Chapter 10

DRAWING PARALLELS BETWEEN LAKE AND COASTAL MARINE ECOSYSTEM MANAGEMENT: Spatial Analysis of the Lake Simcoe Watershed (Ontario, Canada) as a Socio-Ecological System

G. B. Arhonditsis^{1,*}, A. Neumann¹, M. Dittrich¹, J. D. Young², M. E. Palmer², J. G. Winter² and E. Stainsby²

¹Department of Physical & Environmental Sciences, University of Toronto, Toronto, Ontario, Canada ²Ontario Ministry of the Environment & Climate Change, Toronto, Ontario, Canada

ABSTRACT

We present an integrative analysis of the Lake Simcoe watershed, Ontario, Canada, as viewed from the perspective of a socio-ecological system. Drawing parallels with the concept of Hydrological Response Units, we used Self-Organizing Mapping to delineate spatial organizations with similar socio-economic and environmental attributes, also referred to as Socio-Environmental Management Units (SEMUs). Our analysis provides evidence of two SEMUs with contrasting features, the "undisturbed" and the "anthropogenically-influenced", within the Lake Simcoe watershed. The "undisturbed" cluster occupies approximately half of the Lake Simcoe catchment area (45%) and is characterized by low landscape diversity and low average population density <0.4 humans ha⁻¹. By contrast, the socio-environmental functional properties of the "anthropogenically-influenced" cluster highlight the likelihood of a stability loss in the long-run, as inferred from the distinct signature of urbanization activities on the tributary nutrient export, and the loss of subwatershed sensitivity to natural mechanisms that may ameliorate the degradation patterns. We subsequently use empirical evidence and mathematical modelling

^{*} Corresponding Author: georgea@utsc.utoronto.ca.

to examine whether the spatial and temporal variability in Lake Simcoe is primarily driven by the urbanization trends in the watershed or by the internal mechanisms following the establishment of dreissenid mussels and the proliferation of macrophytes. We conclude by discussing the prospect of the lessons learned from the present analysis to guide integrative management in the context of both large lake and marine systems.

ABBREVIATIONS AND ACRONYMS

AWC	available water capacity in top soil layer							
BD-TP	phosphorus in sediments extracted with bicarbonate dithionite							
	solution during the second stage of sequential P fractionation							
CAD (\$)	Canadian dollars							
COM/IND	commercial and industrial areas							
DA	dissemination area of census in Canada							
DO	dissolve oxygen (concentration)							
DW	dry weight							
EA	enumeration area of census in Canada							
ha	hectares, measure of land surface area							
HCI-TP	carbonate-bound P (apatite-P)							
H-LU	Shannon diversity index							
HRU	Hydrological Response Units							
IWM	integrative watershed management							
LSRCA	Lake Simcoe Region Conservation Authority (resource management							
	organization)							
LULC	land use/land cover							
MOECC	Ministry of the Environment and Climate Change of the Province of							
	Ontario, Canada							
MOI	Ministry of Infrastructure of the Province of Ontario, Canada							
MVWHDO	minimum volume-weighted hypolimnetic dissolved oxygen							
	concentration							
NaOH-NRP	organic bound P, calculated as the result of subtraction of NaOH-SRP							
	from total P after digestion during NaOH stage of sequential P							
	fractionation							
NaOH-SRP	P bound to hydrated oxides of aluminum as extracted with NaOH							
	base solution during the third stage of sequential P fractionation							
NH ₄ Cl-TP	loosely adsorbed (labile) P as extracted with NH4Cl solution during							
	the first stage of P fractionation							
Р	phosphorus, one of limiting nutrients for algae growth in inland water							
	bodies							
P_EXPORT	rate of phosphorus export from watersheds							
рН	potential of hydrogen, quantitative measure of solution acidity							
POP	population records							
Refract-P	refractory phosphorus in sediments							
RESIDEN-HD	high density residential areas							
SEM	Structural Equation Modelling							

Socio-Environmental Management Units								
shell-free dry weight of zebra mussels (actual weight of organi								
biomass)								
areas occupied by sod farms and golf courses								
soil albedo of top soil layer								
bulk density of top soil layer								
organic carbon content of top soil layer								
saturated hydraulic conductivity of top soil layer								
Self-Organizing Mapping								
metric tons								
total phosphorus (concentration)								
unified distance matrix in SOM, which visualizes the distances								
between trained neurons								
low density residential areas								

1. INTRODUCTION

Despite decades of active research in the field of watershed science, there are still significant gaps in our understanding of the complex interplay among hydrological factors, landscape features, and spatial patterns of the urban environment and agricultural activities that modulate the export rates of nutrients and contaminants in a watershed context (Rode et al., 2010). In human-dominated catchments, which are heavily affected by intensive farming or urbanization, achieving long-term ecosystem sustainability requires not only knowledge of the major biogeochemical processes, but also understanding of the evolution of social and economic pressures in time and space (Bowen and Riley, 2003). Restoration programs should consider human population dynamics, socio-economic conditions, and cultural traditions alongside with the environmental perspectives (Neumann et al., 2017). Nonetheless, in most watersheds of socioeconomic interest in North America, we lack the knowledge of the multifaceted linkages among anthropogenic stressors and undesirable ecosystem changes (Bowen and Riley, 2003; Liu et al., 2007). One of the imperatives of the contemporary management practices is, therefore, the development of integrative methodological frameworks that can offer insights into the long-term dynamics of urban and agricultural landscapes and subsequently connect them with the receiving waterbodies.

In this study, we present an integrative analysis of the Lake Simcoe watershed, Ontario, Canada, as viewed from the perspective of a socio-ecological system. Lake Simcoe is the sixth largest inland lake in the province of Ontario, Canada, with a surface area of 722 km², a mean depth of 14 m, and a maximum depth of 42 m (Figure 1). It is a dimictic system that completely freezes over in most winters. Lake Simcoe consists of a large main basin and two large bays: the narrow and deep Kempenfelt Bay on the west side of the lake and the shallow Cook's Bay at the south end of the lake. The lake drains through a single outflow at Atherley Narrows and has a flushing time of approximately 11 years (Palmer et al., 2011). Due to the limestone bedrock underlying its catchment, Lake Simcoe is a hard-water lake with mean calcium concentration of 41 mg L⁻¹, mean alkalinity of 116 mg L⁻¹, and mean sulphate concentration of 20 mg L⁻¹. The lake supports a year-round sport fish industry (>1 million angler hours per year)

as well as recreational activities that generate over \$200 million per year. Lake Simcoe is also a drinking water source for several communities within its 2,899 km² watershed.

Agriculture and increasing urbanization activities have impacted the ecological health of the system. In particular, Lake Simcoe currently receives wastewater from fourteen municipal wastewater treatment plants which constitute sources of phosphorus loading (6 \pm 1 tonnes y⁻¹ between 2004 and 2007). Substantial phosphorus loads are also deposited from the atmosphere $(18 \pm 4 \text{ tonnes y}^{-1})$ or stem from other non-point sources, including runoff from agricultural, urban and natural areas (43 ± 5 tonnes y⁻¹) and rural septic systems (4.4 ± 0.1 tonnes y⁻¹). The exogenous phosphorus inputs influence the ambient total phosphorus (TP) levels and subsequently trigger phytoplankton production, while the decomposition of the excessive organic material in the sediments likely contributes to hypolimnetic dissolved oxygen (DO) depletion. Prior to the mid-1990s, end-of-summer hypolimnetic DO levels reached nearly lethal levels for many coldwater fish species ($<3 \text{ mg } L^{-1}$). As a result, fish biomass declined for several commercially or recreationally important fish species, such as lake trout (Salvelinus namaycush), lake whitefish (Coregonus clupeaformis), and lake herring (Coregonus artedi) (Evans, 2007). To alleviate the problem of hypoxia and thus allow for the restoration of a selfsustaining coldwater fishery, the target for the end-of-summer minimum volume-weighted hypolimnetic dissolved oxygen (MVWHDO) was originally established at 5 mg L⁻¹ and recently revised to 7 mg L⁻¹. A combination of empirical knowledge and modeling indicates a phosphorus loading rate of 44 tonnes y⁻¹ is needed to meet the 7 mg L⁻¹ MVWHDO target. Between 2004 and 2007, total phosphorus loading into the lake was 74 ± 3 tonnes y⁻¹, a significant reduction from over 100 tonnes y⁻¹ during the 1980s and early 1990s (Palmer et al., 2011).

In this chapter, we first present an integrative socio-ecological assessment of Lake Simcoe, aiming to establish linkages among demographic shifts, urbanization trends, and nutrient export in a watershed context. We then evaluate to what extent the spatial and temporal variability in Lake Simcoe is driven by the differential supply of nutrients and suspended solids from the local tributaries or by internal mechanisms following the establishment of dreissenids and the proliferation of macrophytes in the nearshore zone. We also examine the hypothesis that the spatial variability of the mechanisms, modulating phosphorus cycling in the water column, shapes the sediment accumulation patterns in the system. We conclude by discussing the prospect of using the lessons learned from the present analysis to maximize the efficiency of mitigation programs of both large lake and coastal marine eutrophication, including the promotion of public awareness and engagement in stewardship initiatives.

2. INTEGRATIVE ANALYSIS OF THE LAKE SIMCOE WATERSHED AS A SOCIO-ECOLOGICAL SYSTEM

2.1. Background

The scope of the first phase of our project involved the development of a holistic framework for integrative watershed management (IWM), which would identify spatial trends in the landscape and socio-economic features within the context of the Lake Simcoe watershed. The current practice of catchment management heavily relies on environmental factors, and

therefore the rapid socio-demographic transformations due to urban or suburban sprawl are not always factored in. The present study, by contrast, proposes a strategy to level off this misbalance by recommending a framework founded upon the equally weighted consideration of environmental values with socioeconomic parameters. Although Lake Simcoe has a relatively small catchment-to-surface area ratio of 5:1 (Figure 1), which typically results in lower delivery rates of the nutrient loading into the receiving water body, it experienced continuous water quality degradation in the 20th century due to exponentially increasing anthropogenic pressure since the 17th century, when the first European immigrants settled in the lake catchment. Lake Simcoe watershed experienced severe pressure stemming from exponential urbanization after 1945, with population growing from 60,000 to (the current) 350,000 residents. With massive deforestation, the resultant watershed phosphorus (P) export into the lake increased from 27 T P year⁻¹ as a pre-settlement baseline up to 300 T P year⁻¹ in the 1960s, which triggered excessive primary production and ultimately hypolimnetic oxygen depletion, lethal for cold-water fish species. Recent P loading to the lake has varied between 72-115 T P year⁻¹ in 2007-2011, compared to a reduction goal of 44 T P year⁻¹ by 2045. Complicating the issue of the lake restoration program, projected population growth in the catchment of 30 percent over the next 20 years raises concerns as to whether the Lake Simcoe watershed can sustain this urbanization rate, while achieving the P reduction target in the future (Palmer et. al., 2011).

2.2. Methods

To proceed with analysis, we applied ArcHydro toolbox to delineate 824 hydrologically connected subwatersheds with an average area of 350 ha. Characteristics of the upper soil layer were acquired from Agriculture and Agri-Food Canada's Detailed Soil Survey (1:50,000). The list of soil characteristics included moist bulk density (SOL_BD, g cm⁻³), available water capacity (SOL_AWC, mm H₂O mm⁻¹ soil), saturated hydraulic conductivity (SOL_K, mm hr⁻¹), organic carbon content (SOL_CBN, percentage of soil weight), and moist soil albedo (SOL_ALB, ratio of solar radiation reflectance). Lake Simcoe Region Conservation Authority (LSRCA) compiled the map of detailed land use cover for 2013. The land-use specific phosphorus export coefficients (kg P ha⁻¹ year⁻¹) followed the LSRCA-approved Phosphorus budget Tool, which corroborated P export rates for each major tributary watershed (Figure 1). The baseline tributary nutrient loading levels (kg P year⁻¹) were calculated by integrating export coefficients over the corresponding areas of land use. We characterized the landscape diversity (or potential patchiness) on a subwatershed scale using the Shannon diversity index (H-LU).

The socio-demographic data were acquired from Statistics Canada for 1996 and 2006 Census records. We selected the smallest spatial resolution of census data to be commensurate with the approximate average subwatershed size of 350 ha; namely, geographic areas with 400-700 residents in the 2006 census (dissemination areas, DA) and 125-650 dwellings in the 1996 census (enumeration areas, EA). In order to match the hydrological boundaries, the census data were aggregated into subwatershed boundaries in proportion to areas of DA and EA within each subwatershed. Total population counts and average family income (in CAD) were selected as two major proxies to describe the socio-economic features of the Lake Simcoe watershed (Chertow, 2000). Examination of the social dynamics was also based on the number of immigrants (cumulative for out-of-province and out-of-country over the past 15 years), age-

group demographics, total labour-force counts by industry for the age group 15 years and older, average value of dwellings (CAD), and number of houses per different types of dwelling structures (Neumann et al., 2017).

We developed a two-step strategy for integrated analysis aiming to (i) reduce the socioenvironmental data and subsequently cluster the subwatersheds into spatially homogeneous groups; (ii) develop structural equation models within each of the identified spatial clusters. Data reduction was based on Self-Organizing Mapping (SOM), which is an un-supervised artificial neural-network algorithm to identify and visualize patterns underlying multidimensional datasets (Kohonen, 2013). In this study, the multivariate data ordination was mapped onto two-dimensional lattices, whereby subwatersheds with similar socioenvironmental characteristics occupied adjacent cells (Figure 2a). We also applied a post-hoc hierarchical cluster analysis to delineate the dominant patterns in the data using weight vectors of U-matrix (Kohonen, 2013; Figure 2b). As a result, SOM served to downsize the complexity of the catchment by assigning subwatersheds with similar socioenvironmental characteristics of using subwatersheds with similar socioenvironmental characteristics to subwatersheds with similar socioenvironmental characteristics to subwatersheds with similar socio-environmental characteristics to neighboring cells, in contrast to subwatersheds with the greatest differentiation, which were separateFd by the largest distances in a 2D lattice. More information about the SOM implementation in Lake Simcoe can be found in Neumann et al. (2017).



Figure 1. (Continued)



Figure 1. (a) Lake Simcoe basin subdivided into subcatchments based on pour points of the main tributaries. The subcatchments are defined as the land draining into the main watercourse of a tributary. Dashed lines represent the segments of the lake ecosystem model, which accommodate the horizontal variability in Lake Simcoe. Arrows represent bi-directional exchange flows between model segments. (b) Main types of land uses and land cover in the Lake Simcoe catchment. Color grade represent the known phosphorus export gradient from black (maximum) to light grey (minimal) according to P Budget Tool (MOECC, 2012). Dots represent long-term environmental monitoring stations.

501,80	0.833 SCL AWC	0.333 SCK. K	4.09 SOL CON	2.68 50L ALB	0.168
	0.584	0.228	3.34	1.84	0.107
	0.336	0.122	2.59	0.993	0.045
SLOPE	2.06 CROPLAND	0.494 HAMPAST	0.418 GRASSLAND	0.224 FOREST	0.475
	1.5	0.262	0.212	0.119	0.265
	0.943	0.0308	0.006	0.0139	0.054
WETLAND	0.489 QUARRY	0.057 WATER	0.0682 00000	0.244 URB-LD	0.082
	0.254	0.0285	0.0353	0.127	0.044
20000000	0.0199		0.0024	0.0097	0.007
SOD/GOUF	0.268 RESIDENHID	0.403 POP	7.11 INCOME	11.5 P.EOPORT	0.76
	0.135	0.202	4.8	11.2	0.422
	0.0009	0.0008	2.49	10.8	0.084
HU	1				
	0.787				
10 C	0.569				

(a)

Figure 2. (Continued)



Figure 2. (a) Self-organizing maps (SOM) for Lake Simcoe watershed parameters in log-transformed scale, where SOL_BD - soil bulk density (g cm⁻³); SOL_AWC - available water capacity of the top soil layer (mm H₂O mm⁻¹ soil); SOL_K - saturated hydraulic conductivity (mm hr⁻¹); SOL_CNB - organic carbon content (% soil weight); SOL_ALB - moist soil albedo; SLOPE - slope; CROPLAND - various crop types (henceforth LULC as % of subwatershed); HAY/PAST - hay and pasture areas; GRASSLAND - grassland areas; FOREST - all types of forests; WETLAND - wetland areas including bogs and marsh areas; QUARRY - excavated quarry areas; WATER - all water bodies including lakes and ponds; COM/IND – commercial and industrial areas; URB-LD - urban low density areas; SOD/GOLF - sod farms and golf courses; RESIDEN-HD - residential high density areas; POP - population census (2006); INCOME - family income before taxes (2005); P_EXPORT - phosphorus export coefficient (kg P ha⁻¹ year⁻¹); H-LU - Shannon index of land use diversity; (b) dendrogram of the identified SOM clusters based on Euclidean distances; and (c) resultant map of the eight SOM clusters.

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Structural equation modeling (SEM) was subsequently applied to identify the minimal number of socio-environmental variables controlling phosphorus export from the subwatersheds. SEM is a multivariate statistical method that encompasses both factor and path analysis, which allows decomposing multiple causal pathways and quantifying direct and indirect relationships among variables (Arhonditsis et al., 2006; Ullman, 2006). Another advantage of SEM is its ability to explicitly incorporate uncertainty due to measurement error and/or accommodate the discrepancy between conceptual catchment properties and observed variables that can be directly measured. SEM is also an a priori statistical method whereby a hypothetical structure of the studied system, reflecting the best knowledge available, is tested against the observed covariance structure. Drawing parallels with the reverse-engineering approach (Lobo and Levin, 2015), we tested multiple a priori models until an optimal fit was achieved with minimal residuals when comparing hypothesized and observed covariance model structures (Arhonditsis et al., 2006). Box-Cox power transformations were implemented to stabilize the data variance and effectively linearize the bivariate relationships examined within the SEM structure (Neumann et al., 2017).

2.3. Results-Discussion

SOM maps enabled the comparison of the spatial clustering of subwatersheds based on different watershed input parameters (Figure 2a). Subwatersheds with rich organic carbon in the top layer (SOL_CBN) became concentrated in the upper-left corner of the grid lattice. A similar aggregation pattern was found with wetland-dominated subwatersheds (WETLAND) characterized by minimal patchiness (H-LU), while a negative correlation exists with soil bulk density and albedo (SOL_BD and SOL_ALB). Watersheds with steeper slopes (SLOPE) also associated with soils of light colors and high irradiation reflectance (SOL_ALB), low available water capacity (SOL_AWC), and high values of saturated hydraulic conductivity (SOL_K); all of which suggest slope instability consistent with a history of intense erosional processes. Areas with low values of saturated hydraulic conductivity (SOL_K) partly overlap with high density residential areas (RESIDEN-HD). This combination typically exacerbates the intensity of surface run-off, thereby increasing nutrient export (P_EXPORT) from urbanized watersheds.

Anthropogenically transformed landscapes, primarily located at the bottom of the SOM lattice, overlap with areas of high intensity of socio-economic attributes. In particular, subwatersheds dominated by high-density residential areas, lower left corner of RESIDEN-HD map on Figure 2a, correspond to high population records (POP). COM/IND cells representing commercial/ industrial areas in terms of similarity of their socio-environmental parameters occupy the same cells as highly urbanized areas in the SOM lattice. Interestingly, both urbanized land use/land cover (LULC) types (RESIDEN-HD and COM/IND) are characterized by relatively lower landscape fragmentation (H-LU index), which bears resemblance to the single-use, homogeneous land use features of the urban sprawl in Toronto region (Hess and Sorensen, 2015). Finally, several residential low-density subwatershed nodes (URB-LD), located in the right part of SOM lattice, partially overlap with areas of protected natural heritage woodlands (FOREST in the lower right corner), areas with high slope and the highest family-income. These subwatersheds meet the criteria for Toronto exurbia, defined as areas beyond the suburbs of the city, inhabited by wealthy professionals and executives who seek natural

"wilderness" and equestrian life styles, in contrast to middle-class suburban areas (Cadieux and Taylor, 2013).

After hierarchical clustering of U-matrix, two distinct spatial groups were identified (Figure 2b), each consisting of four socio-environmental subwatershed clusters (Figure 2c). The first group, consisting of clusters #1, 4, 5, and 8 (Table 1), is primarily occupied by significant portions of woodland (10-63%), wetlands (15-47%), and reservoirs (1-5%). Furthermore, this group reflects the low ends of population density and landscape patchiness (POP<0.4 humans ha-1, H-LU=0.9-1.3), rich with organic carbon content top soil (3.3-12.0%), and below-average family income (\$52,700 - \$79,000), and therefore this spatial cluster was labeled as "undisturbed". In delineating the cluster-specific features, we note that cluster #1 encompasses wetlands (47%) with extremely high organic matter composition (12% of organic carbon in soil weight) and lowest bulk density (0.6 g cm-3); cluster #4 – is occupied by wetlands and forested areas with golf clubs and sod farms, where residents have the highest family income within this group (\$79,000); cluster #5 – by less intensive agricultural areas, such as hay and pastures; cluster 8 – by forested areas.

The second cluster group comprises "anthropogenically-influenced" clusters, which have experienced severe landscape transformations typically associated with anthropogenic activities (Table 1): cluster #7 is dominated by high-intensity agriculture (row crops); cluster #6 is inhabited by low-density communities with the highest average family income across the entire Lake Simcoe watershed (\$100,500); cluster #3 represents urbanized cores with maximum population density of up to 18.5 person ha⁻¹; cluster #2 encompasses suburban areas around urban cores. As a transient zone between clusters #4, 6, 7 and the highly urbanized cluster #3, subwatersheds in cluster #2 incorporate a mix of different LULC types, such as farmland (28%), forest (20%), and wetlands (11%), which gradually experience subdivision and conversion to residential lots. The common feature of the second spatial cluster is their high landscape patchiness (H-LU = 1.2-1.7) and the - plausibly - high population density (>0.4 person ha⁻¹).

Drawing parallels with the concept of Hydrological Response Units (HRU), as cross-basin spatial organizations with common hydrological behavior (Zehe et al., 2014), the identified SOM clusters were characterized as Socio-Environmental Management Units (SEMU). Interestingly, this SOM clustering bears resemblance to the subwatershed ranking based solely on the dominant LULC (Figure 3a-b), especially in areas with high spatial homogeneity and minimal population density, such as the cropland belt in West Holland tributary or hay/pasture in Ramara Creeks. Beyond dominant LULC, other parameters that can shape watershed classification are the soil characteristics (low soil bulk density in Black River watershed) or family income (forested areas in southern East Holland). The landscape diversity index (H-LU) also played an important role in the SOM decision process (Neumann et al., 2017).

Table 1. Characteristics of spatial clusters derived with Self-Organizing Map analysis inLake Simcoe catchment. These variables have been used as model inputs for

unsupervised learning with artificial neural network. The cell shade color from white to dark gray represent min-max gradient, while numbers in white font indicate the highest values for each variable among the eight clusters

Variable	Unit	Mean	Undisturbed clusters				Anthropogenically- influenced clusters			
			1	4	5	8	2	3	6	7
Proportion of area	%	12.5	7.2	16.0	14.3	5.5	15.6	2.8	15.5	23.2
Available water capacity (AWC)	Unitless	0.23	0.22	0.20	0.23	0.24	0.24	0.26	0.15	0.27
Bulk density (SOL_BD)	g cm ⁻³	1.12	0.61	1.17	1.14	1.07	1.18	1.17	1.24	1.13
Organic carbon content (SOL_CNB)	% (weight)	4.0	12.0	3.2	3.9	4.5	2.9	3.0	2.5	3.5
Saturated hydraulic conductivity (SOL_K)	mm hr-1	38.2	33.8	40.2	26.7	27.6	43.4	31.9	53.5	37.3
Slope (SLOPE)	Degree	3.5	2.6	2.6	2.5	2.7	4.4	4.5	5.7	3.4
Soil albedo (SOL_ALB)	Ratio	0.10	0.11	0.06	0.08	0.10	0.10	0.08	0.16	0.09
Cropland (CROPLAND)	%	20.5	9.5	10.3	19.3	4.8	16.9	2.0	13.9	50.7
Forested areas (FOREST)	%	19.1	12.9	18.9	9.9	63.3	19.4	8.2	34.3	11.2
Grassland (GRASSLAND)	%	4.2	3.5	7.5	2.0	4.3	4.8	2.4	4.5	2.6
Hay and pasture (HAY/PAST)	%	17.5	19.2	8.2	48.9	0.3	10.8	4.8	23.2	16.0
Quarries (QUARRY)	%	0.8	0.5	0.9	0.5	0.5	0.7	0.0	2.7	0.1
Water covered areas (WATER)	%	2.2	4.6	4.3	1.0	3.4	2.4	1.7	0.7	0.5
Wetlands (WETLAND)	%	19.6	46.5	35.5	14.6	21.0	11.4	3.9	10.0	11.4
Commercial/Industrial areas (COM/IND)	%	4.3	1.0	1.9	1.1	1.0	11.6	23.7	1.6	2.1
Residential low density areas (URB-LD)	%	3.3	1.6	3.4	1.1	0.8	5.8	1.8	6.3	3.0
Residential areas (RESIDEN-HD)	%	5.9	0.4	1.4	0.8	0.5	13.6	50.8	1.0	1.2
Sod farms/Golf farms (SOD/GOLF)	%	2.6	0.4	7.7	0.8	0.1	2.5	0.9	1.9	1.2
Shannon Index (H-LU)		1.3	1.1	1.2	1.3	0.9	1.7	1.2	1.5	1.3
Population density (POP)	human ha ⁻¹	1.3	0.2	0.3	0.3	0.1	3.4	18.5	0.4	0.5
Average Family Income (INCOME)	\$K family ⁻¹	82	69	79	66	53	86	79	101	77
Phosphorus export (P_EXPORT)	kg P ha ⁻¹	0.29	0.09	0.13	0.12	0.07	0.46	1.14	0.14	0.20

Our integrative socio-environmental analysis offered a preliminary tool for the identification of "hot-spots" with increased likelihood of nutrient export rates in Lake Simcoe watershed. Three subwatershed clusters, #2, 3, and 7, were identified as major P sources across the entire basin (68% of total tributary P export). In particular, our study pinpointed the subcatchments of West Holland, East Holland, Black River, and Pefferlaw Brook as the largest P contributors in the area. Our spatial clustering also sheds light on the water quality impairment in Cook's Bay at the southwestern end of Lake Simcoe, as this embayment is both geographically and hydrologically connected to the previously mentioned West (agricultural cluster #6) and East Holland Rivers (urbanized clusters #2 & 3, Figure 3a). The Kempenfelt Bay in the west of Lake Simcoe is another area of impairment, which is primarily affected by the surrounding urban cluster of the City of Barrie (cluster #2-3). Given the ever-growing population and infrastructural expansion plans (MOI, 2011), the latter findings highlight the challenges in successfully implementing management plans in these locations.

To elucidate the functional relationships between nutrient export from watershed and socio-environmental catchment characteristics, we identified two distinct structural equation models (SEMs) with acceptable goodness-of-fit statistics for the undisturbed (Figure 4a) and anthropogenically-influenced cluster (Figure 4b). The SEM for the first cluster connected areal nutrient export rates (kg P ha⁻¹ year⁻¹) with the proportion of the subwatersheds occupied by different LULC types, i.e., primarily commercial/industrial and high-density residential areas, followed by lakes and ponds, and then all types of forests, wetland areas including bogs and marsh areas, and various crop types. Importantly, P export is particularly sensitive to the relative amount of anthropogenically transformed areas, such as infrastructural and urbanized locations (standardized path coefficients of 0.47 and 0.44), artificial on-stream reservoirs (0.30), and croplands (0.23). This spatial cluster contains the largest inventory of forests and wetlands, the known natural landscape mediators to control P mobilization from catchments. Nonetheless, the standardized paths from forests and wetlands (\approx -0.17) are weaker relative to those from anthropogenically affected areas (0.23-0.47). Thus, to maximize the attenuation effects of this land use coverage, it is critical not only to faithfully comply with the LSRCA stipulation that forests and wetlands should not fall below a minimum of 40% of total basin area but also that this threshold should be consistently met in all major local tributaries (Neumann et al., 2017).

In the second SEM, absolute rates of nutrient fluxes (kg P year⁻¹) were controlled by actual area sizes of human-associated LULC (m² subwatershed⁻¹), such as hay and pasture areas, various crop types, residential high-density areas, commercial and industrial areas, and then the number of residents (persons subwatershed⁻¹), latitude, and landscape diversity index. In terms of the importance of different LULC types, commercial/industrial and urbanized high-density areas exert significant control over catchment P budget, whereas croplands and hay/pastures appear to play a secondary role. The extent of residential areas is directly associated with catchment demographics (pathway strength of 0.83). The strong positive covariance between the residual variability in population and infrastructural LULC (correlation coefficient between residuals e3-e8 equal to 0.77) is conceptually on par with the notion that community infrastructure expansion closely follows population growth in Ontario (MOI, 2011). Additionally, the infrastructural expansion and land-use diversity (H-LU) appear to have a tight association (0.32) and collectively this pathway is the second strongest modulator of P export (total effect equal to 0.23 = 0.32 x 0.72). It is therefore reasonable to assume that the effect of

basin population growth and ecosystem degradation is magnified by the concurrent increase in infrastructure and industrial developments.



(b)

Figure 3. Spatial distribution of LULC in Lake Simcoe watershed: (a) according to SOM clustering; (b) based on dominant LULC within each tributary watershed. Dark colors correspond to higher P export rates from the corresponding cluster and LULC type.



Figure 4. Structural Equation Model (SEM): (a) for the "undisturbed" clusters, where RESIDEN-HD and COM/IND, WETLAND, FOREST, WATER, CROPLAND and HAY/PASTURE - in %; P_Export - in kg P ha⁻¹ year⁻¹; (b) for the "anthropogenically-influenced" clusters, where RESIDEN-HD and COM/IND - in m²; CROPLAND and HAY/PASTURE - in %; P_Export - in kg P year⁻¹ subwatershed⁻¹. Numbers correspond to the standardized path coefficients, depicting the relative importance of the causal relationships. Circled e1-e7 represent the measurement or structural errors associated with a particular variable. Double-headed arrows represent the covariance between connected variables or errors. More information about structural equation modeling can be found in Arhonditisis et al. (2006).

Interestingly, the optimal SEM for the "anthropogenically-influenced" clusters does not identify any pathways with negative regression coefficients, which could provide offsetting mechanisms for human-induced P mobilization and therefore socio-environmental sustainability, in the long run, cannot be ensured. The latter finding allows us to speculate about two critical conditions that may solidify the shift between the two contrasting watershed states, i.e., "undisturbed" versus "anthropogenically-influenced": (i) establishment of a distinct signature of demographics on the tributary nutrient export, effectively accelerating nutrient export rates for every incremental addition of new residents and/or conversion to urban/infrastructural land use in the watershed; and (ii) the loss of subwatershed sensitivity to natural (counterbalancing) mechanisms that may curb nutrient export.

3. THE INFLUENCE OF DREISSENID MUSSELS AND SUBMERGED MACROPHYTES IN SHAPING THE SPATIO-TEMPORAL PHOSPHORUS DYNAMICS IN LAKE SIMCOE

3.1. Background

The invasion of dreissenid mussels has been responsible for a major restructuring of the biophysical environment in many parts of the Laurentian Great Lakes, with profound alterations on the nutrient dynamics in the littoral zone. The nearshore shunt (sensu Hecky et al., 2004) has been identified to profoundly impact the fate and transport of particulate matter, and subsequently, alter the relative productivity of inshore sites along with their interactions with the offshore areas. Dreissenid mussels may filter twice as many food particles as they can actually ingest, while a large portion of the filtered food items is subsequently excreted in soluble form or released as (pseudo)feces. This particulate matter may then be subject to bacterial mineralization, and therefore the dreissenids are likely to mediate the nutrient cycling and may significantly modulate the nearshore nutrient concentrations.

In Lake Simcoe, the initial year with discernible dreissenid production was 1994. Abundant colonies of juvenile and adult mussels first occurred on rocky substrates throughout the spring and summer growing season in 1996. In its main basin, dreissenid mussel distribution is determined by a complex interplay among lake depth, substrate availability, and exposure to wave disturbance (Ozersky et al., 2011). Specifically, the highest dreissenid biomass levels are typically found at areas of intermediate depth, where water movement is high enough to ensure that the lake bottom is dominated by rocky substrate but not excessively high to cause catastrophic disturbances to the dreissenid community. Not surprisingly, the same sites are characterized by higher amount of periphyton biomass, primary production, and community respiration relative to sites where mussels are fairly low. The improved water transparency has also extended the area of submerged macrophyte coverage in Lake Simcoe, which in turn further influenced the biogeochemical processes. The second phase of the project aimed to examine the hypothesis that the phosphorus variability in Lake Simcoe is predominantly driven by internal mechanisms, after the establishment of dreissenids and the proliferation of macrophytes (Gudimov et al., 2015). An important implication of the likelihood of a strong causal linkage among dreissenids, macrophytes, and nutrient variability will be the weakening of the role of external loading in determining the lower food web dynamics in Lake Simcoe.

3.2. Methods

Phosphorus cycling in Lake Simcoe was simulated with a TP mass-balance model, which represented the system as seven completely mixed tank reactors to accommodate the horizontal variability in Lake Simcoe as well as the stratification patterns typically shaping the water quality in Kempenfelt Bay, Cook's Bay, and the main basin (Figure 5). The four epilimnetic segments are interconnected through bi-directional hydraulic exchanges to account for wind-driven flows and tributary discharges from adjacent watersheds. The embayment outflows comprise the watershed inflow discharges and the horizontal advection movement due to wind-induced wave propagation and current drifts controlled by the water surface shear stress. Wave movements were calculated based on the premise that the wave height is a function of wind speed, fetch, and storm duration, while drift currents were assumed to follow the Ekman exponential decline of current speed with depth and are also driven by the Coriolis force (Smith, 1979). The bi-directional circulation patterns across the interface between the main basin and the two embayments meet equilibrium conditions by considering backflows that counterbalance the displaced volume of water (Gudimov et al., 2015).

The model follows the approach presented by Kim et al. (2013) to improve the fidelity of epilimnetic TP simulations through detailed specification of internal P recycling pathways (Figure 5), such as the macrophyte dynamics and dreissenid activity as well as the fate and transport of phosphorus in the sediments, including the sediment resuspension, sorption/desorption in the sediment particles, and organic matter decomposition (Gudimov et al., 2015).

The role of macrophytes in the phosphorus cycle was based on the dry-mass biomass submodel introduced by Asaeda et al. (2000) with modifications from Kim et al. (2013). The governing macrophyte equation considered biomass growth through roots P uptake of segment-specific interstitial inorganic P in sediment; mortality with deposition of senesced plant tissues to the sediment organic P pool, and the plant respiration through tubers to release P back into the water column. The macrophyte submodel was calibrated against empirical macrophytes biomass estimates (g DW/m²), while their proliferation extent was based on the Ginn's (2011) study.

The dreissenid equation followed the Schneider (1992) and Bierman et al. (2005) bioenergetic description of individual mussel physiological activity. The dreissenid activity in the sediment-water column was simulated by considering their filtration rates, food ingestion, respiration, excretion metabolism, production of faeces, pseudofeces, and dissolved P as endproducts (Figure 5). Filtering rate represents the volume of water swept clear of particles per unit time, which was modelled following Bierman et al. (2005) assumption that mussels maintain a maximum ingestion rate for all food concentrations below a saturation value and are negatively related to food abundance when this threshold is exceeded (Sprung and Rose, 1988). The filtration capacity of dreissenid bed to affect the entire water column is known to be dependent upon the wind-induced turbulent mixing and the resultant eddy diffusivity in the water column (Edwards et al., 2005). This process can suppress the dreissenid filtration effect on algae and other biogenic particles from littoral to pelagic zones, resulting in the formation of boundary layers near dreissenid mussel beds in stratified waters (Boegman et al., 2008). The latter effect is introduced in the model with a segment-specific and depth-dependent scaling clearance rate coefficient (Daunys et al., 2006). The rejected suspended solids and the remaining biodeposited particulate material are distributed between the water column and

sediments (Yu and Culver, 1999). Counter to the Bierman et al. (2005) study, our approach does not explicitly consider age cohort classes, while the dynamics of individual dreissenid mussels are converted to an ecosystem-scale effect by multiplying the areal mussel density by a prespecified site-specific colonization area (Ginn, 2011).



Figure 5. Simulated phosphorus fluxes (tonnes P year⁻¹) in epilimnion, hypolimnion, and sediment layer at the seven spatial compartments of Lake Simcoe. The net *TP* contributions (sources or sinks) represent the mass of phosphorus associated with the various compartments (water column, sediments, macrophytes, dreissenids) averaged over the 1999-2007 period.

Segment/Model	Cook's Bay		Kempenfelt Bay		Eastern End		Main Basin		Total	
Endpoint	Model	Obs.	Model	Obs.	Model	Obs.	Model	Obs.	Model	Obs.
Macrophytes abundance, g DW/m ^{2*}	35-116	75	21-67	20-40	32-95	70	32-95	20-40	-	-
Macrophytes colonization area, km ²	17.8	17.8	1.5	-	24.9	-	11.6	-	56	56
Macrophytes biomass, tonnes DW	1,000	-	58	-	1,500	-	700	-	3,300	-
Macrophytes P content, kg	2,800	1,169**	120	-	3,600	-	1,500	-	8,000	-
Dreissenids biomass, tonnes SFDM***	600	450	200	200	3,200	3,600	7,000	7,400	11,000	11,500
Sediment OP (fast degradable) accumulation, mg P g DW ⁻¹	0.11	0.12	0.25	0.22	-	-	0.14	0.17	-	-
TP in water column, $\mu g P L^{-1}$	16.1	14-23	18.0	15.0	16.0	13.7	15.2	14.1	-	
Flux from sediments, mg P m ⁻² day ⁻¹	0.07-0.11	0.10	0.18-0.21	0.20	0.07-0.08	-	0.07-0.08	0.07	-	-

Table 2. Model predictions and measured values for aquatic macrophytes, dreissenids, ambient total phosphorus concentrations and sediment fluxes

* Dry weight; **Estimated in 1988 under eutrophic conditions; ***Shell-free dry mass;

The sediment submodel considered particulate organic and inorganic phosphorus as well as phosphorus dissolved in the interstitial waters. The model approximates the dynamic P transformation processes in the upper sediment layers with an active P pool constrained by measured data by Dittrich et al. (2013). The organic P pool in sediments was accounting for settling flux of organic matter from the water column as well as mussel-mediated biodeposition. The main diagenetic process considered was the temperature-dependent decomposition of the organic fraction along with the burial in deeper layers. The soluble fraction was subject to diffusion and sorption-adsorption to/from the sediment particles. The sediment pool supports the macrophytes by supplying soluble P to their roots. The sediment accumulation depths in most model segments extend beyond the simulation time period of 9 years (1999-2007) with 10 years of sediment accumulation history in Cook's Bay, 22 years in Kempenfelt Bay, and 36 years in Main Basin (Hiriart-Baer et al., 2011).

3.3. Results-Discussion

Comparison of model predictions and measured values for aquatic macrophytes, dreissenids, ambient total phosphorus concentrations and sediment fluxes is provided in Table 2, while the various external and internal TP flux rates in Lake Simcoe are presented in Figure 5. In the main basin, the dreissenids filter 103.1 tonnes P year⁻¹ and approximately 90% of that amount (93.5 tonnes P year⁻¹) is returned into the water column as pseudofeces or other metabolic excreta. In the same area, external TP loading accounts for about 21.7 tonnes P year ¹, while an average of 12.1 tonnes P year⁻¹ are exported through the outflows into Lake Couchiching. Our model postulates that the burial into the deeper sediment layers of the main and eastern basin represents a significant pathway (15.6-39.1 tonnes P year⁻¹) through which phosphorus is permanently lost from the system. Kempenfelt Bay receives 9.3 tonnes P year⁻¹ from exogenous sources, while 7.3 tonnes P year⁻¹ are transported into the main basin. The total net loss to the sediments accounts for 1.6 tonnes P year⁻¹, while dreissenids on average reduce the ambient TP levels by 0.8 tonnes P year⁻¹. In Cook's Bay, the phosphorus budget is predominantly driven by the external sources (phosphorus loading: 18.3 tonnes P year⁻¹) and sinks (outflows: 13.1 tonnes P year⁻¹). Dreissenids approximately filter 68.5 tonnes P year⁻¹ from the water column and subsequently egest 58.5 tonnes P year⁻¹ via their metabolic excretion and particle rejection, whereas an additional 6.7 tonnes P year⁻¹ of pseudofeces are deposited onto the sediments. Interestingly, our model suggests that the sediments (resuspension and diffusion from the sediments to water column minus particle settling) act as a net sink in this segment (2.7 and 1.2 tonnes P year⁻¹ in the epilimnion and hypolimnion, respectively). Macrophyte intake of phosphorus from the interstitial waters is responsible for a net loss of 8.6 tonnes P year⁻¹ from the sediments, and an approximately equal amount is returned into the water column through respiration/excretion. Likewise, macrophyte intake minus the amount of P regenerated from the decomposition of the dead plant tissues can take away 12.7 tonnes P year⁻¹ from the sediments in the eastern part of Lake Simcoe, while the subsequent release of their metabolic by-products is responsible for 12.8 tonnes P year⁻¹. The particulate P settling clearly dominates over the resuspension and diffusion from the sediments to the water column with the corresponding net fluxes being equal to 5.8 tonnes P year⁻¹.

The macrophyte community in Lake Simcoe is dominated by *Ceratophyllum demersum* (39.1% of the total biomass), the invasive species *Myriophyllum spicatum* (27.4%), *Elodea*

canadensis (10.7%) and Chara spp. (9.7%) (Ginn, 2011). The controlling factors of the submerged macrophyte distribution and abundance are the depth, fetch/wave exposure, sediment texture and stability, and P loading from the closest tributary along with the size of the area drained (Ginn, 2011). A nearly threefold increase in aquatic plant biomass has been recorded since 1984, with macrophytes proliferating into much deeper (from 6.0 m in 1984 to 10.5 m in 2008) waters with increasing water clarity (Ginn, 2011). Submerged macrophytes obtain P both from the water column and the sediment substrate, but under normal pore and ambient P concentrations, nutrient intake from the sediments dominates. In doing so, they can provide a significant pathway for the rapid transport of the nutrients assimilated from the sediments into the water column, a process known as "nutrient pump effect" (Asaeda et al., 2000; Howard-Williams and Allanson, 1981). In accordance with empirical evidence, our model consistently predicts that macrophyte intake from the interstitial waters is responsible for a significant loss of P from the sediments. For example, in Cook's Bay, Johnson and Nicholls (1989) found a sediment TP \approx 1040 µg g⁻¹ relative to a recently reported mean value of 518 µg g^{-1} , with $\approx 300 \ \mu g \ g^{-1}$ in the southern area of this embayment where the highest plant biomass was recorded (Ginn, 2011). Our study also postulates that approximately equal P mass is returned into the water column as metabolic excreta. Interestingly, due to its bathymetry, the deep and narrow Kempenfelt Bay has minimal area of potential habitat for macrophytes, compared to Cook's Bay and Eastern End and it is, therefore, the only part of the lake, where their role in the phosphorus cycle appears to be negligible.

A recent in-vitro experiment with eutrophic water from Holland River confirmed a rapid change in color from murky water to transparent due to active mussel filtration (LSRCA, 2012). However, our model calibration results suggest caution before extrapolating small-chamber experiments to the entire lake, as dreissenids are predicted to filter a considerable amount of particulate phosphorus from the water column (6.2-238 tonnes P year⁻¹), but the effective clearance rate is significantly lower (0.8-22.8 tonnes P year⁻¹) with a substantial amount of the filtered particles (>85%) returned into the water column as feces, pseudofeces or other metabolic excreta. The latter finding is not surprising as the ratio between zebra mussel filtration and effective clearance rate can vary between 3.4 and 6.9 (Yu and Culver, 1999). In particular, our model highlights the critical role of dreissenids in the shallow eastern end of Lake Simcoe, where they filter 238.5 tonnes P year⁻¹ from the water column and subsequently egest 215.0 tonnes P year-1, while an additional 22.4 tonnes P year-1 of metabolic excreta are deposited onto the sediments (Figure 5). Because of its shallow morphometry, a large portion of the eastern area is located within the euphotic and well-mixed zone, and therefore the elevated benthic photosynthesis and access of the dreissenids to sestonic algae create favorable conditions for biodeposition and nutrient recycling (Ozersky et al., 2013). Importantly, the large fetch of Lake Simcoe, the relatively deep epilimnion, and the fairly rapid horizontal mixing often induce hydrodynamic conditions that may allow the localized impacts of dreissenids to shape ecosystem-scale patterns (Schwalb et al., 2013).

Along the same line of reasoning, North (2013) provided evidence that six out of eleven predicted effects of the nearshore P shunt hypothesis are supported by the long-term patterns in Lake Simcoe. For example, the littoral benthos has been characterized by an increase in abundance and diversity (Ozersky et al., 2011), while the biomass of non-dreissenid profundal benthos demonstrates decreasing trends (Rennie et al., 2012). Our model also corroborates the prevailance of dreissenids mediated flux of sestonic material to the near-shore sediments which leads to material and energy transfer from the water column to littoral zone (Figure 5). Counter

to the expected responses though (Higgins and Zanden, 2010), there was no evident change in the ice-free TP concentrations, phytoplankton biovolume levels, and relative abundance of filamentous benthic algae. Regarding the TP concentrations, the same study attributed the lack of a declining trajectory to the year-to-year variability of the exogenous TP loading that tends to prevail over the nearshore dreissenid filtration effects. Given the current mesotrophic state of Lake Simcoe, it is not unreasonable to assume a stronger reliance of the ambient TP dynamics upon the point and non-point nutrient subsidies from the watershed. However, our modelling analysis also suggests that the presence of active nutrient recycling pathways, potentially magnified by the particular morphological features and hydrodynamic patterns of Lake Simcoe, could be the reason why the system has not experienced distinct decreasing trends in regards to its TP levels.

4. DYNAMICS OF PHOSPHORUS BINDING FORMS IN LAKE SIMCOE SEDIMENTS

4.1. Introduction

Except for macrophytes and dreissenid mussels, lake sediments play a critical role in determining the fate and vertical transport of phosphorus, thereby modulating the actual magnitude of internal P loading. Phosphorus can be present in many chemical forms in the sediments and each form contributes differently to the internal loading depending on the prevailing conditions (Christophoridis and Fytianos, 2006). Hence, drawing robust predictions of internal P loading requires quantification of the different P forms present in the sediments. P mobilization in sediments has been extensively investigated in many eutrophic lakes, but there are only a few studies on P retention in mesotrophic systems, and thus the mechanisms are currently not fully understood. In general, P release is dependent on the ability of the sediments to retain P, the conditions of the overlying water, and the productivity status of the lake (Abdel-Satar and Sayed, 2010). The main driving factors are temperature, redox conditions, pH, dissolved oxygen, and the concentrations of other inorganic species, such as nitrate and sulfate in the sediments and water column (Ribeiro et al., 2008). P can be released through a wide array of physical, chemical, and biological processes, including ligand exchange mechanisms, mineralization, and release of dying cells (Christophoridis and Fytianos, 2006).

The reduction of external P loading has not always rendered a prompt recovery from eutrophication (Ahlgren et al., 2005; Carey and Rydin, 2011). Such delayed responses typically stem from the positive feedback between eutrophication-driven anoxia and internal P release (Gachter and Muller, 2003; Schindler, 2006). By contrast, internal loading in oligotrophic lakes is typically limited and the sediments are capable of greater P burial (Nürnberg, 1988). However, Lake Simcoe as a mesotrophic lake represent a transitional state between oligo- and eutrophic lakes, and as such investigations on P diagenesis processes in conjunction with its loading and land-use history can improve our fundamental understanding of the relative importance and effective control of internal loading.

In the third phase of the project, Dittrich et al. (2013) set out to study the spatio-temporal variability of P binding forms in Lake Simcoe. In doing so, the goal was to understand the mechanisms of internal P release under a wide range of loading conditions, diverse spatial

settings, ranging from flat, macrophyte-dominated to deep glacier-formed basins, and different periods of the year. The focus of the study was on three basins with different loading histories: Cook's Bay, Kempenfelt Bay, and Main Basin (Hiriart-Baer et al., 2011; Landre et al., 2011). The catchment area of the shallow Cook's Bay is characterized by both agricultural and urban land uses, and has been subjected to river channelization and wetland draining since the beginning of the 19th century. In the deep Kempenfelt Bay, the land-use and P loading history reflect the urbanization activities associated with the City of Barrie's population growth after the 1950s (Hiriart-Baer et al., 2011). The catchment of the main basin experienced gradual deforestation, which has been the main driver of the P loading variability.

4.2. Methods

As previously mentioned, the three sampling sites were located in main basin (K45), Kempenfelt Bay (K42) and Cook's Bay (C9) (see stations in Figure 1). The concentrations of five phosphorus-binding forms were measured in sediment cores down to 28 cm depth at two distinctly different periods of the year, before the stratification onset (March 2011) and toward the end of thermal stratification (September 2011). The P forms separated in the sequential fractionation method include loosely adsorbed (labile) P (extracted with NH₄Cl, NH₄Cl-TP), redox-sensitive bound P (extracted with bicarbonate dithionite, BD-TP), P bound to hydrated oxides of aluminum (extracted with NaOH, NaOH-SRP), organic bound P (extracted with NaOH-NRP), carbonate-bound P (apatite-P) (extracted with HCl, HCl-TP) and refractory P (Refract-P) (Psenner and Pucsko, 1988). Redox conditions (pH and oxygen profiles) were also measured in-vitro at the sediment-water interface with high (0.5 mm) vertical resolution. The total carbon was estimated as Loss of Ignition/2.5 (%) (Heiri et al., 2001). For each measurement two samples were prepared and measured in replicates, the data presented in this study are averaged values for these measurements, while the standard deviations were less than 7%. More details about the sampling protocol and analytical methodology of the sediment phosphorus binding form study can be found in Dittrich et al. (2013).

4.3. Results-Discussion

Lake Simcoe is a dimictic lake with strong summer stratification and ice coverage between January-March. The first sampling was conducted in March, when there was minimal replenishment of O_2 from atmosphere due to ice cover. The bottom O_2 concentrations in March were the highest in main basin and Cook's Bay with 5 mg L⁻¹ and lowest in Kempenfelt Bay with 3 mg L⁻¹ (Figure 6). In the end of summer stratification period, before the autumn overturn, the bottom concentrations were 6 mg L⁻¹ in main basin, 7 mg L⁻¹ in Cook's Bay, and 3.8 mg L⁻¹ in Kempenfelt Bay. pH varied from 7.0 to 7.5 in Cook's Bay, and 6.6 to 7.5 in Kempenfelt Bay, while the respective pH values in main basin were varying between 7.0 and 7.3. There were instances when these pH values were 0.2-0.6 units higher than those measured in the bottom water, possibly due to the carbonate dissolution in the sediments, which may also modulate the Ca²⁺ and HCO₃⁻ fluxes into overlying waters.

The three basins demonstrated significant spatial variation of the P binding forms in both March and September 2011 (Figure 7). The dominant binding form of phosphorus in the main

basin was carbonate-bound (HCl-TP), which contributed 35-50% to the total P content in the sediment (Figure 7). The redox-sensitive form (BD-P) was the second most abundant form (20% of total P), especially in the top sediment layer, though it distinctly decreased toward the deeper sediment. The NaOH-fraction contributed significantly to P content in the sediment surface. The dominant part of this fraction was organic-bound, NaOH-NRP fraction, approximately representing 20% of the total phosphorus, which is primarily driven by vertical flux of settling organic matter and sediment transported from shallow nearshore areas. Both refractory (Refract-P) and easily adsorptive phosphorus (NH₄Cl-TP) did not change with the sediment depth, contributing about 7% to the total phosphorus pool (Figure 7).

The surficial sediment TP in Kempenfelt Bay is higher, 0.8-1.9 mg P g DW⁻¹, than in the main basin, 0.7-1.1 mg P g DW⁻¹ (Figure 8). The P binding forms are also distributed differently in Kempenfelt Bay, in that a significant part of phosphorus (42%) was bound as a redox-sensitive component (BD-TP), which was the highest amount among all the stations sampled in Lake Simcoe (Figure 7). HCl-fraction was about 20% of the total phosphorus throughout the sediment depths studied. The redox-sensitive fraction declined from 42% of the total P at the sediment surface to around 3% in 20 cm depth, while organic-bounded P (NaOH-NRP) declined from 20% to 2%, and refractory phosphorus from 6.7% to 1.8%.

In Cook's Bay, the TP content was the lowest among the investigated stations, 0.5-1.0 mg P g DW⁻¹ (Figure 8). Interestingly, the carbonate-bounded (HCl-TP) fraction was the predominant one, accounting for up to 48% of the total phosphorus, which indicate the massive catchment erosion from highly intensive agricultural subwatersheds of West and East Holland rivers. The second important fraction was the organic-bound P (NaOH-NRP), which could be exacerbated by elevated primary production in Cook's Bay and macrophytes senescence. Approximately 50% of the P content in the deeper sediment was decreased due to the depletion of the BD-TP fraction and about 40% was associated with a decrease of the NaOH-NRP form, which indicates a strong internal loading from sediments to water column. The other fractions did not demonstrate notable changes over depth.

Depth profiles of the organic carbon and total phosphorus content in the three basin indicate that the highest concentrations of organic carbon were in surface sediments with values in Kempenfelt Bay and Main Basin to be comparable (7-8%), while the organic carbon content in Cook's Bay was lower (5-6%) (Figure 8). With increasing depth the organic carbon in Kempenfelt Bay and main basin decreased steadily from ca. 8% to ca. 5%, which indicated that the settled organic matter was not solely buried in the deeper layers, but also experienced bacteria-mediated mineralization. Sediment total P was very similar in March and September for all basins, with the highest P measured in Kempenfelt Bay, lower values in the main basin, and the lowest ones in Cook's Bay (Figure 8). P increased toward the surface of the sediment in all of the Lake Simcoe cores. Total P was elevated within the top 8-10 cm of the sediment cores, which chronologically correspond to 1970 in Main Basin, 1950 in Kempenfelt Bay, and 1990 in Cook's Bay.

A critical piece of information for the potential of Lake Simcoe to experience internal loading is the characterization of the sediment diagenesis processes between those occurring in short (fast release) and long time (slow release) scales (Figure 9). The fast P release rates at three sites were estimated by comparing the P-fraction content in the two uppermost layers, while the slow P release rates were calculated as a difference between P at the surface and deep sediment layers (Hupfer and Lewandowski, 2005).



Figure 6. Oxygen and pH profiles at the sediment-water interface for three study sites: Main Basin (a, b), Kempenfelt Bay (c, d), and Cook's Bay (e, f) for March (open symbols/left panel) and September (closed symbols/right panel).



Figure 7. Depth profiles of phosphorus binding forms in Lake Simcoe sediment cores sampled at the Main Basin (a, b), Kempenfelt Bay (c, d), and Cook's Bay (e, f) for March (left panel) and September (right panel).

NaOH-NRP is a good measure for organic P and poly-phosphate and its decrease is typically the result of microbial degradation. The organic fraction is usually the predominant P form of the sedimenting material (Guede and Gries, 1998). Together with HCl-P fraction, organic P is the main source for fast diagenesis. The most important source of this fraction is the erosion process associated with the land-use changes in the carbonate-rich Lake Simcoe watershed during the last decades, especially due to deforestation with the subsequent conversion to intensive agriculture and/or the urban sprawl. The accumulation of this fraction in surface sediments may be explained by the high pH values (>7.3) in the main basin sediments as well as the overall pH increase at the sediment-water interface compared to deep-water layers.



Figure 8. Organic carbon (circles) and total phosphorus (squares) in sediments of the Main Basin (a), Kempenfelt Bay (b) and Cook's Bay (c). Open symbols indicate March sampling and closed symbols represent September sampling.



Figure 9. Phosphorus release from sediment: dynamics of phosphorus binding forms responsible for the slow and rapid phosphorus release in Main Basin (a, b), Kempenfelt Bay (c, d) and Cook's Bay (e, f).

In the same context, Dittrich et al. (2013) showed a small difference in total release rates between fast (40 mg m⁻² year⁻¹) and slow processes (52 mg m⁻² year⁻¹), which indicates that almost half (44%) of P releases in a short-time scale. P release in the main basin is driven by the continuous flux of settling P from the epilimnion as well as the inventory of P stored in the sediments. Diagenesis in the upper sediment layers is fast enough and is approximately twice as high as P loading from air deposition (23-30 mg m⁻² year⁻¹) (LSRCA, 2013).

In contrast to the main basin, Dittrich et al. (2013) found that the BD-P fraction in Kempenfelt Bay contributes up to 67% and 54% of P release in long- and short-term scales, respectively. The other two significant fractions that contributed to P release are NaOH-NRP

and HCl-TP. The proportions of these binding-forms in total P release correspondingly are 24% and 9% in a long-term time scale and 16 and 2% in a short time scale. The high amount of BD-P fraction distinguishes the Kempenfelt Bay sediments from the Main Basin and Cook's Bay. The long history of hypolimnetic anoxia and deep morphology of Kempenfelt Bay may have led to the depletion of the redox-sensitive fraction, BD-P, in the deeper sediment and the accumulation of BD-P at the surface sediments. A difference in total release rates between fast and slow processes (97 versus 133 mg m⁻² year⁻¹) indicates that 42% of P releases occur within a short time scale, but a substantial fraction (58%) of diagenetically mobile P sediments represents a long-term P source in the system.

The TP content in the sediments of Cook's Bay is the lowest among the three studied basins in Lake Simcoe, and the limited P accumulation could be attributed to the higher sedimentation rates that may dilute P concentration as well as the substantial amount of P flushed out from Cook's Bay in the form of decaying macrophytes biomass. The main P binding form that appears to be mobilized through diagenesis is HCI-TP fraction, which is also the dominant fraction of TP in Cook's Bay. This fraction contributes 42% and 39% to the P release from the sediments in a long- and short-time time scale (Dittrich et al., 2013). The accelerated erosion in the catchment of Cook's Bay may be responsible for the predominance of this fraction. Furthermore, the low TP content provides evidence that the high sedimentation rates and natural watershed sources lead to the "dilution" of P in the sediment dry matter.

By comparing tributary loading with sediment P accumulation estimates, Dittrich et al. (2013) attempted to infer about the spatial variability of P retention. During the period 2007-2009, Cook's Bay reportedly received 570-930 mg P m-2 year-1 (25 tonnes P year-1 in 2009 with 0.52 km3/yr of precipitation and 42 tonnes P year-1 in 2008 with 0.77 km3/yr of precipitation), while the sediments accumulated P in the top 0-2 cm layer with an annual rate of ~520 mg m-2 year-1, which is lower than post-1970 estimate of 650 mg m-2 year-1 in Hiriart-Baer et al.'s (2011). Therefore, overall 50-420 mg P m-2 year-1 were transported to the main basin in 2007-09 and the level of retention for Cook's Bay was 56-92%, which means that the tributary loading from the highly urbanized and agriculturally intensive watersheds of Holland River has also a direct effect on the water quality of the main basin. In contrast, Dittrich et al. (2013) found that the retention for Kempenfelt Bay increased to 54-70% in 2007-09 compared to 25% in the 1980s (Johnson and Nicholls, 1989). The main explanation for the higher retention value in Kempenfelt Bay may be the lower external P loading since the 1990s (Winter et al., 2007), fewer events of severe oxygen depletion over profundal sediments since 1990s (Johnson and Nicholls, 1989), and higher end-of-summer dissolved oxygen levels in 2000-2003 (3.8-4.6 mg L-1) than the long-term average (3.3 mg L-1) at the 39 m water depth (Eimers et al., 2005). During the last two decades, point sources in the urbanized area of Kempenfelt Bay have been successfully removed, and this change combined with the morphology of the basin may have led to an increase of P retention. The main basin retained 72-95% of P compared to 54% in the 1980s (Johnson and Nicholls, 1989) and exported to the outlet basin with a rate of 15-52 mg m-2 year-1, which corresponds to total lake retention of 87-93% in 2007-09. This P retention estimates are approximately similar to a retention value for the whole lake, 88%, calculated independently from an inventory of inputs and outputs (Young et al., 2010).

To recap, Lake Simcoe is characterized by significant spatial heterogeneity in respect to P retention. While in the two deep basins, Kempenfelt Bay and Main Basin, the P retention increased compared to the eutrophic years (1980s), it decreased in the shallow Cook's Bay. The

increase of P retention in Kempenfelt and main basin caused mainly by their deep morphology and land-use changes. On the other hand, despite the recent decline of P loading in Cook's Bay catchment, its intensive agricultural land-use in the past, its morphology with flat bottom, the colonization of the embayment by dreissenids and/or the recent proliferation of macrophytes, may led to decrease of P retention. Therefore, P retention in Lake Simcoe evolved differently in three main basins, depending on the morphology, history, and land-use practices in their catchments.

5. CONCLUSION

We have presented an integrative spatial analysis aiming to connect watershed with downstream biogeochemical processes in Lake Simcoe. The need for such a modelling exercise stemmed from the emerging management questions related to contemporary climate and land use changes that may challenge the achievability of the goal to reducing nutrient loading from 72-115 T P year⁻¹ in 2007- 2011 to 44 T P year⁻¹ by 2045. Using Self- Organizing Mapping of biophysical and socio-economic data, we delineated Socio-Environmental Management Units as a basic organizational unit for integrated watershed management planning. Integrating social, economic, and environmental data enabled to distinguish between "undisturbed" (or reference) and "anthropogenically-influenced" subwatersheds. In the latter group, affordable housing appears to be a strong accelerating factor of residential mobility. There is a significant disparity between average dwelling prices in the Lake Simcoe watershed and the Greater Toronto Area, whereas family incomes between 1996 and 2006 were ranging from \$85,000 to \$125,000 in Lake Simcoe catchment versus a contemporaneous annual average income of \$97,000 in Toronto (Neumann et al., 2017). Moreover, qualitative changes in the productivity mode, characterized by a shift from the manufacturing industry to a post-industrial service economy, appear to magnify socio-economic interactions and thus attract more residents in the Lake Simcoe basin. Bearing also in mind the increasing urbanization pressure in the area, another key finding of our analysis is that the "anthropogenically-influenced" subcatchments have some distinct functional properties, such as the presence of a tight relationship between demographics and tributary nutrient export, and absence of natural mechanisms to control environmental degradation, which collectively cast doubt on their sustainability.

Given the ever-growing population and infrastructural expansion plans, the latter finding underscores the challenges for a successful nutrient control in locations classified into the "anthropogenically-influenced" group. In particular, the subcatchments of West Holland and East Holland were identified as the largest P contributors in the area, which are also geographically and hydrologically connected to Cook's Bay at the southwestern part of Lake Simcoe. Importantly, phosphorus levels in Cook's Bay are relatively higher than any other location in Lake Simcoe, partly reflecting the elevated P from the highly agricultural Holland Marsh (Gudimov et al., 2012). The latter assertion is also reinforced by the fact that the predominant fraction of TP in the sediments of that embayment is carbonate-bound P (apatite-P) mainly due to the accelerated erosion in the adjacent catchment (Gudimov et al., 2015).





Figure 10. (a) Comparative diagram of P sinks at sediment–water interface (tonnes P year⁻¹); (b) Sankey diagram for a comparative description of the phosphorus flows from exogenous and endogenous P sources (tonnes P year⁻¹). Width of the flow pathways is proportional to annual estimates of relevant fluxes. Dreissenids pathways indicate negative fluxes associated with the particle rejection/egestion of metabolic excreta minus particle filtration.

(b)

Thus, it is essential for the local agricultural operations to comply with the key principles established by the local Water Quality Trading systems (e.g., Lake Simcoe Phosphorus Offset Program); namely, first meet baseline nutrient reduction requirements and then generate nutrient credits through crop conversions, agronomic practices (cover crops, reduced fertilizer application, and manure export), and structural best management practices (riparian buffers, livestock fencing).

Differences in the socio-environmental patterns within Lake Simcoe watershed can also be used to gauge the residents' potential engagement in stewardship programs for nutrient loading reduction initiatives. A characteristic example was the spatial cluster characterized by highest family income and dwelling values in the basin (cluster #6). These residents deliberately opt for quasi-rural settlements in order to connect with nature, which may imply an aptitude to support conservation programs. Thus, these sites could be identified as a priority target for catchment stewardship initiatives (Cadieux and Taylor, 2013). By contrast, areas holding an extensive inventory of wetlands (14.6-46.5% of subwatershed areas) are also occupied by the low end of family-income spectrum (clusters #1, 5, and 8). This distinct land use-family income patterns may be used to optimize the efficiency of local Nutrient Trading Programs by establishing economic incentives for nutrient loading reductions and subsequently offsetting new or increased discharges from other sources within the Lake Simcoe watershed (Neumann et al., 2017). For example, the cluster #6 could buy nutrient credits from clusters #1, 5, and 8 that will be used to further occupy the latter subcatchments by wetlands and forested areas and phase out hay, pasture, and other agricultural lands. In doing so, there will be greater financial interest in wetland mitigation programs (Bendor, 2009), thereby maximizing the environmental benefits in the studied area.

Nonetheless, it is important to note that the success of the on-going restoration efforts in Lake Simcoe can be significantly modulated by the presence of significant feedback loops associated with nutrient recycling (dreissenid activity, macrophyte proliferation, and the interplay between water column and sediments) that shape the relationship between external loading and ecosystem response in both space and time. P diffusive fluxes from the sediments account for about 30–35% of the P loading in Lake Simcoe (Figure 10). The sediments in the main basin are mostly driven by fast diagenetic processes of settling organic matter from the epilimnion, resulting in internal P loading of 9.2 tonnes P year⁻¹. In a similar manner, the hypolimnetic sediments in Kempenfelt Bay are responsible for a fairly high diffusive P flux into the water column (\approx 1.7 tonnes P year⁻¹), presumably reflecting the highest proportion of the redox-sensitive P sediment pool compared to other lake segments.

Both empirical evidence and modelling projections suggest that macrophyte intake is responsible for a significant loss of P from the interstitial waters, thereby providing a significant pathway for the rapid transport of the nutrients assimilated from the sediments into the water column. Dreissenids filter also a significant amount of particulate P from the water column, but the effective clearance rate is significantly lower with a substantial amount of the filtered particles (>85%) returned into the water column as feces, pseudofeces or other metabolic excreta. This pattern is particularly pronounced in the shallow eastern end of Lake Simcoe, where a large portion is located within the euphotic and well-mixed zone, and therefore the elevated benthic photosynthesis and access of the dreissenids to sestonic algae create favourable conditions for biodeposition and nutrient recycling. Importantly, the large fetch of Lake Simcoe and the fairly rapid hydrodynamic mixing may facilitate the localized impacts of dreissenids to modulate ecosystem-scale patterns. The latter pattern may also be responsible

for the absence of a decreasing trend in the lake P concentrations after the invasion of dreissenid mussels along with the presence of active nutrient recycling pathways, and therefore there will inevitably be some uncertainty in accurately linking management actions in the watershed with the response of the receiving waterbody.

On a final note, drawing parallels among the challenges that pose threats to the integrity of large lakes and coastal areas, Shimoda et al. (2011) asserted that our contemporary understanding of the effects of anthropogenic activities and climate change on lake phenology has been primarily based on empirical evidence from offshore areas, while the interactions with the nearshore zones have largely been neglected. In many large lakes, the most degraded areas are nearshore zones above the summer thermocline adjacent to the mouths of large rivers and enclosed embayments with restricted mixing with offshore water masses. Similar to the coastal zone, these areas are intermediate zones in that they can receive polluted inland waters from watersheds with significant agricultural, urban and/or industrial activities while mixing with offshore waters having different biological and chemical characteristics. Climate-induced shifts in air temperature, rainfall and wind forcing can potentially influence lake mixing and currents, because they determine both the rate and magnitude of warming/cooling and the magnitude and frequency of runoff. The interaction of surface hydrological patterns with in-lake hydrodynamics thus dictates to a large degree the in-lake dispersal of pollutants and consequently the spatial extent and magnitude of associated ecological impacts that incoming inflows are likely to have. Thus, the advancement of our understanding of human and/or climate-induced changes on ecosystem integrity should be based on integrative methodological tools that consider as one of the focal points the interplay among watershed, nearshore, and offshore areas. Viewed from this perspective, we believe that the advancement of the management paradigm of large lakes and coastal areas is in principle a bidirectional and recursive process (Arhonditsis et al., 2003). As such, the spatial analysis framework presented herein is conceptually suitable in assisting with the design of restoration programs and management planning for both large lake and marine systems.

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