MPI-M) in the FORTRAN IEG format, we also included tools of the CDO open source software (provided by MPI-M, version 1.5.9) in our desktop solution. CDO was developed for standard processing of climate model output, including simple statistical and arithmetic functions, data selection and subsampling, as well as spatial interpolation tools (Schulzweida et al., 2012). After pre-processing, to match the necessary input format of the hydrodynamic model DYRESM, the data was translated into netCDF format. NetCDF is an information-rich, machine-independent Binary file format, which is commonly used for the storage of field and simulation data in the oceanography and atmospheric science communities (Antenucci and Imerito, 2003; Hipsey et al., 2013).

3. Tools developed

The current study deals with the development of user-friendly, lightweight and automated software-tools for downloading and pre-processing input data, managing of data operations necessary for model run and coupling, implementation of spatial operations, as well as post-processing, visualisation and assessment of hydrodynamic model results. In this way, we can simplify and accelerate the procedure when investigating different study areas, to explore the impacts of climate change on lakes and their catchment area, which are regionally different, owing to morphometric, climatologic and land-use conditions, etc. The single steps, like mentioned as objectives in the Introduction part (1.), are illustrated in Figure 1. All the developed scripts and macros are presented in the following.

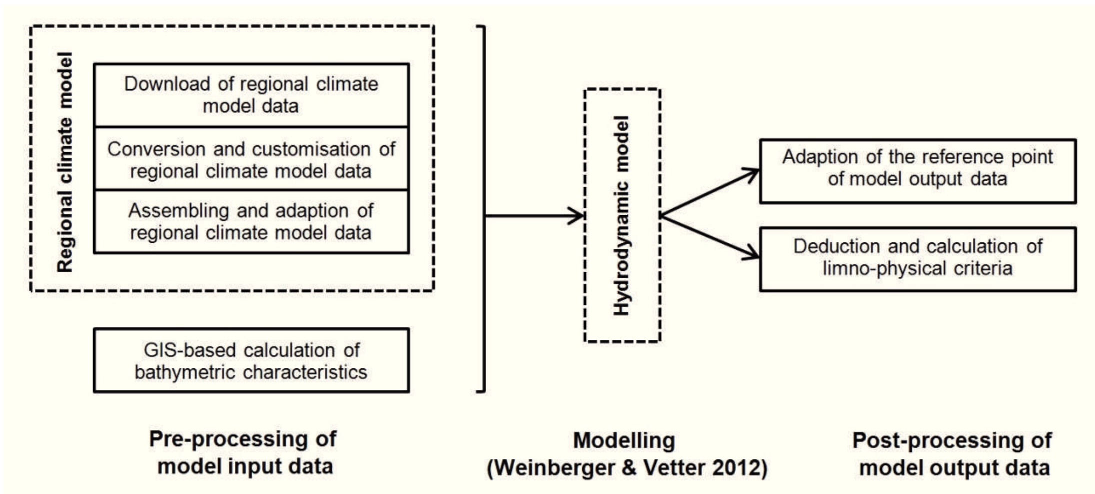

Figure 1: Automated steps from the output data of a regional climate model to hydrodynamic modelling and assessment of limnological conditions in the future.

3.1. Shell script for REMO data

As an initial step we created a Shell script in the Linux operating system, which is able to convert and customise meteorological data automatically from the regional climate model REMO, using commands of the open-source CDO software (version 1.5.9). The meteorological REMO series used for our hydrodynamic modelling approach include projections for the variables shortwave radiation, cloud cover, air temperature, vapour pressure, wind speed and precipitation. The processes integrated in this automated tool can be seen in the flowchart in Figure 2.

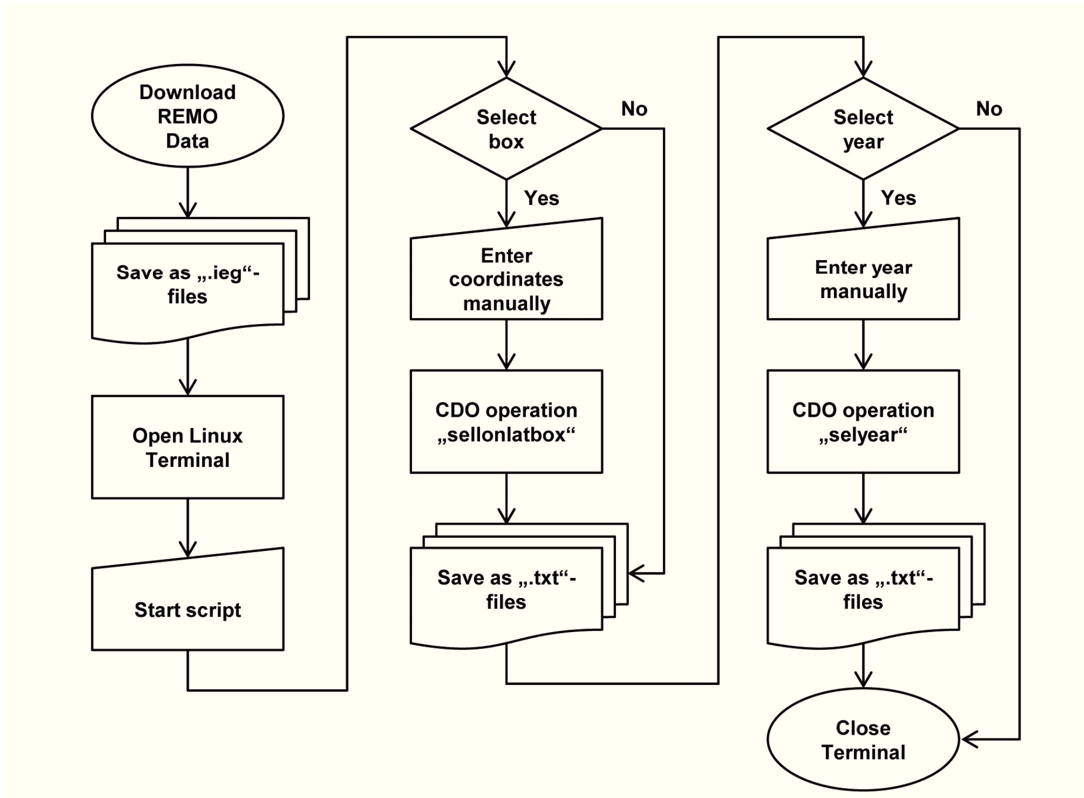

Figure 2: Flowchart of processes integrated in the Linux Shell script to convert and customise meteorological data automatically from the regional climate model REMO.

After the REMO data was downloaded from the CERA database of the World Data Center of Climate (FORTRAN IEG format) the script can be started manually in the terminal by entering the command ‘sh shellscript.sh’. Initially, the user should decide whether they want to select a single box of the area covered by REMO. In this way, it is possible to obtain a spatially customised data set for the respective study site of the modelling investigation. Therefore, a query line appears where the geographic coordinates of the requested 10 x 10km box should be entered, more precisely, western longitude, eastern longitude, southern latitude and northern latitude. Following this step, the REMO data is cut to the requested box by using the CDO operation 'sellonlatbox' and saved automatically. Afterwards, a second query line appears, where the user can enter year numbers, on which the data should be limited. Thus the CDO operation 'selyear' customises the data set temporally, and the resulting data set is saved in the ASCII format. All the commands implemented in the Shell script are listed in Table 1.

Table 1
Commands used in Linux Shell script to customise REMO data; example for air temperature (temp) at Lake Ammersee, based on emission scenario A1B, period 2041-2050

Operation	Command '…'
Start Shell script in terminal	'sh shellscript.sh'
Customise spatially (box of region)	'cdo sellonlatbox A1B_temp_2041-2050.ieg A1B_temp_2041-2050_Ammersee.ieg'
Customise temporally (single year)	'cdo selyear A1B_temp_2041-2050_Ammersee.ieg A1B_temp_2043_Ammersee.ieg'
Convert IEG-file to TXT-file	'cdo info A1B_temp_2043_Ammersee.ieg > cdo info A1B_temp_2043_Ammersee.txt'

3.2. Macro for data pre-processing

To match the input format necessary for the hydrodynamic model, the meteorological data customised and saved by the script mentioned before needs to be pre-processed. This was realised by developing a user-friendly, flexible and modifiable macro in MS VBA program language, which is a time-saving instrument when adapting data for spreadsheet software such as MS Excel. The resulting data format fits the standards of the meteorological input file of the hydrodynamic model

DYRESM, which was used in our study at Lake Ammersee (Weinberger and Vetter, 2012).

The pre-processing of meteorological input-data in the VBA routine includes different steps. At the beginning, when opening the MS Excel file, the script starts automatically with the appearance of a message box (Figure 3). This graphical user interface (GUI) contains important information regarding the required path and names of the input files of REMO-data, created by running the Shell script mentioned before.

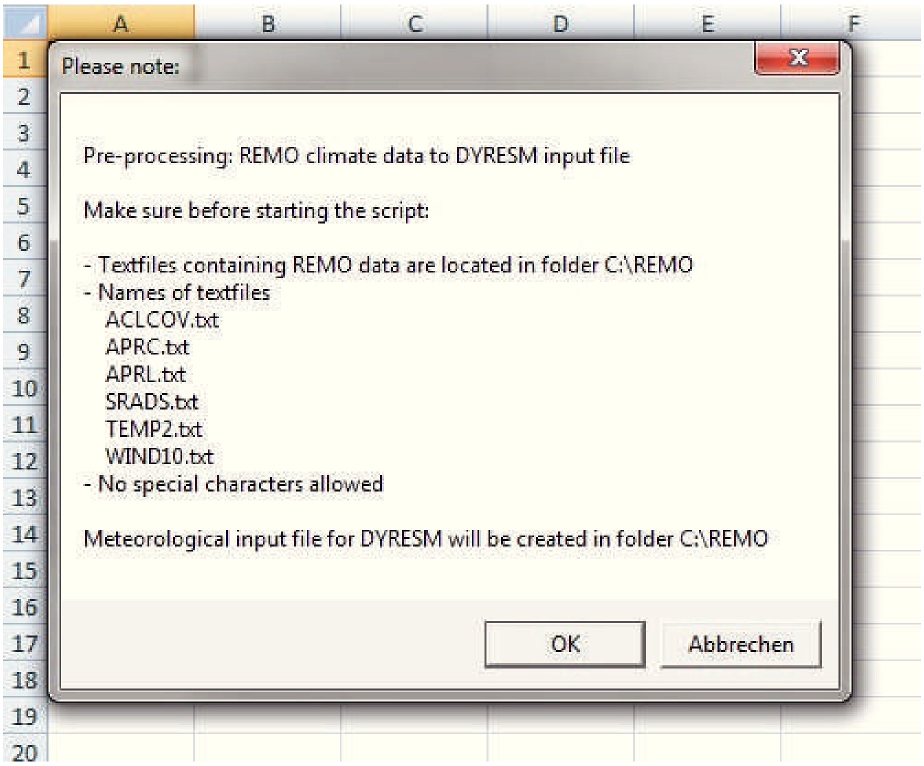

Figure 3: GUI that appears when starting the MS VBA macro to pre-process meteorological data.

At first, when the routine is started, the REMO text files are imported to the spreadsheet program, including the variables total cloud cover (ACLCOV), convective precipitation (APRC), large-scale precipitation (APRL), net surface solar radiation (SRADS), air temperature (TEMP) and wind speed (WIND). Afterwards the columns in the datasheets and the date format, which in the original REMO files is counted in months, starting from January 2001, are adapted. In a next step, the macro adapts the units of all meteorological variables, and calculates the overall precipitation by summarizing large-scale (APRL) and convective (APRC) precipitation, which are provided separately by the REMO model. Also, an automatic calculation of vapour pressure, with respect to the air temperature and humidity correlation, is operated, and the variables are assembled in one general datasheet. As last steps, the routine deletes redundant datasheets and exports the resulting input file for the hydrodynamic model as a text file to a specified directory. The essential parts of the code of the VBA macro are provided in Listing 1.

3.3. GIS macro for bathymetry

Another software tool included in this workflow is a GIS macro for the automatic calculation of bathymetric characteristics of the water body, which is presented by the flowchart in Figure 4. This GIS-based macro is able to evaluate the volumes of different horizontal layers on the basis of bathymetric data, which are required to prepare the morphometry input file (.stg) for the hydrodynamic model. For the creation of this automated tool, we used the software ESRI ArcGIS, together with the 3D Analyst and Spatial Analyst extensions as well as ESRI ModelBuilder visual programming language. To start the operation, the surface information data of the shore line and of the lake bed (measured by echo sounder by the Bavarian State Office for Survey and Geo-Information) are required in dbf-tables, containing spatial coordinates, as well as the absolute altitude of each measuring point. At the beginning, it is also necessary to define a spatial reference, which in our case study was the projected ‘DHDN 3 Degree Gauss Zone 4’ coordinate system. The dbf-tables are then the basis to create spatial point layer files (.lyr) out of the shore line and echo-sounder source tables, using the tool ‘Make XY Layer’ provided by the ArcGIS toolbox. Afterwards, these two point layers are combined using the ArcGIS tool 'Merge' and saved considering their spatial surface information as a point shape file (.shp).

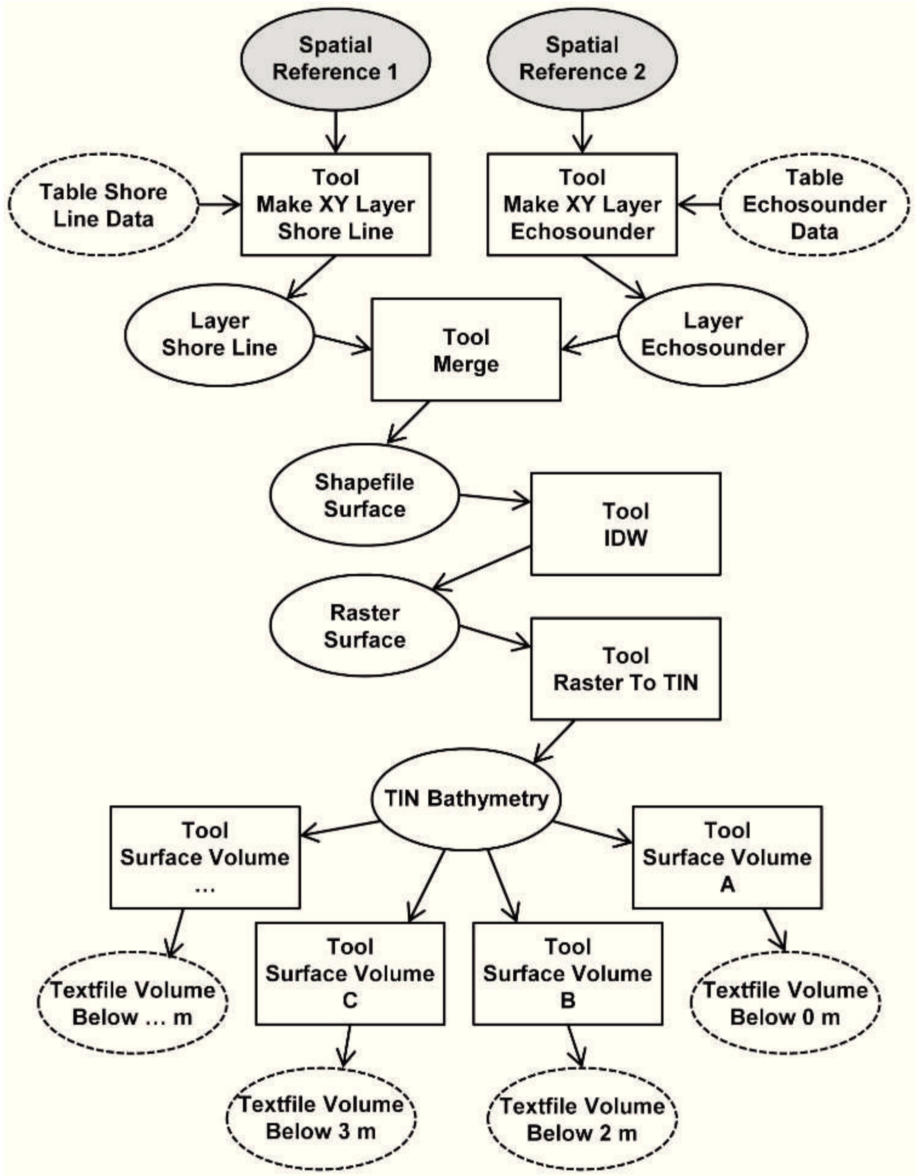

Figure 4: Flowchart of GIS macro for the automatic calculation of bathymetric characteristics of the water body, using ESRI ArcGIS ModelBuilder; Oval-shaped white fields represent spatial GIS files, oval-shaped white and dashed fields represent in-and output data, oval-shaped grey fields represent spatial references and rectangular fields represent spatial GIS tools.

Next, the macro uses the ArcGIS Spatial Analyst tool 'Inverse Distance Weighted (IDW)' to interpolate a surface raster out of the aforementioned point shape file. In this way, an inverse distance weighted technique is applied for data interpolation, and the resulting plane is saved as a raster data set. Afterwards, the raster is converted to a vector-based file (.TIN) by means of the ArcGIS 3D Analyst tool 'Raster to TIN'. This TIN (triangulated irregular network) contains all the spatial and absolute altitude coordinates (three-dimensional) of the lake bottom. On the basis of this three-dimensional file, the 3D Analyst tool 'Surface Volume' is used to calculate the area and volume of the TIN surface below a given reference plane, and exports the resulting data as a text file. Lastly, it is necessary to calculate the difference between the volumes to obtain the volume of a specific layer; e.g. between 2 and 3 metres of depth. So it is possible to determine the surface and volumes of each horizontal layer defined in the hydrodynamic model.

3.4. Macro to adapt water level reference point

To compare water temperatures in the water column independent of changing water levels after a hydrodynamic model run with DYRESM, it is necessary to adapt the reference point of the DYRESM output file from the lake bottom to the surface (re-indexing the vector). This was done by an additional MS VBA script, which uses the DYRESM output data format as its basis, and can be taken as an example for investigations using alternative hydrodynamic models. In doing so, we are able to compare water temperatures in the water column independent of changing water levels. In Figure 5, we provide a user-friendly overview of the functionality of this VBA script. This overview is based on our case study at Lake Ammersee. For example, we modelled the water temperatures for the years 2001-2007, using the DYRESM model. The resulting output file provides the water temperatures in the vertical profile for a daily time step and at different depths. If variations appear in the water level of the lake, owing to changing amounts in the inflow and withdrawal file of the model, these are indicated at the top of the water column. This means, that the horizontal layers of the model are counted originally from the bottom to the top of the lake, and the depth of each layer is indicated as the height above the bottom. To compare water temperatures of different model runs, and to use the model output for further statistical evaluation, it is necessary to count the horizontal layers from the surface to the bottom, using the water surface as the new reference point. In this way, the user is able to use the upper water layers for further limno-physical or ecological investigations, independent of changes in water level, as mentioned before.

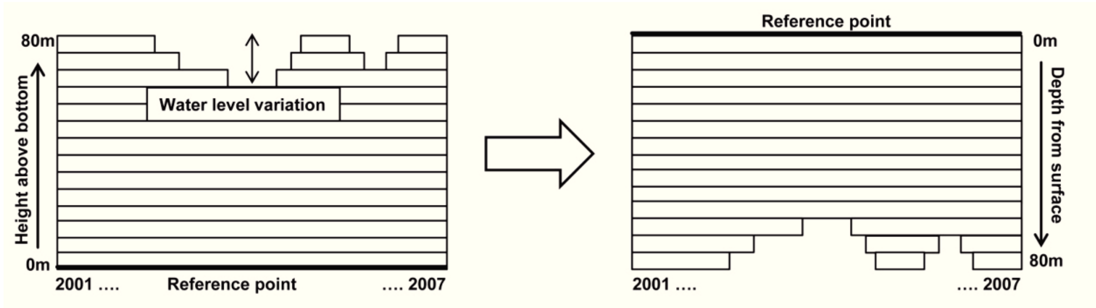

Figure 5: Overview over the functionality of MS VBA script to adapt the reference point of the DYRESM output file from the lake bottom to the surface automatically.

3.5. VBA-macros to deduce limno-physical criteria

The innovative simulation of future water temperatures, using a regional climate model, is a sound basis for deducing potential future physical changes in a water body. This is a result of the fact that a possible heating of the vertical water column leads, in turn, to substantial changes in the physical properties of the lake; more precisely, in terms of mixing processes, stratification characteristics and heat content (Danis et al., 2004; Austin and Colman, 2008; Rimmer et al., 2011; Vetter and Sousa, 2012). These limno-physical changes are thus crucial for further investigations, as they influence nearly all biological and chemical processes directly; e.g. substantial trophic- and species-dependent changes in lakes (Wagner and Adrian, 2009; Rinke et al., 2010; Gallina et al., 2011). To show how the user could save time when post-processing the results of different model runs, we generated dynamic MS Excel sheets and auxiliary routines in VBA. Using these tools, it is possible to compute automatically the heat content in different layers of the lake, as well as density and thermal stability in the water column from temperature and conductivity data.

The dynamic spreadsheet to deduce heat content is based on the formula published by Schwoerbel and Brendelberger (2005), who calculated the total lake heat content (*W*) by summing the heat content of single layers (from lake surface to lake bottom), based on its mean water temperatures:

[1] $$W = \int_0^{Zmax} T(z) c_p(z) \rho(z) A(z) d(z) \ ,$$

where T(z) is the mean water temperature (°C) at depth z, $c_p(z)$ is the specific heat capacity (kJ kg^{-1} K^{-1}) at depth z, ρ(z) is the density of water (kg m^{-3}) at depth z, A(z) is the isobath plane (m^2) at depth z and d(z) is the depth interval. The procedure of calculating total heat content using the dynamic MS Excel sheet is simplified in Figure 6.

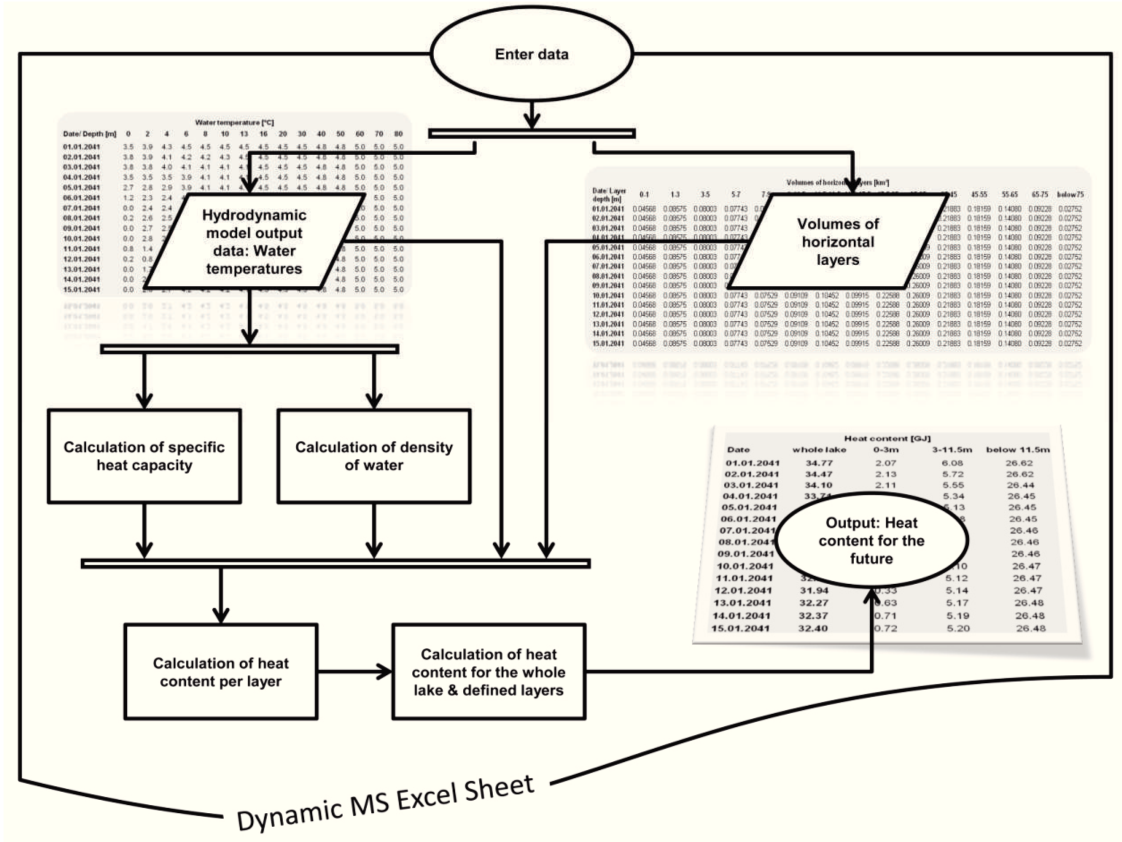

Figure 6: Flowchart of the procedure to calculate total heat content using a dynamic MS Excel sheet.

To derive the thermal stability of the water column, we embedded the equation of Idso (1973) in a VBA macro, to calculate values of Schmidt stability (S):

[2] $$S = g{A_0}^{-1}\int_0^{Z_{max}}(z - z^*)(\rho(z) - \rho^*)A(z)d(z) ,$$

where A_0 is the lake surface area (m^2), A(z) is the lake area (m^2) at depth z, ρ(z) is density ($kg\ m^{-3}$) calculated from temperature at depth z, ρ* is the volume-weighted mean density of the water column ($kg\ m^{-3}$), z* is the depth (m) at which mean density occurs, d(z) is the depth interval (m), and g is acceleration owing to gravity ($m\ s^{-2}$). The Schmidt stability represents the work that would be required to transform a thermally stratified lake into a lake characterised by isothermal conditions (Gaiser et al., 2009). For calculation of this limno-physical parameter, the determination of lake water density and conductivity is required. Thus, the formula according to Chen & Millero (1986) is also included in the macro, which is used to calculate density at different depths, while conductivity is determined using the relationship of temperature, density and water pressure in the water column (UNESCO, 1987). Some results of our limno-physical study at Lake Ammersee, including estimations on the basis of the regional climate model REMO, are published in Weinberger & Vetter (2014). The source code of the macro can be seen in Listing 2.

4. Discussion and Conclusion

As a result of the ever-increasing amount of data and the need for knowledge acquisition in the field of environmental research and modelling, it is necessary to call for the use of automated and smart tools (Weinberger, 2011) to handle and interpret the environmental data flood efficiently. This applies especially to input and output data of regional impact models, which are coupled with regional climate models. Only by means of computer-assisted, innovative tools it is possible to simplify and accelerate the analysis of big data produced by environmental model approaches at the interface between geo- and biological sciences. By developing and using the automated IT-tools, presented in this paper, we were able to contribute to the simplification of the process of gaining knowledge in the aquatic modelling community and to integrate GIS in an environmental modelling workflow. The steps from the output of a regional climate model to the simulation of limnological conditions in the future, and the interoperability between complex Earth system models were improved in a user-friendly way.

Nevertheless, in the future it is necessary to work out IT best practise approaches to community research. These should deal with data interoperability, reusability and the added value of open source and commercial software, which are the subject of current controversial discussions. In our study, we aimed to improve different issues in a lake modelling workflow and made out, that a mix of open source (e.g. CDO, Linux) and widely used commercial software (e.g. ESRI ArcGIS, MS Excel) therefore could be a good solution. However, for some other members of the community, it is easily conceivable that a different, generalized framework could be better, such as a holistic open source software stack. In general, to ensure a sustainable future support of such workflows, it is necessary to focus on the biggest needs of the community that have the highest potential for reuse.

The regional climate model data in our study area is available in the IEG format and was downloaded to the desktop for automated pre-processing. Other familiar formats of climate models output include for example NetCDF or GRIB and could be more popular in other regions of interest. Hence, to apply our pre-processing scripts to different climate model output formats, it would be desirable to create a gridded climate output format transducer, which supports all the popular input types and allows the users to specify various output types. Thereby it would be important to create this tool as server-client solution that could pre-subset the data spatially and temporally before it arrives on the desktop. In doing so, we could avoid downloading whole fine resolution climate datasets, which could, in some cases, be in the multi terabyte range. Regarding our GIS macro for the automatic calculation of bathymetric characteristics of the water body it has to be said, that this tool is very useful whenever bathymetric information is available and stored in compatible file formats, as existing for our investigation at Ammersee. Unfortunately, it is not very common to have such detailed echo sounder data available.

In general, our approach can be described as scientific workflow for pre-processing, managing, analysing and post-processing climatic and hydrodynamic model data, as is already adapted for processes in other fields of environmental modelling research (Viviroli et al., 2009; Akbar et al., 2013; David et al., 2013; Laniak et al., 2013; Turuncoglu et al., 2013). In this way, it is able to save time and to substantially simplify procedures for investigating and comparing the impact of climate change on different water bodies worldwide. Consequently, additional calibration and validation runs can be conducted within these investigations, which would otherwise not have been possible because of missing human and temporal resources. Also, our workflow is not limited to individual software, but can be used as an example when dealing with different hydrodynamic models. All the scripts and macros are wholly transparent, and can be used or changed by members of the aquatic modelling community, by applying widely used software packages and data formats as mentioned in the models and methods section (2.).

Nevertheless, it should be a future objective to secure the ongoing progress of these tools, considering the particular state of the art, and developing new processes to simplify modelling within the community. Thereby also web services should be considered for data processing in the future (Zhao et al., 2012; Delipetrev et al., 2014). In this way, it is possible to go on improving and accelerating existing integrated modelling approaches, instead of 'reinventing the wheel' (Trolle et al., 2012).

Acknowledgements

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Listing 1

Code of MS VBA macro for automated REMO data pre-processing

```
'Script starts automatically when opening the file and
opens GUI
Sub Auto_open()
  Dim byValue As Byte
  'Content message box
  byValue = MsgBox("REMO climate data to DYRESM input
  file" &_
  vbCrLf & vbCrLf &_
   "Make sure before starting the script:"&_
  vbCrLf & vbCrLf & _
  "- Textfiles containing REMO Data are located in folder
  C:\REMO" &_
   vbCrLf &_
  "- Names of Textfiles:" &_
   vbCrLf & _
  "    ACLCOV.txt" &_
   vbCrLf &_
  "    APRC.txt" &_
   vbCrLf &_
  "    APRL.txt" &_
  vbCrLf &_
  "    SRADS.txt" &_
  vbCrLf &_
  "    TEMP2.txt" &_
  vbCrLf & _
  "    WIND10.txt" &_
  vbCrLf &_
  "- No special characters allowed" &_
  vbCrLf & vbCrLf &_
  "Meteorological input file for DYRESM will be created in
  folder C:\REMO"_
  , 1, "Please note:")
  If byValue = 1 Then
  Call REMO_Makro
   'ElseIf byValue = 2 Then
  'Application.Quit
  End If
  End Sub

'Conversion and customisation of REMO data
Sub REMO_Makro()
'Customisation of separators in MS Excel
With Application
  .DecimalSeparator = "."
  .ThousandsSeparator = ","
  End With

'Step 1: Import of text files containing REMO data: total
cloud cover (ACLCOV), convective precipitation
(APRC), large scale precipitation (APRL), net surface
solar radiation (SRADS), air temperature (TEMP) and
wind speed (WIND)
  Sheets.Add After:=Sheets(Sheets.Count)
  Sheets.Add After:=Sheets(Sheets.Count)
  Sheets.Add After:=Sheets(Sheets.Count)
  Sheets("Table1").Select
  'REMO data: Example total cloud cover (ACLCOV)
  ‘This step is repeated for all REMO variables
  With ActiveSheet.QueryTables.Add(Connection:=_
    "TEXT;C:\REMO\Remo_Excel\ACLCOV.txt",
    Destination:=Range("$A$1"))
    .Name = "ACLCOV"
    .FieldNames = True
    .RowNumbers = False
    .FillAdjacentFormulas = False
    .PreserveFormatting = True
    .RefreshOnFileOpen = False
    .RefreshStyle = xlInsertDeleteCells
    .SavePassword = False
    .SaveData = True
    .AdjustColumnWidth = True
    .RefreshPeriod = 0
    .TextFilePromptOnRefresh = False
    .TextFilePlatform = 850
    .TextFileStartRow = 1
    .TextFileParseType = xlDelimited
    .TextFileTextQualifier = xlTextQualifierDoubleQuote
    .TextFileConsecutiveDelimiter = True
    .TextFileTabDelimiter = True
    .TextFileSemicolonDelimiter = False
    .TextFileCommaDelimiter = False
    .TextFileSpaceDelimiter = True
    .TextFileColumnDataTypes = Array(1, 1, 1, 1, 1, 1, 1, 1,
    1, 1, 1, 1, 1)
    .TextFileTrailingMinusNumbers = True
    .Refresh BackgroundQuery:=False
  End With

'Step 2: Adaption of columns, example Wind speed
‘This step is repeated for all columns containing
imported REMO variables
  Sheets("Table6").Select
  Columns("A:C").Select
  Selection.Delete Shift:=xlToLeft
  Columns("C:G").Select
  Selection.Delete Shift:=xlToLeft
  Range("C1").Select
  ActiveCell.FormulaR1C1 = "Mean"
  Sheets("Table6").Select
  Sheets("Table6").Name = "WIND"

'Step 3: Adaption of date format
  'Adaption of number of lines
  Dim Rows As Long
  Rows = Cells(Rows.Count,
 1).End(xlUp).Row
  Sheets.Add After:=Sheets(Sheets.Count)
  Sheets("ACLCOV").Select
  Columns("A:B").Select
  Selection.Copy
  Sheets("Table7").Select
  ActiveSheet.Paste
  Columns("B:B").Select
  Application.CutCopyMode = False
  Selection.NumberFormat = "0.000"
  Range("C2").Select
  ActiveCell.FormulaR1C1 = "=YEAR(RC[-2])"
  Range("C2").Select
  Selection.AutoFill Destination:=Range("C2:C" &  Rows)
  Range("D2").Select
  ActiveCell.FormulaR1C1 = "=TEXT(RC[-3]-
  DATE(YEAR(RC[-3]),1,1)+1,""000"")"
  Range("D2").Select
  Selection.AutoFill Destination:=Range("D2:D" &  Rows)
  Range("E2").Select
  ActiveCell.FormulaR1C1 = "=(RC[-2]&RC[-1])+RC[-3]"
  Columns("E:E").Select
  Selection.NumberFormat = "0.000"
  Range("E2").Select
  Selection.AutoFill Destination:=Range("E2:E" & Rows)
  Range("E1").Select
  ActiveCell.FormulaR1C1 = "YrDayNum"
  Columns("E:E").Select
  Selection.Copy
  Columns("F:F").Select
  Selection.PasteSpecial Paste:=xlPasteValues,
  Operation:=xlNone,
  SkipBlanks _:=False, Transpose:=False
  Application.CutCopyMode = False
  Selection.NumberFormat = "0.000"
  Columns("A:E").Select
  Selection.Delete Shift:=xlToLeft
  Range("F6").Select
  Sheets("Table7").Select
  Sheets("Table7").Name = "Overall"

'Step 4: Adaption of units, calculation of overall
precipitation and vapour pressure, assembling in 1
sheet
  'Calculation of overall precipitation
  Sheets("APRL").Select
  Columns("C:C").Select
  Selection.Copy
  Sheets("APRC").Select
  Columns("D:D").Select
  Selection.PasteSpecial Paste:=xlPasteValues,
  Operation:=xlNone,
  SkipBlanks _:=False, Transpose:=False
  Range("E2").Select
  Application.CutCopyMode = False
  ActiveCell.FormulaR1C1 = "=RC[-2]+RC[-1]"
  Range("E2").Select
  Selection.AutoFill Destination:=Range("E2:E" & Rows)
  ActiveWindow.SmallScroll Down:=-21
  ActiveCell.FormulaR1C1 = "=(RC[-2]+RC[-1])/1000"
```

```
Range("E2").Select
Selection.AutoFill Destination:=Range("E2:E" & Rows)
Range("E1").Select
ActiveCell.FormulaR1C1 = "Rain [m]"
Range("E1").Select
ActiveCell.FormulaR1C1 = "Rain_[m]"
Columns("E:E").Select
Selection.Copy
Sheets("Overall").Select
Columns("G:G").Select
Selection.PasteSpecial Paste:=xlPasteValues,
Operation:=xlNone,
SkipBlanks _:=False, Transpose:=False
'Adaption of net surface solar radiation unit
Sheets("SRADS").Select
Application.CutCopyMode = False
ActiveCell.FormulaR1C1 = "SW_[W/m^2]"
Columns("C:C").Select
Selection.Copy
Sheets("Overall").Select
Columns("B:B").Select
Selection.PasteSpecial Paste:=xlPasteValues,
Operation:=xlNone,
SkipBlanks _:=False, Transpose:=False
'Adaption of total cloud cover unit
Sheets("ACLCOV").Select
Range("C1").Select
Application.CutCopyMode = False
ActiveCell.FormulaR1C1 = "CloudCover"
Columns("C:C").Select
Selection.Copy
Sheets("Overall").Select
Columns("C:C").Select
Selection.PasteSpecial Paste:=xlPasteValues,
Operation:=xlNone,
SkipBlanks _:=False, Transpose:=False
'Adaption of 2m temperature unit
Sheets("TEMP").Select
Range("D2").Select
Application.CutCopyMode = False
ActiveCell.FormulaR1C1 = "=RC[-1]-273.15"
Range("D2").Select
Selection.AutoFill Destination:=Range("D2:D" & Rows)
Range("D1").Select
ActiveCell.FormulaR1C1 = "Tair_[°C]"
Columns("D:D").Select
Selection.Copy
Sheets("Overall").Select
Columns("D:D").Select
Selection.PasteSpecial Paste:=xlPasteValues,
Operation:=xlNone,
SkipBlanks _:=False, Transpose:=False
'Adaption of wind speed unit
Sheets("WIND").Select
Application.CutCopyMode = False
ActiveCell.FormulaR1C1 = "Wind_Speed_[m/S]"
Columns("C:C").Select
Selection.Copy
Sheets("Overall").Select
Columns("F:F").Select
Selection.PasteSpecial Paste:=xlPasteValues,
Operation:=xlNone,
SkipBlanks _:=False, Transpose:=False
'Calculation of vapour pressure and adaption of unit
Sheets("TEMP2").Select
Range("E1").Select
Application.CutCopyMode = False
ActiveCell.FormulaR1C1 = "Vapour_press_[hPA]"
Range("E2").Select
ActiveCell.FormulaR1C1 = "=6.1*10^((7.5*RC[-1])/(RC[-
1]+237.2))"
Range("E2").Select
Selection.AutoFill Destination:=Range("E2:E" & Rows)
Columns("E:E").Select
  Selection.Copy
  Sheets("Overall").Select
  Columns("E:E").Select
  Selection.PasteSpecial Paste:=xlPasteValues,
  Operation:=xlNone,
  SkipBlanks _:=False, Transpose:=False

'Step 5: Adaption of format and adding file heading of
DYRESM meteorological input file
  Columns("A:A").ColumnWidth = 13
  Cells.Select
  Application.CutCopyMode = False
  With Selection
    .HorizontalAlignment = xlLeft
    .VerticalAlignment = xlBottom
    .WrapText = False
    .Orientation = 0
    .AddIndent = False
    .IndentLevel = 0
    .ShrinkToFit = False
    .ReadingOrder = xlContext
    .MergeCells = False
  End With
  Range("B3").Select
  Columns("B:B").ColumnWidth = 14
  Columns("C:C").ColumnWidth = 13
  Columns("E:E").ColumnWidth = 20
  Columns("F:F").ColumnWidth = 20
  Rows("1:5").Select
  Selection.Insert Shift:=xlDown,
  CopyOrigin:=xlFormatFromLeftOrAbove
  Range("A1").Select
  ActiveCell.FormulaR1C1 = "<#3>"
  Range("A2").Select
  ActiveCell.FormulaR1C1 = "Meteorology Lake Ammersee"
  Range("A3").Select
  ActiveCell.FormulaR1C1 = "3600 # Met input data time
  step"
  Range("A4").Select
  ActiveCell.FormulaR1C1 = "CLOUD_COVER # longwave
  radiation indicator (NETT_LW, INCIDENT_LW,
  CLOUD_COVER)"
  Range("A5").Select
  ActiveCell.FormulaR1C1 = "FIXED_HT 90 # sensor type
  (FLOATING, FIXED_HT), height in metres (above water
  surface, above lake bottom)"
  Range("B3").Select

'Step 6: Delete redundant sheets
  Application.DisplayAlerts = False
  Sheets("WIND").Select
  ActiveWindow.SelectedSheets.Delete
  Sheets("TEMP").Select
  ActiveWindow.SelectedSheets.Delete
  Sheets("SRADS").Select
  ActiveWindow.SelectedSheets.Delete
  Sheets("APRL").Select
  ActiveWindow.SelectedSheets.Delete
  Sheets("APRC").Select
  ActiveWindow.SelectedSheets.Delete
  Sheets("ACLCOV").Select
  ActiveWindow.SelectedSheets.Delete

'Step 7: Export file as text file
  ChDir "C:\REMO\Remo_Excel"
  ActiveWorkbook.SaveAs
  Filename:="C:\REMO\Remo_Excel\Meteo.prn",
  FileFormat _:=xlTextPrinter, CreateBackup:=False
  MsgBox "Data conversion  successful!" &
  strText, 0, "Hinweis"
  Application.Visible = False
  Workbooks("Meteo.prn").Close SaveChanges:=False
  Application.DisplayAlerts = True
End Sub
```

Listing 2

Code of MS VBA macro for automated calculation of thermal stability

```
Sub calculation_density()
      'Name of worksheet containing initial data
      (DYRESM output)
      source1 = "temperature"
      source2 = "conductivity"
      'Name of worksheet for resulting table
      target = "density"
      schmidt = "Schmidt stability"
      finalvalue = 1000
      'Number of measurements in vertical profile
      f = 16
      'Number of days of measurements
      sp = 370
      'Volume of Lake Ammersee [m³]
      totalvolume = 1750010000
      'Surface area of Lake Ammersee [km²]
      surface = 46600000#
    a = 2
    b = 3
    c = 4
    E = 3
  For d = 1 To sp
    For i = 1 To f
      Sheets(source1).Select
      Cells(a, b).Select
      'Columns containing temperature measurements
      (tempms)
      tempms = Cells(a, b)
      Selection.Copy
        'Enter date to table of Schmidt stability
        If a = 2 Then Sheets(schmidt).Select
        Cells(a, b).Select
        ActiveSheet.Paste
        Sheets(target).Select
        Cells(a, c + 1).Select
        ActiveSheet.Paste
        End If
      Sheets(source2).Select
      Cells(a, b).Select
      'Columns containing conductivity measurements
      (cms)
      cms = Cells(a, b)
      Sheets(target).Select
      c = c + 1
      Cells(a, c).Select
      texponent3 = tempms * tempms * tempms
      texponent2 = tempms * tempms
      'Circumvent the date
      If a > 2 Then
        'Calculation of density and mean density [kg m-3
        10-3] as well as depth at which mean density
        occurs [m]
        term3 = ((0.059385 * (tempms * tempms * tempms) -
        8.56272 * (tempms * tempms) + 65.4891 * tempms) *
        0.000001 + 0.99984298) + 0.64 * 0.000001 * (cms *
        (-0.00001222651 * (tempms * tempms * tempms) +
        0.00114842 * (tempms * tempms) - 0.0541369 *
        tempms + 1.72118))
        ActiveCell.FormulaR1C1 = term3
        sum_density = sum_dichte + term3
      End If
      a = a + 1
      c = c - 1
    Next i
        c = c + 1
        Cells(a, c).Select
      mean_density = sum_density / (f - 1)
      ActiveCell.FormulaR1C1 = mean_density
    schmidtstability = diff * totalvolume * volweightedsum *
    1000 * 9.81
    schmidtstabilsurface = schmidtstability / surface
    Sheets(schmidt).Select
      Cells(3, E).Select
      ActiveCell.FormulaR1C1 = schmidtstabilsurface
      E = E + 1
    volwithdensitysum = 0
    voldensitysum = 0
    s = 0
    s0 = 0
    diff = 0
    volwithsum = 0
    schmidtstability = 0
    volweightedsum = 0
    sum_density = 0
    a = 2
    b = b + 1
  Next d
End Sub

Sub schmidtstability()
'Ensure that Sub calculation_density runs first
      source1 = "temperature"
      source2 = "conductivity"
      target = "density"
      schmidt = "Schmidt_stability"
      finalvalue = 1000
      f = 16
      sp = 370
      totalvolume = 1750010000
      surface = 46600000#
    a = 2
    c = 6
    E = 3
  For d = 1 To sp
    For i = 1 To f
    If a > 2 Then
    'Calculation of Schmidt stability [KJ m-2]
    Sheets(target).Select
    mean_density = Cells(18, c)
    depth_mean_density = Cells(19, c)
    term = (Cells(a, c) – mean_density) * (Cells(a, 2) *
    (Cells(a, 3) – depth_mean_density))
    termsum = term + termsum
    End If
    a = a + 1
  Next i
      schmidtstability = (termsum / surface) * 9.81
      Sheets(schmidt).Select
      Cells(3, E).Select
      ActiveCell.FormulaR1C1 = schmidtstability
      E = E + 1
      schmidtstability = 0
    a = 2
    c = c + 1
    termsum = 0
  Next d
End Sub
```

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Anhang B

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