Numerical modeling of eutrophication dynamics in the shallow coastal ecosystem: A case study in the Maryland and Virginia coastal bays

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NUMERICAL MODELING OF EUTROPHICATION DYNAMICS IN THE SHALLOW COASTAL ECOSYSTEM: A CASE STUDY IN THE MARYLAND AND VIRGINIA COASTAL BAYS

A Dissertation
Presented to
The Faculty of the School of Marine Science
The College of William and Mary in Virginia

In Partial Fulfillment
Of the Requirements for the Degree of
Doctor of Philosophy

by

Taiping Wang

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This dissertation is submitted in partial fulfillment of
the requirements for the degree of
Doctor of Philosophy

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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>viii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>ix</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>xv</td>
</tr>
<tr>
<td>CHAPTER I INTRODUCTION</td>
<td></td>
</tr>
<tr>
<td>I-1 Background</td>
<td>2</td>
</tr>
<tr>
<td>I-2 Study site – Maryland and Virginia Coastal Bays</td>
<td>4</td>
</tr>
<tr>
<td>I-3 Key issues</td>
<td>6</td>
</tr>
<tr>
<td>I-3-1 The importance of physical processes</td>
<td>6</td>
</tr>
<tr>
<td>I-3-2 The spatial water quality gradient</td>
<td>7</td>
</tr>
<tr>
<td>I-3-3 Modeling of benthic macroalgae – formulation and computation</td>
<td>8</td>
</tr>
<tr>
<td>I-3-4 The influence of benthic macroalgae on phytoplankton, nutrient, and oxygen dynamics in the MVCBs</td>
<td>8</td>
</tr>
<tr>
<td>I-3-5 The impact of benthic microalgae (BMA) in shallow coastal waters</td>
<td>10</td>
</tr>
<tr>
<td>I-4. Objectives and hypotheses</td>
<td>10</td>
</tr>
<tr>
<td>CHAPTER II APPLICATION OF A HYDRODYNAMIC MODEL IN THE MARYLAND AND VIRGINIA COASTAL BAYS</td>
<td>17</td>
</tr>
<tr>
<td>II-1 Introduction</td>
<td>17</td>
</tr>
<tr>
<td>II-2 Model description</td>
<td>19</td>
</tr>
<tr>
<td>II-3 Model setup</td>
<td>23</td>
</tr>
<tr>
<td>II-3-1 Grid generation</td>
<td>23</td>
</tr>
<tr>
<td>II-3-2 Model forcing</td>
<td>24</td>
</tr>
<tr>
<td>II-4 Model calibration results</td>
<td>26</td>
</tr>
<tr>
<td>II-4-1 Water level calibration</td>
<td>26</td>
</tr>
<tr>
<td>II-4-2 Velocity calibration</td>
<td>27</td>
</tr>
<tr>
<td>II-4-3 Salinity calibration</td>
<td>28</td>
</tr>
<tr>
<td>II-5 Conclusion</td>
<td>29</td>
</tr>
<tr>
<td>CHAPTER III DETERMINATION OF HYDRODYNAMIC TRANSPORT TIME SCALES FOR THE MARYLAND AND VIRGINIA COASTAL BAYS</td>
<td>47</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>-----------------------------------------------------------------------</td>
</tr>
<tr>
<td>III-1</td>
<td>Introduction</td>
</tr>
<tr>
<td>III-2</td>
<td>Concept of different transport time scales</td>
</tr>
<tr>
<td>III-2-1</td>
<td>Definition of flushing time, age, and residence time</td>
</tr>
<tr>
<td>III-2-2</td>
<td>Selection of transport time scales in MVCBs</td>
</tr>
<tr>
<td>III-3</td>
<td>Application of flushing and residence time scales in MVCBs using a</td>
</tr>
<tr>
<td></td>
<td>numerical model</td>
</tr>
<tr>
<td>III-3-1</td>
<td>Flushing time</td>
</tr>
<tr>
<td>III-3-2</td>
<td>Residence time</td>
</tr>
<tr>
<td>III-3-3</td>
<td>Biogeochemical feature and residence time in MVCBs</td>
</tr>
<tr>
<td>III-4</td>
<td>Discussion and conclusions</td>
</tr>
<tr>
<td>IV-1</td>
<td>Introduction</td>
</tr>
<tr>
<td>IV-2</td>
<td>Field data collection</td>
</tr>
<tr>
<td>IV-3</td>
<td>Results and discussion</td>
</tr>
<tr>
<td>IV-3-1</td>
<td>Spatial water quality gradient in the MVCBs</td>
</tr>
<tr>
<td>IV-3-2</td>
<td>Water quality profiles along Turville Creek – Isle of Wight Bay transect</td>
</tr>
<tr>
<td>IV-3-3</td>
<td>High frequency continuous measurements in Turville Creek</td>
</tr>
<tr>
<td>IV-4</td>
<td>Summary</td>
</tr>
<tr>
<td>V-1</td>
<td>Introduction</td>
</tr>
<tr>
<td>V-2</td>
<td>Model development</td>
</tr>
<tr>
<td>V-2-1</td>
<td>Description of the general water quality model framework</td>
</tr>
<tr>
<td>V-2-2</td>
<td>Major assumptions for the benthic macroalgal module</td>
</tr>
<tr>
<td>V-2-3</td>
<td>Formulations of the benthic macroalgal module</td>
</tr>
<tr>
<td>V-2-4</td>
<td>Parameter evaluation</td>
</tr>
<tr>
<td>V-3</td>
<td>Simulating benthic macroalgae kinetics using a box-model</td>
</tr>
<tr>
<td>V-3-1</td>
<td>The effect of flushing time on algal species competition</td>
</tr>
<tr>
<td>V-3-2</td>
<td>Seasonal patterns of benthic macroalgae</td>
</tr>
<tr>
<td>V-3-3</td>
<td>A comparison between Droop and Monod kinetics</td>
</tr>
</tbody>
</table>
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## List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 2-1. Field stations used for hydrodynamic model calibration (station information was obtained from MDNR, NOAA and XTIDE websites)</td>
<td>30</td>
</tr>
<tr>
<td>Table 3-1. Flushing times for the MVCBs</td>
<td>65</td>
</tr>
<tr>
<td>Table 5-1. Water column state variables in CE-QUAL-ICM</td>
<td>133</td>
</tr>
<tr>
<td>Table 5-2. Benthic macroalgal module parameters – Ulva lactuca</td>
<td>134</td>
</tr>
<tr>
<td>Table 5-2 (Cont’d). Benthic macroalgal module parameters – Ulva lactuca</td>
<td>135</td>
</tr>
<tr>
<td>Table 5-3. Benthic macroalgal module parameters – Gracilaria vermiculophylla</td>
<td>136</td>
</tr>
<tr>
<td>Table 5-3 (Cont’d). Benthic macroalgal module parameters – Gracilaria vermiculophylla</td>
<td>137</td>
</tr>
<tr>
<td>Table 5-4. Box model configurations for Experiment 1</td>
<td>138</td>
</tr>
<tr>
<td>Table 5-5. Model results for Experiment 1 – phytoplankton only</td>
<td>139</td>
</tr>
<tr>
<td>Table 5-6. Model results for Experiment 1 – benthic macroalgae only</td>
<td>140</td>
</tr>
<tr>
<td>Table 5-7. Model results for Experiment 1 – both phytoplankton and benthic macroalgae present</td>
<td>141</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fig. 1-1. Map of the study site – the Maryland and Virginia Coastal Bays (taken from Wazniak et al., 2004a).</td>
<td>14</td>
</tr>
<tr>
<td>Fig. 1-2. The mean and maximum bottom dissolved oxygen (DO, mg L(^{-1})) in the MVCBs. Data are from MDE and MDNR for the period of 1992-2003.</td>
<td>15</td>
</tr>
<tr>
<td>Fig. 1-3. The mean and maximum surface chlorophyll a ((\mu g L^{-1})) in the MVCBs. Data are from MDE and MDNR for the period of 1992-2003.</td>
<td>16</td>
</tr>
<tr>
<td>Fig. 2-1. Hydrodynamic model grid of the Maryland and Virginia Coastal Bays (MVCBs).</td>
<td>31</td>
</tr>
<tr>
<td>Fig. 2-2. Comparisons between different versions of shoreline used for model grid generation for the MVCBs (see text for data sources).</td>
<td>32</td>
</tr>
<tr>
<td>Fig. 2-3. Map showing the subwatershed boundary, hydrodynamic model grid, NOAA weather stations, and USGS flow gages (station information were obtained from USGS and NOAA websites).</td>
<td>33</td>
</tr>
<tr>
<td>Fig. 2-4. An example plot of the daily freshwater discharge calculated from two USGS flow gages. The flow rate is for per unit square mile drainage area (raw flow data were downloaded from USGS website).</td>
<td>34</td>
</tr>
<tr>
<td>Fig. 2-5. Non-tidal water level fluctuations extracted from two NOAA field monitoring stations located in Lewes, DE and Chesapeake Bay Bridge Tunnel (CBBT), DE, respectively (data were downloaded from NOAA websites).</td>
<td>35</td>
</tr>
<tr>
<td>Fig. 2-6. The field stations used for tide, salinity, and current calibrations in the MVCBs (station information is given in Table 2-1).</td>
<td>36</td>
</tr>
<tr>
<td>Fig. 2-7(a). Tidal calibrations in the northern bays.</td>
<td>37</td>
</tr>
<tr>
<td>Fig. 2-7(b). Tidal calibrations in the southern bays.</td>
<td>38</td>
</tr>
<tr>
<td>Fig. 2-7(c). Tidal calibrations in the middle and southern bays.</td>
<td>39</td>
</tr>
<tr>
<td>Fig. 2-8. Along-bay tidal profiles (left panel: (M_2) amplitude; right panel: (M_2) phase).</td>
<td>40</td>
</tr>
<tr>
<td>Fig. 2-9. Water level verification at four water level field monitoring stations in the MVCBs (A: Ocean City Inlet, field data were downloaded from NOAA; B: South Point, field data were provided by MGS; C: Harbor of Refuge, field data provided by MGS; D: Turville Creek, field data were downloaded from MDNR website). Model – red solid line; Field – blue dotted line. See Table 2-1 for corresponding station information.</td>
<td>41</td>
</tr>
<tr>
<td>Fig. 2-10. An example plot of the wind data during the one-month period of current calibration in the MVCBs (data were downloaded from NOAA website).</td>
<td>42</td>
</tr>
<tr>
<td>Fig. 2-11. Current calibration results at three stations in the MVCBs (A: Isle of Wight Bay Channel; B: Sinepuxent Bay Channel; C: Chincoteague Channel). Model – red</td>
<td></td>
</tr>
</tbody>
</table>
solid line; Field – blue dash line. Current measurements were provided by MDNR.

Fig. 2-12(a). Salinity calibration results in the northern MVCBs (salinity observations were provided by MDNR, see Table 2-1 for station information) ........................................ 43

Fig. 2-12(b). Salinity calibration results in the northern MVCBs (salinity observations were provided by MDNR, see Table 2-1 for station information) ........................................ 44

Fig. 2-12(c). Salinity calibration results in the southern MVCBs (salinity observations were provided by MDNR, see Table 2-1 for station information) ........................................ 45

Fig. 3-1. A diagram explaining the definitions of age and residence time ........................................ 66

Fig. 3-2. Coastal Bays segmentation for flushing time calculation ........................................ 67

Fig. 3-3. The relationship between flushing time for the entire MVCBs and freshwater discharge rate. Black solid line denotes linear regression fit ........................................ 68

Fig. 3-4. An example plot showing the track of two particles released in Isle of Wight Bay (top) and Newport Bay (bottom). Green dots denote particle initial release locations. The whole simulation lasts about 10 days ........................................ 69

Fig. 3-5. Local residence time distributions in the MVCBs under four different flow conditions (unit for the color map is day) ......................................................... 70

Fig. 3-6. An example plot of the along-bay local residence time (LRT) profile under the mean flow condition .............................................................. 71

Fig. 3-7. Average peak concentration of brown tide at each Coastal Bays sample station between 1999 and 2001. The figure taken from Wazniak et al. (2004b) ................. 72

Fig. 3-8. Water Quality Index for the MVCBs (Jones et al., 2004) ........................................ 73

Fig. 4-1. A map showing MDNR monthly water quality monitoring stations in the MVCBs .............................................................. 86

Fig. 4-2. A map showing field monitoring stations along Turville Creek – Isle of Wight Bay – Ocean City Inlet transect .............................................................. 87

Fig. 4-3 (a). Average monthly monitoring water quality parameter values in the MVCBs (top panel – salinity; bottom panel – Secchi depth). Error bars represent one standard deviation. Raw data were collected by MDNR ........................................ 88

Fig. 4-3 (b). Average monthly monitoring water quality parameter values in the MVCBs (top panel – DO; bottom panel – chlorophyll a). Error bars represent one standard deviation. Raw data were collected by MDNR ........................................ 89

Fig. 4-3 (c). Average monthly monitoring water quality data in the MVCBs (top panel – NH_{4}^{+}-N; center panel - NO_{3}^{-}-N; bottom panel – PO_{4}^{3-}-P). Error bars represent one standard deviation. Raw data were collected by MDNR ........................................ 90

Fig. 4-3 (d). Average monthly monitoring water quality data in the MVCBs (top panel – DOC; middle panel – DON; bottom panel – DOP). Error bars represent one standard deviation. Raw data were collected by MDNR ........................................ 91

Fig. 4-4 (a). A bi-plot of the principal component analysis (PCA) result (x-axis – PC1 (65.5%); y-axis – PC2 (26.5%)) in the MVCBs. Data labels denote water quality monitoring stations in Fig. 4-1. Raw data were collected by MDNR ........................................ 92

Fig. 4-4 (b). Loadings of the 6 water quality variables on PC1 and PC2 ........................................ 93

Fig. 4-5 (a). Time series plot of 6-year (2000-2005) monthly chlorophyll a concentrations along the transect of Turville Creek – Isle of Wight Bay (from top to bottom are
monthly monitoring Stations 1 – 6 in Fig. 4-2). Raw data were collected by MDNR.

Fig. 4-5 (b). Time series plot of 6-year (2000-2005) monthly DO concentrations along the transect of Turville Creek – Isle of Wight Bay (from top to bottom are monthly monitoring Stations 1 – 6 in Fig. 4-2). Raw data were collected by MDNR.

Fig. 4-6 (a). Monthly averaged chlorophyll a and NH\textsubscript{4}\textsuperscript{+} profiles along the transect of Turville Creek – Isle of Wight Bay (error bars represent one standard deviation). From top to bottom are Stations 1-6 in Fig. 4-2. Raw data were collected by MDNR.

Fig. 4-6 (b). Monthly averaged NO\textsubscript{x} and PO\textsubscript{4}\textsuperscript{3-} profiles along the transect of Turville Creek – Isle of Wight Bay (error bars represent one standard deviation). From top to bottom are Stations 1-6 in Fig. 4-2. Raw data were collected by MDNR.

Fig. 4-7 (a). Time series plot of high-frequency water quality data in the upstream of Turville Creek. Raw data were collected by MDNR.

Fig. 4-7 (b). Time series plot of high-frequency water quality data in the upstream of Turville Creek. Raw data were collected by MDNR.

Fig. 4-8. Time series plot of summer high-frequency water quality data (left panel) and corresponding periodicity profiles (right panel) in the upstream of Turville Creek.

Fig. 4-9. Calculated daily net ecosystem metabolism (NEM) rates with four constant surface reaeration rates. Legend denotes the surface reaeration rate $k_a$.

Fig. 4-10. Calculated monthly mean net ecosystem metabolism rates vs. surface reaeration rates. The squares are monthly mean net ecosystem metabolism rate calculated under four constant $k_a$ (error bars represent ± one standard deviation), and the straight line denotes the best-fit linear regression line.

Fig. 5-1. Conceptual diagram showing hypothetical pattern of change in the relative contribution by three major groups of primary producers (phytoplankton - P; macroalgae - M; seagrass - S) in response to changes in nitrogen loading rate and residence time in shallow temperate estuaries (adopted from Valiela et al., 1997).

Fig. 5-2. Kinetic processes to be incorporated into the proposed benthic macroalgal module (BMAC – benthic macroalgae; DOM – dissolved organic matter; POM – particulate organic matter; DO – dissolved oxygen).

Fig. 5-3. Predicted light attenuation coefficient $k_e$ vs. measured values. Black solid line denotes the linear regression fit, and the pink dotted line denotes the 1:1 relationship.

Fig. 5-4. Temporally and spatially variable macroalgal N content as found in Hog Island Bay, VA. (Top panel: Ulva lactuca, Tyler et al., 2001; Bottom panel: Gracilaria vermiculophylla, Tyler and McGlathery, 2006).

Fig. 5-5. Net growth (biomass increment) of Gracilaria vermiculophylla under different temperature conditions after a 12-day incubation experiment (error bar stands for ± SE). Top panel – Experiment conducted in April, 2009; Bottom panel – Experiment conducted in May, 2009.

Fig. 5-6. Observed benthic macroalgal characteristics in Isle of Wight Bay, MD (data courtesy of Amber Hardison, VIMS).
Fig. 5-7. Observed macroalgal biomass at three monitoring stations in the MVCBs. Stations M-1 and M-2 were located in Turville Creek, and station M-3 was in Isle of Wight Bay. Data courtesy of Amber Hardison. (Legend: G – Gracilaria vermiculophylla; U – Ulva lactuca; O – other macroalgae). .................................................. 148

Fig. 5-8(a). Maximum photosynthesis rates $P_m$ (top panel) and respiration rates $R$ (bottom panel) measured for macroalgal samples taken in different months from Hog Island Bay, VA. Data courtesy of Juliette Giordano ......................................................... 149

Fig. 5-8(b). Maximum photosynthesis rates $P_m$ (top panel) and respiration rates $R$ (bottom panel) measured for macroalgal samples taken in different months from Isle of Wight Bay, MD. Data courtesy of Juliette Giordano .............................................. 150

Fig. 5-9. Diagram showing box model configurations. The water column has a fixed volume = $1 \times 1 \times 1 \text{ m}^3$. The bottom sediment layer consists of two sublayers (upper oxic layer (brown color in the figure) thickness = $\approx 0.1 \text{ cm}$ and lower anoxic layer (grey color in the figure) thickness = $\approx 0.1 \text{ m}$; thus, the total sediment layer thickness = $0.1 \text{ m}$). ............................................................................................... 151

Fig. 5-10. Solar radiation (top panel) and temperature (bottom panel) forcing for the 2nd numerical experiment .............................................................................................................. 152

Fig. 5-11(a). Seasonal variations of benthic macroalgal biomass, intracellular N:C mass ratio, and phytoplankton concentrations during a 2-year model simulation period. ................................................................................................................................. 153

Fig. 5-11(b). Seasonal variations of DO, DOC, and POC concentrations in the water column during a 2-year model simulation period ................................................................................................................................. 154

Fig. 5-11(c). Seasonal variations of DIN, DON, and PON concentrations in the water column during a 2-year model simulation period ................................................................................................................................. 155

Fig. 5-11(d). Seasonal variations of sediment fluxes of NH$_4^+$, COD (chemical oxygen demand in the form of H$_2$S), and SOD during a 2-year model simulation period.. 156

Fig. 5-12. Comparisons between Droop and Monod kinetics in the 3rd box-model experiment ................................................................................................................................. 157

Fig. 6-1. Map showing watershed model configurations and the linkage between watershed and the hydrodynamic model grid. The raw ArcView shape files of outfalls, streams, and watershed were provided by Dr. Angelica Gutierrez-Magness (UMD) ..................................................................................................................... 175

Fig. 6-2. Total annual nonpoint source loading rates calculated by the watershed model for the entire MVCBs (top panel – total nitrogen; bottom panel – total phosphorus). The raw data were provided by Dr. Angelica Gutierrez-Magness (UMD) .......... 176

Fig. 6-3: A comparison between HSPF predicted daily flow vs. USGS measurements (top panel – USGS1148471320; bottom panel - USGS01484719. See Fig. 2-3 for station locations). The model results were provided by Dr. Angelica Gutierrez-Magness (UMD) ................................................................................................................................. 177

Fig. 6-4. The spatial pattern comparisons between model predicted benthic macroalgal distribution at the end of 2003 (green color denotes the occurrence of benthic macroalgae) vs. MDNR field survey data (McGinty et al., 2004) .......... 178

Fig. 6-5. A spatial pattern comparison between MDNR survey data (left panel, McGinty et al, 2004) and model predicted maximum Gracilaria biomass (right panel, unit in g C m$^{-2}$) in Turville Creek and Isle of Wight Bay. ................................................................................................................................. 179
Fig. 6-6(a). Model predicted temporal variations of benthic macroalgal biomass and intracellular N:C mass ratio at three macroalgal survey stations in Fig. 6-9........... 180

Fig. 6-6(b). Model predicted temporal variations of water column chlorophyll a and DO at three macroalgal survey stations in Fig. 6-9....................................................... 181

Fig. 6-7(a). Model predicted seasonal (2004) variations of Ulva lactuca biomass (unit: g C m$^{-2}$) in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution).................................................................. 182

Fig. 6-7(b). Model predicted seasonal (2004) variations of Ulva lactuca intracellular N:C mass ratio in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution). ................................................................. 183

Fig. 6-7(c). Model predicted seasonal (2004) variations of Gracilaria vermiculophylla biomass (unit: g C m$^{-2}$) in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution). ................................................................. 184

Fig. 6-7(d). Model predicted seasonal (2004) variations of Gracilaria vermiculophylla intracellular N:C mass ratio in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution). ................................................................. 185

Fig. 6-8(a). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). All the filed data were collected by MDNR................... 186

Fig. 6-8(b). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). .......................................................................................... 187

Fig. 6-8(c). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). .......................................................................................... 188

Fig. 6-8(d). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). .......................................................................................... 189

Fig. 6-8(e). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). .......................................................................................... 190

Fig. 6-8(f). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). .......................................................................................... 191

Fig. 6-8(g). Water quality model calibration – comparisons between model predictions (blue line) and field observations (red star). Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). .......................................................................................... 192

Fig. 6-9. Map showing additional water quality model calibration stations in the MVCBs. .................................................................................................................. 193

Fig. 6-10(a). Water quality model calibration for selected stations in the MVCBs (Fig. 6-3) – comparisons between model predictions (blue line) and field observations (red star). ...................................................................................................................... 194

Fig. 6-10(b). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions (blue line) and field observations (red star). ...................................................................................................................... 195
Fig. 6-10(c). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions (blue line) and field observations (red star). ................................................................. 196

Fig. 6-10(d). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions (blue line) and field observations (red star). ................................................................. 197

Fig. 6-10(e). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions (blue line) and field observations (red star). ................................................................. 198

Fig. 6-10(f). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions (blue line) and field observations (red star). ................................................................. 199

Fig. 6-10(g). Water quality model calibration for selected stations in the MVCBs. ...... 200

Fig. 7-1. Model estimated temporal (2004) variations of total benthic macroalgal biomass (top panel) and intracellular nitrogen (bottom panel) retained by benthic macroalgae in the entire MVCBs ............................................................................................... 210

Fig. 7-2. Comparisons of water column profiles for chlorophyll a and DO (base scenario with benthic macroalgae – blue dotted line; sensitivity test scenario without benthic macroalgae – red solid line). ................................................................................................. 211

Fig. 7-3(a). With benthic microalgae activated as well, model results for benthic macroalgal biomass and N:C mass ratio. ........................................................................................................... 212

Fig. 7-3(b). With benthic microalgae module activated as well, model results for water column chlorophyll a, benthic microalgae, and DO. ................................................................................................. 213

Fig. 7-4. Model results for sediment oxygen demand (SOD) and chemical oxygen demand (COD) (with MA – blue solid line; no MA – red solid line). ................................................................. 214

Fig. 7-5(a). Benthic macroalgae simulation results in year 2003, note mortality rate sharply increases at Stations M-1 and M-2. ................................................................................................. 215

Fig. 7-5(b). Water column profiles of chlorophyll a and DO in year 2003, note low DO events occurred concurrently with benthic macroalgae dieoff events at Stations M-1 and M-2. ................................................................................................. 216

Fig. 7-6. Model sensitivity test results indicating the effect of surface reaeration rates on DO simulations at three benthic macroalgal survey stations. Red line represents the model results with the default surface reaeration rate k_r calculated by ICM; Blue line represents the model results with increased surface reaeration rates under super-saturation conditions. See text for details. ................................................................. 217
Shallow coastal bays and lagoons (mean depths <2-3 meters) are important buffer zones and links between terrestrial and deep marine ecosystems. They are inherently vulnerable to eutrophication, and are normally dominated by benthic primary producers such as seagrass, benthic micro- and macroalgae. There is an urgent need for quantitative models that are specifically designed for studying eutrophication dynamics in shallow coastal ecosystems.

In this study, a hydrodynamic and water quality modeling system consisting of the hydrodynamic model UnTRIM and the water quality model CE-QUAL-ICM was applied to a representative shallow coastal bay ecosystem, the Maryland and Virginia Coastal Bays (MVCBs). A high-resolution unstructured model grid was generated to resolve the complex geometry. To address the important role played by benthic macroalgae, a benthic macroalgal module, which assimilated macroalgal kinetics from literature and recent laboratory studies, was incorporated into the water quality model framework. The module includes two representative macroalgal species, Ulva lactuca and Gracilaria vermiculophylla, common in the MVCBs, and employs the internal nutrient-limited growth kinetics proposed by Droop.

The numerical modeling system has been calibrated against a comprehensive field monitoring data collected by the Maryland Department of Natural Resources in the MVCBs. The data include water level, current velocity, salinity, and major water quality variables, such as chlorophyll a, dissolved oxygen, and nutrients. The calibrated hydrodynamic model was used to calculate the physical transport time scales. The model estimated flushing time for the entire system is on the order of 2-3 months, which are much longer than typical time scales required by most biological processes. In addition, the local residence time is found to be extremely variable throughout the system. Depending on locations, the local residence time can vary from 0 to more than 200 days. The calculated transport time scales were further compared with spatial water quality distributions in the system. The comparisons demonstrate that physical circulations could substantially modulate biological processes in the system.

By using the Droop equation, the benthic macroalgae’s unique property, the so-called luxury uptake, was satisfactorily captured. Furthermore, the characteristic boom-and-bust life cycle of benthic macroalgae was qualitatively simulated using a box model. The expanded water quality model that includes the benthic macroalgal module reproduced both temporal and spatial distributions of observed benthic macroalgae and major water quality variables reasonably well in the MVCBs. The model results indicate that benthic macroalgae are highly important in regulating ecosystem metabolism in areas where they are abundant. Moreover, spring phytoplankton bloom was substantially suppressed when benthic macroalgae were present. The incorporation of a benthic macroalgal module also improved the model’s predictive capability in simulating dissolved oxygen in shallow ecosystems affected by benthic macroalgae. In terms of
nutrient budget, the model estimated that benthic macroalgae retain approximately 10% of annual nonpoint source nitrogen inputs from the watershed based on the simulation of year 2004. This is lower than that contributed by benthic microalgae reported in other shallow coastal bays such as the Lynnhaven Bay. It is suspected that the restricted distribution of benthic macroalgae in the MVCBs limited their role from the whole bay perspective. With the incorporation of a benthic macroalgae module, the overall water quality model prediction capability is improved.
NUMERICAL MODELING OF EUTROPHICATION DYNAMICS IN THE SHALLOW COASTAL ECOSYSTEM: A CASE STUDY IN THE MARYLAND AND VIRGINIA COASTAL BAYS
CHAPTER I INTRODUCTION

I-1 Background

Shallow coastal bays and lagoons are important land-margin ecosystems constituting at least 13% of the world’s coastlines (Nixon, 1982). They are in general relatively shallow (e.g., <3 m in Kjerfve, 1986), brackish bodies of water, separated by barrier islands, sandbanks, or coral reefs through limited tidal inlets from the open seas (http://en.wikipedia.org/wiki/Lagoon). For instance, shallow coastal bays and lagoons are common along the US East Coast from New York to Florida including: Great South Bay in New York, Barnegat Bay in New Jersey, Indian River and Rehoboth Bay in Delaware, Isle of Wight Bay in Maryland, Hog Island Bay in Virginia, Albemarle and Pamlico Sound in North Carolina, and Indian River and Banana River in Florida.

As important buffer zones and linkages between terrestrial and deep marine ecosystems, shallow coastal bay and lagoon ecosystems are extremely dynamic, both biologically and physically (e.g., Flindt et al., 1999). Because light can reach the sediment in most shallow lagoons and support photosynthetic activities there, phytoplankton photosynthesis is supplemented with, or even dominated by, a rich assemblage of benthic primary producers, including seagrasses, macroalgae, and benthic microalgae (Peckol and Rivers, 1996; Solidoro et al., 1997b; Valiela et al., 1997; Anderson et al., 2003; Dalsgaard, 2003). The high productivity is sustained by nutrient enrichment from direct land and atmospheric inputs as well as strong benthic recycling.
Therefore, the responses of different primary producers to excess nutrient input are the key to our understanding of the role played by shallow coastal ecosystems as coastal filters (e.g., McGlathery et al., 2007). Besides, shallow coastal waters have another characteristic physical feature, the vertically well-mixed water column. Efficient water column mixing driven by both winds and tides promotes effective exchanges inside the water body as well as at the air-water interface. This not only results in enhanced benthic-pelagic coupling, but also prevents the formation of persistent hypoxia/anoxia. Lastly, the complex shoreline geometry plus spatially varying nutrient input often leads to strong water quality gradients, which are difficult to investigate without a full understanding of the system-wide hydrodynamic properties.

The shallow coastal bay and lagoon systems provide important ecological functions for living resources, but are increasingly under stress due to anthropogenic effects caused by recreational, commercial, and navigation activities. The United Nation Environmental Program of World Health Organization reported that increasing human activities in coastal zones are causing coastal ecosystem disturbance – from river basin to the coastal marine ecosystem - that is trans-boundary and could inadvertently trigger change with catastrophic consequences (UNEP/GPA, 2006). Whereas shallow coastal ecosystems are inherently vulnerable to eutrophication resulting from the rapid human development in the coastal zone, to date there is still a lack of quantitative models to predict the ecosystem responses to increased nutrient inputs (McGlathery et al., 2007). To understand the eutrophication dynamics of shallow coastal bay and lagoon ecosystems, a system approach that integrates studies on watershed characteristics, hydrodynamics, and
water quality processes is highly warranted. Most complex numerical water quality models (e.g., Cerco and Cole, 1993; Rajar and Cetina, 1997; Park et al., 2005) have been applied to phytoplankton-based deep ecosystems rather than shallow, nearshore coastal waters that are more dominated by benthic primary producers; thus, there is at present a pressing need to develop system-specific numerical models suitable for shallow coastal waters. This has been the motivation for my dissertation.

I-2 Study site – Maryland and Virginia Coastal Bays

The Maryland and Virginia Coastal Bays (MVCBs), along the Atlantic Coast of the Delmarva Peninsula, extend approximately 200 km from Delaware to the mouth of Chesapeake Bay (Fig. 1-1). The MVCBs are a collection of shallow water bodies, which include Assawoman Bay, Isle of Wight Bay, Sinepuxent Bay, Newport Bay, and Chincoteague Bay. They represent a class of small estuaries that are comprised of many shallow, backbarrier island lagoons and salt marshes.

Based on physical geography, the MVCBs system is shallow and connected to the Atlantic Ocean through two inlets: the Ocean City Inlet to the north and the Chincoteague Inlet to the south. Its depth is generally less than 3 m, draining from a watershed with an area of approximately 450 km$^2$. The lagoons are characterized by extensive shoals (intertidal to 1 m below MLW) draining into deeper channels (Orth et al., 2006). River discharge is, in general, low and freshwater input is primarily from groundwater inflow. Hydrodynamics in the system are mainly controlled by tides and winds. Tidal range near
the Ocean City Inlet is larger than 1 m, while it drops to 0.1 m in the middle of the Chincoteague Bay and 0.5 m in Assawoman Bay. Strong mixing usually occurs due to wind in these shallow waters. Because of the limited connection to the Atlantic Ocean and moderate freshwater input, flushing in the bays is very slow. It usually takes months to replace all of the water within the bays by freshwater and ocean exchange. In general, these bays tend to trap both nutrients and sediments and, thus, are especially susceptible to eutrophication.

The water quality of the MVCBs is considered degraded as evidenced by elevated nutrients, low dissolved oxygen, and high bacteria concentrations, and are projected to experience environmental stress (Maryland Department of Natural Resources (MDNR), 2004; Maryland Department of the Environment (MDE), 2005). Figs. 1-2 and 1-3 show the averaged Bay-wide bottom DO and surface chlorophyll a measurements collected during 1992-2003 by MDNR and MDE. Since 1995, the MVCBs have been listed as one of the 28 estuaries in EPA’s National Estuary Program (NEP). The NEP program described the current status of the MVCBs as: “excessive levels of nitrogen resulting in algal blooms that reduce oxygen levels in bay waters; loss of natural habitats for fish, crabs, birds, and other wildlife; declines in numbers of fish, clams, crabs, and other important species; local bacterial contamination; and negative impacts from boating, dredging, and other water-based activities” (USEPA, 2007). Hence, there is a great need to search for solutions to these environmental problems. More importantly, as a typical shallow coastal ecosystem, the MVCBs provide an excellent site for studying ecological responses of the shallow coastal ecosystem to eutrophication.
In this dissertation, the study site focuses on the areas from Chincoteague Inlet to Assawoman Bay, which include Chincoteague Bay, Newport Bay, Sinepuxent Bay, Isle of Wight Bay, and Assawoman Bay (Fig. 1-1). These bays together form a system that connects to the Atlantic Ocean via Ocean City Inlet in the north and Chincoteague Inlet to the south. The state line between Maryland and Virginia cuts through the middle of Chincoteague Bay and separates the system into the Maryland Coastal Bays (MCBs, including the northern part of Chincoteague Bay and the remaining bays in Maryland) and the southern part of Chincoteague Bay in Virginia.

I-3 Key issues

I-3-1 The importance of physical processes

Physical processes (e.g., water circulations) play an important role in determining the ecological responses of coastal ecosystems to nutrient enrichment. Transport time scales, such as flushing time and residence time, have been widely used by estuarine ecologists to quantify hydrodynamic effects on biogeochemical processes in coastal environments (e.g., Hagy et al., 2000). Boynton et al. (1995) argued that residence time is such a critical attribute that it should be the basis for comparative analysis of ecosystem-scale nutrient budgets. Nixon et al. (1996) showed that the net transport of nutrients through estuaries to the continental shelf is negatively correlated with residence time of the water in the system. Short residence time in many estuaries may modify, and sometimes alleviate, the effects of eutrophication from nutrient enrichment (e.g., Monbet,
Interestingly, compared to river-dominated estuaries, shallow coastal lagoons are often characterized by a long residence time, which normally lasts for weeks to months (e.g., Hog Island Bay, VA, Fugate et al., 2006). The long residence time favors the entrapment of nutrients and sediments from terrestrial input and thereby intensifies the function of coastal bays and lagoons as “natural filters” for adjacent oceans. However, on the other hand, the accumulation of nutrients would inevitably cause water quality degradation inside the bays and lagoons. Therefore, a quantitative understanding of transport time scales is a high priority task in studying shallow coastal ecosystems.

I-3-2 The spatial water quality gradient

The distribution of salinity and water quality in shallow coastal systems often exhibits strong spatial variability. Compared to deep marine ecosystems, the spatial variability in shallow systems is mostly in the horizontal directions rather than in the vertical. In some shallow ecosystems, severe water quality degradation is often restricted to local areas. It is believed that the combination of watershed characteristics (e.g., pollutant loadings) and hydrodynamic settings (e.g., residence time) must play a leading role in determining water quality responses (e.g., Josefson and Rasmussen, 2000). In Isle of Wight Bay and Assawoman Bay, the gradients are most pronounced from the tributaries to the Ocean City Inlet; whereas, in Chincoteague Bay, there is a gradient between the western and eastern shores. The different characteristics highlight the necessity of applying a systematic approach to the study of this coastal lagoon ecosystem.
I-3-3 Modeling of benthic macroalgae – formulation and computation

Unlike deep water ecosystems that are dominated by free-floating phytoplankton species, the major primary producers in shallow ecosystems are usually bottom-dwelling species such as benthic microalgae, macroalgae, and seagrass (Nixon et al., 2001). McGlathery et al. (2001) established that, in the Virginia Coast Reserve Long-Term Ecological Research Site (Hog Island Bay, VA), macroalgae are responsible for most of the autotrophic production in spring and early summer, during which they serve as the dominant temporary sink for nitrogen. In order to understand how benthic macroalgae affect the shallow water dynamics quantitatively, it is essential to develop the capability to model the fundamental properties of benthic macroalgae such as light and nutrient requirements, boom-and-bust life cycle. Issues to be addressed include (1) the factors that affect its growth rate including availability of nutrients, temperature, and light levels, (2) the appropriate formulation for uptake (Monod vs. Droop formula), (3) the factors that contribute to its respiration and mortality, and (4) integration with the general eutrophication modeling framework.

I-3-4 The influence of benthic macroalgae on phytoplankton, nutrient, and oxygen dynamics in the MVCBs

The proliferation of ephemeral macroalgal communities in temperate, nutrient-rich coastal waters worldwide has been recorded and related to coastal eutrophication for decades (Curiel et al., 2004; Sfriso et al., 1992; Valiela et al., 1997;
Middelboe et al., 1998; Granger et al., 2000; McGlathery, 2001; Krause-Jensen et al., 2007). The occurrence of macroalgae in shallow coastal ecosystems has many ecosystem-level impacts. McGlathery (2001) reviewed the effects of macroalgal blooms on the decline of seagrass in nutrient-enriched coastal waters. She concluded that massive and persistent macroalgal blooms play an important role in shading light away from seagrass and eventually in displacing seagrass as the dominant benthic autotrophs in nutrient-enriched waters. Moreover, benthic macroalgae are especially effective in disrupting benthic-pelagic coupling by intercepting nutrient flux from the sediment to the water column due to their unique location between water-sediment interfaces (McGlathery et al., 1997; Valiela et al., 1997; Tyler et al., 2001).

The difference in life cycle and growth strategy between macroalgae and phytoplankton will affect the phytoplankton population in the coastal and lagoon systems. Most notably, macroalgae can outgrow phytoplankton during the spring/summer season and become a dominant source of nitrogen for phytoplankton as they decompose in later summer. Macroalgae can also substantially affect nutrient dynamics through high rates of production, respiration and decomposition (McGlathery et al., 2001). The extremely dynamic DO fluctuations in a shallow ecosystem are one of the most striking features resulting from the occurrence of macroalgae (e.g., D'Avanzo and Kremer, 1994; Peckol and Rivers, 1996; Park et al., 2003; Shen et al., 2008). Hence, to study the unique role played by benthic macroalgae in regulating nutrient recycling and ecosystem metabolism is indispensable to our understanding of the ecological responses of shallow coastal bays to eutrophication.
In addition to benthic macroalgae, benthic microalgae have been found to be another important benthic primary producer in shallow coastal ecosystems (Sundbäck, 1986; Dalsgaard, 2003; Tyler et al., 2003). Benthic microalgae are efficient in intercepting benthic nutrient fluxes and thus can retain nutrients within the sediment (Anderson et al., 2003). Using numerical models, Cerco and Seitzinger (1997) demonstrated that benthic microalgae had a major impact in the intra-annual cycling of nitrogen and phosphorus, especially in late winter and spring. Li (2006) also found that benthic microalgae's presence in Lynnhaven Bay could decrease the overall export of nitrogen and phosphorus to Chesapeake Bay. However, due to limited time and resources, this dissertation work will mainly focus on the role played by benthic macroalgae in the MVCBs. The potential impact of benthic microalgae on eutrophication dynamics will be briefly discussed later on.

I-4. Objectives and hypotheses

Interesting and important scientific questions on shallow coastal ecosystems are numerous. The development of both conceptual and quantitative models for the effects of eutrophication in shallow coastal bays lags significantly behind that for deeper estuarine ecosystems (McGlathery et al., 2007). The central goal of this dissertation was to develop a system-specific numerical modeling system that is more suitable for shallow coastal ecosystems. The calibrated modeling system will be further applied to address a series of
scientific questions and hypotheses that are difficult to answer with laboratory studies. Specifically, I have the following three major objectives:

1) To conduct a comprehensive hydrodynamic modeling study for representative shallow coastal bay and lagoon ecosystems, and to examine how key transport properties (e.g., residence time) affect the biogeochemical processes in these systems.

2) To develop a proper benthic macroalgal module using updated laboratory experimented results and algorithm(s). To integrate benthic macroalgae, as a major primary producer, into a system-specific water quality model and apply to the MVCBs.

3) To identify the combined roles played by physical transport and benthic primary producer (such as benthic macroalgae) on the phytoplankton, nutrient, and oxygen dynamics in shallow coastal bays and lagoons.

Accordingly, the following hypotheses have been postulated:

1) Transport properties (e.g., transport time scales) play a key role in controlling environmental gradients in shallow coastal ecosystems.

In shallow coastal ecosystems, physical processes including freshwater discharge and tidal flushing play a crucial role in modulating water quality and ecological
responses to increased nutrient loadings. The transport time scales, such as flushing time and residence time, are at least partially responsible for the spatially varying water quality gradients commonly observed in shallow coastal ecosystems.

2) Benthic macroalgae tend to dominate ecosystem metabolism when they occur abundantly in shallow coastal ecosystems. In addition, benthic macroalgae can outcompete phytoplankton in areas with high light availability and short residence time.

Benthic macroalgae will dominate ecosystem metabolism due to their much higher biomass than phytoplankton and benthic microalgae once they become abundant in shallow coastal ecosystems. The competition between benthic macroalgae and phytoplankton will be largely determined by spatially varying light availability and flushing capability.

3) Active growing benthic macroalgae increase the mean residence time of inorganic nutrients within shallow coastal ecosystems and thus intensify the “filter” function of shallow coastal ecosystems.

Benthic macroalgae can accumulate a large portion of nutrients within their tissue and thus retain more nutrients inside shallow coastal ecosystems. However, this retention is temporary. Once benthic macroalgae die off and decompose, the stored nutrients are released to the system and become an important nutrient source for other
primary producers. In addition, the retention effect is only significant in areas with high benthic macroalgal biomass.

4) A system-level numerical modeling system is necessary in addressing both temporally and spatially varying, system-wide eutrophication dynamics in shallow coastal ecosystems.

By using a system-level numerical modeling approach, the effects of both nutrient loadings and hydrodynamic properties on eutrophication can be better addressed within the same framework.
Fig. 1-1. Map of the study site – the Maryland and Virginia Coastal Bays (taken from Wazniak et al., 2004a).
Fig. 1-2. The mean and maximum bottom dissolved oxygen (DO, mg L\(^{-1}\)) in the MVCBs. Data are from MDE and MDNR for the period of 1992-2003.
Fig. 1-3. The mean and maximum surface chlorophyll a (µg L$^{-1}$) in the MVCBs. Data are from MDE and MDNR for the period of 1992-2003.
CHAPTER II APPLICATION OF A HYDRODYNAMIC MODEL IN THE MARYLAND AND VIRGINIA COASTAL BAYS

II-1 Introduction

Ecosystem modeling in the coastal bays and lagoons is inherently a multi-disciplinary process. In order for nutrient cycling processes, oxygen dynamics, and phytoplankton production to be modeled accurately in a shallow water ecosystem, one requires the freshwater discharge and nutrient loadings from the watershed model; water velocity, diffusion, and exchange rate with ocean from the hydrodynamic model; and, the proper diagenesis processes to generate sediment oxygen demand and nutrient fluxes from the sediment diagenesis model. Specifically, the MVCBs is a coastal inlet-lagoon system that experiences physical forcings from river input, tide, wind stress, precipitation, and evaporation and responds differently in time and space to those forcings. Physical processes play an important role in modulating the biological and chemical processes in the system. Monsen et al. (2002) demonstrated that the spatial variability of residence time (and exposure time) from a hydrodynamic model provides strong clues in shaping the spatial patterns of non-conservative quantities such as chlorophyll \( a \) and dissolved oxygen (DO). Because natural waters receive influxes of matter from external sources, there is little doubt that accurate representation of the physical processes by the hydrodynamic model is critical in providing accurate transport fields to the water quality model.
A number of 3-D hydrodynamic models are available to simulate tide- and wind-driven circulations in estuarine and coastal waters (e.g., Princeton Ocean Model (POM), Blumberg and Mellor, 1987; Curvilinear Hydrodynamics in Three Dimensions (CH3D), Sheng, 1987; Regional Ocean Model System (ROMS), Shchepetkin and McWilliams, 2005; Environmental Fluid Dynamics Code (EFDC), Hamrick, 1992 and 1994; Unstructured Tidal, Residual, and Intertidal Mud-flat Model (UnTRIM), Casulli and Walters, 2000; Eulerian – Lagrangian Circulation Model (ELCIRC), Zhang et al., 2004; Finite Volume Coastal Ocean Model (FVCOM), Chen et al., 2006). Depending on model grid types, these models can be classified into two categories, structured grid models (e.g., POM, ROMS, and EFDC) and unstructured grid models (e.g., UnTRIM, ELCIRC, and FVCOM). In general, unstructured grid models have a significant advantage over structured grid models in representing water bodies because of their flexibility in grid configurations. In particular, use of the unstructured grid allows one to “zoom in” on areas of keen interest by increasing the spatial resolution of grid cells locally. Hence, unstructured grid models have been increasingly popular in studying hydrodynamics of shallow coastal waters characterized by complex coastlines and bathymetry. For example, in the Venice Lagoon of Italy, a highly complex coastal lagoon ecosystem, nearly all the hydrodynamic modeling studies were conducted using unstructured grid models (e.g., Umgieesser et al., 2003 and 2004; Bajo et al., 2007).

In this dissertation, the UnTRIM model (Casulli and Walters, 2000) was used to investigate the general hydrodynamic circulation patterns in the MVCBs. A high-resolution, unstructured model grid was generated to represent the MVCBs and the
adjacent coastal ocean. Sections II-2 and II-3 describe the model formulation and model setup, respectively. Section II-4 summarizes the model calibration processes for surface elevation, current and salinity simulations. The model results demonstrated that a high-resolution hydrodynamic model has been successfully developed for the MVCBs and is readily available for use in studying eutrophication dynamics in the shallow coastal ecosystem.

II-2 Model description

The hydrodynamic model of UnTRIM was originally developed by Prof. Casulli of Trento University, Italy and implemented extensively in the natural environment by the United States Department of the Interior, Geological Survey, and the German Federal Waterways Engineering and Research Institute. A detailed description of the governing equations and numerical algorithm can be found in these references (Casulli and Zanolli, 1998; Casulli and Walters, 2000; Casulli and Zanolli, 2002 and 2005). The UnTRIM model solves the three-dimensional shallow water equations on an unstructured orthogonal grid in the horizontal domain. In the vertical, it uses a z-grid discretization with user-defined vertical layer thickness. The governing equations are solved using a finite difference – finite volume method that allows mass conservation to be satisfied both locally and globally.

In the UnTRIM numerical scheme, a finite volume method is used to discretize the free-surface two-dimensional continuity equation at each polygon. In this fashion, local and global volume conservation is guaranteed. The Eulerian–Lagrangian method
(ELM), also known as the semi-Lagrangian method, is applied to solve the momentum equations. It allows one to achieve a very accurate discretization of the nonlinear advection terms. ELM is especially efficient when applied to unstructured grids (Casulli and Walters, 2000; Casulli and Zanolli, 2002). The transport equations are solved by using an upwind difference scheme, or using a higher-order scheme – flux limiter method (Casulli and Zanolli, 2005) with a sub-cycle time step to ensure that mass is also conserved locally and globally.

In addition, UnTRIM also has the capability of simulating the wetting and drying process, which is crucial for shallow coastal waters characterized by a significant portion of intertidal areas. The model has been widely used to study hydrodynamics and pollutant transport in estuarine and coastal systems worldwide (Cheng and Casulli, 2002; Sisson et al., 2005; Celebioglu and Piasecki, 2006; Li, 2006; Shen et al., 2006; Liu et al., 2007 and 2008).

The UnTRIM model provides users the flexibility to formulate their own bottom friction and surface wind stress. The commonly used quadratic drag law is adopted here:

\[ \vec{\tau} = \rho C_d |\vec{u}| \vec{u} \]  

(2-1)

where \( \vec{\tau} \) = shear stress (Pa) induced by bottom sediment or surface wind; \( \rho \) = water or air density (kg/m\(^3\)); \( C_d \) = bottom or surface drag coefficient, and \( \vec{u} \) = wind or current
velocity vector (m/s). The bottom drag coefficient $C_b$ was formulated using the following equation (Hamrick, 1992) by assuming that a logarithmic current profile holds for the bottom layer:

$$C_b = \frac{\kappa^2}{\left(\ln\left(\frac{\Delta z_b}{2z_0}\right)\right)^2}$$  \hspace{1cm} (2-2)

where $C_b$ is the bottom drag coefficient; $\kappa$ is the von Karman constant = 0.4; $\Delta z_b =$ bottom layer thickness (m), and $z_0 =$ bottom hydraulic roughness height (m). In calibrating the model, $z_0$ was adjusted spatially, based on the bottom sediment property as well as the model calibration results for surface elevation and current velocity. The value of $z_0$ ranges from 0.002 to 0.02 m spatially.

The surface wind drag coefficient, $C_a$, was formulated as follows, according to the equation used in EFDC (Hamrick, 1992):

$$C_a = 1.2 \times 10^{-6} \left(0.8 + 0.065 \left|\frac{-u}{|u|}\right|\right)$$  \hspace{1cm} (2-3)

Eddy viscosity and diffusivity are calculated based on a turbulence closure scheme using the mixing length concept. The Richardson number-dependent scheme formulae were adopted to calculate the influence of stratification and shear on vertical eddy viscosity and diffusivity (Park, 1996; Liu et al., 2007):
where $A_z = \text{vertical eddy viscosity (m}^2/\text{s})$; $K_z = \text{vertical eddy diffusivity (m}^2/\text{s})$; $Z =$ distance from the surface (m); $h =$ total water depth (m); $u =$ horizontal current velocity (m/s); $a$ and $\beta$ are constants to be determined empirically via model calibration, and $R_i$ is the local Richardson number to characterize stability due to vertical stratification, and is defined as:

$$R_i = -\frac{g}{\rho} \left( \frac{\partial \rho}{\partial z} \right)$$

(2-6)

The water density was calculated using the equation of state:

$$\rho = \rho_0 \left( 1 + kS \right)$$

(2-7)

where $\rho =$ seawater density (kg/m$^3$); $\rho_0 =$ freshwater density = 1000 kg/m$^3$; $k = 7.8 \times 10^{-4}$ ppt$^{-1}$, and $S =$ salinity (ppt).
Open boundary forcing consists of tides and salinity. The tides comprising the ocean boundary condition consisted of the M\(_2\), N\(_2\), S\(_2\), K\(_2\), K\(_1\), O\(_1\), P\(_1\), and Q\(_1\) constituents, as described in detail in Section II-3-2.

The open boundary condition for salinity was treated using an upwind difference scheme such that, during the flood, an ocean salinity value of 33 ppt is prescribed for incoming flow and, during the ebb, freshwater inside the domain can be advected out by the ebb flow.

II-3 Model setup

II-3-1 Grid generation

A high-resolution unstructured orthogonal model grid consisting of both quadrilateral and triangular grid cells was generated for the MVCBs using the software program JANET. The grid covers the entire MVCBs and a substantial portion of the adjacent coastal ocean (Fig. 2-1). Whenever possible, quadrilateral cells were used to represent deep channels where the major axis of the current velocities normally coincides with the channel direction. Because the MVCBs have active shoreline migrations, four versions of shoreline data were used for grid generation. These shoreline data include: (1) medium-resolution shoreline data from NOAA (http://rimmer.ngdc.noaa.gov/mgg/coast/getcoast.html), (2) more recent shoreline data for the entire MVCBs provided by the Maryland Geological Survey (MGS) (Ms. Darlene Wells, personal communication), (3) high-resolution shoreline data from Worcester County, MD and the Maryland Geological Survey, which only cover the areas in
Maryland (http://www.mgs.md.gov/coastal/maps/shorevect.html), and (4) shoreline data extracted from Virginia Baseline Mapping Program’s (http://gisdata.virginia.gov/Portal/ptk?command=openchannel&channel=33) high-resolution aerial photograph for the southern Chincoteague Bay (Virginia Baseline Mapping Program, 2006). The NOAA shoreline data served as the baseline because of its broader coverage that included both VA and DE portions of the Coastal Bays. The two versions of shoreline data provided by MGS were used to better characterize and refine the portions located within Maryland because of their higher resolution and accuracy. An example of comparisons of different versions of shoreline data is given in Fig. 2-2.

High-quality bathymetric data are another crucial element required for hydrodynamic model grid generation. Since 2004, MGS has been conducting intensive bathymetry surveys in the MVCBs. These data provided essential depth information for the model domain inside the MVCBs. For the adjacent coastal ocean, the 3-second Coastal Relief Model bathymetric data from NOAA’s NGDC (National Geophysical Data Center) were used. All the bathymetric data were interpolated to grid depths using the bilinear interpolation method in JANET.

II-3-2 Model forcing

The major forcing functions for a hydrodynamic model include tides, winds, bottom friction, and freshwater inflow. The tidal forcing for each open boundary grid cell includes 8 major tidal constituents, namely $M_2$, $N_2$, $S_2$, $K_2$, $K_1$, $O_1$, $P_1$, and $Q_1$, which were extracted from the U.S. Army East Coast 2001 database of tidal constituents (Mukai
et al., 2002). The hourly wind data were downloaded from the National Climate Data Center (NCDC) online database at the two stations in Ocean City Municipal Airport, MD and Wallops Island, VA (Fig. 2-3). The freshwater discharge from each sub-watershed adjacent to the MVCBs was calculated using an area-weighted method based on the daily flow measurements from two USGS gauge stations (USGS 01484719 and USGS 0148471320, Fig. 2-3). The entire MVCBs watershed was first delineated into 157 sub-watersheds based on a 30-m resolution digital elevation model (DEM) and a medium-resolution stream network downloaded from USGS. The freshwater discharge for each sub-watershed was then calculated by multiplying its drainage area with the unit area flow rate obtained from the two USGS gauges. An example plot of the unit area flow rate for the year of 2004 is shown in Fig. 2-4.

To simulate water level, current, and salinity under real conditions, hourly wind data from NOAA were applied to the model domain. Additionally, the non-tidal surface elevations obtained from two nearby NOAA field water level monitoring stations (Lewes, DE and Chesapeake Bay Bridge Tunnel, VA) were linearly interpolated to the open boundary grid cells. The non-tidal surface elevations at the two NOAA stations were calculated by subtracting predicted hourly water levels from observed water levels (Fig. 2-5). The estimated daily freshwater discharge from each sub-watershed was distributed into adjacent hydrodynamic model grid cells.
II-4 Model calibration results

II-4-1 Water level calibration

The MVCBs hydrodynamic model was calibrated for water level, current velocity, and salinity by comparing model simulation results against field measurements. Inside the MVCBs, there is only one active water level monitoring station maintained by NOAA (Ocean City Inlet, MD, NOAA Station #08570283). Obviously, it is insufficient for water level calibration. In comparison, the online tidal prediction program XTIDE provides a much better coverage in the MVCBs (Fig. 2-6 and Table 2-1). The water level prediction provided by XTIDE is solely based on the astronomical harmonic constituents and does not include meteorological effects. However, because regular, short-term (with period of hours-day) water level fluctuations inside the MVCBs are mainly controlled by astronomical tides, to calibrate UnTRIM simulated tidal fluctuation against the XTIDE prediction is sufficient to prove the model's performance. Hence, the XTIDE prediction provides an important alternative for water level calibration inside the MVCBs.

In 2004, MGS conducted a brief survey of field water level measurements at selected sites in the MVCBs together with its bathymetry survey (Fig. 2-6 and Table 2-1). In 2005, MDNR deployed a YSI™ water quality data logger at its continuous monitoring station in Turville Creek. The data logger had a depth sensor recording water depth changes every 15 minutes. These additional field monitoring data were used for model verification, which was done in conjunction with salinity and current calibrations described as follows.
To calibrate surface elevation changes induced by tides, the UnTRIM model was run in a vertically integrated mode (2-D). The model calculations of tidal elevation were compared against XTIDE predictions at 9 stations throughout the MVCBs (Fig. 2-7(a-c)). In general, the model results match XTIDE predictions very well except for the station at Assateague Beach, Tom's Cove, which is located behind Chincoteague Inlet (Fig. 2-7(b)). The under-prediction of the tidal range at this station is probably due to the inaccuracy of local geometry. As can be seen from Fig. 2-2, the shoreline around this area is continuously changing, judging from different shoreline data sources.

Similar to other inlet systems, the tidal signal dampens out quickly as it propagates inside from the inlets. In the MVCBs, the tidal range decreases significantly from the regions right outside the inlets in the Atlantic Ocean (~1.6 m) to less than 0.2 m at the Public Landing Station, located in the Northern Chincoteague Bay (Fig. 2-6). Fig. 2-8 shows the along-bay profile of the M₂ tidal constituent, which accounts for the majority of the astronomical tidal forcing in this area. Clearly, the amplitude decreases inside from the two inlets while the phase shifts behind. The water level simulation was further verified with field measurements collected in 2004 and 2005. The comparison is shown in Fig. 2-9. Again, the model results compared very well with field observations.

II-4-2 Velocity calibration

Wind has been shown to have a key influence on currents in shallow water regions such as the MVCBs. High-frequency wind data, as shown in Fig. 2-10, were recorded at Ocean City and Wallops Island and used in the velocity calibration of the
UnTRIM model. Fig. 2-11 shows the calibration results of surface current velocity (2 m below surface) at three monitoring stations located in the deep channels of Chincoteague Bay (inside Chincoteague Inlet), Isle of Wight Bay (northern passage near Ocean City Inlet), and Sinepuxent Bay (southern passage near Ocean City Inlet), respectively. The current velocity was projected along its primary axis to obtain the along-channel component and the positive values denote the flooding stage. As can be seen from the comparisons, the model results are in good agreement with field measurements. The model slightly underestimated the velocity magnitude at the two stations located in Chincoteague Inlet and Isle of Wight Bay (A and C in Fig. 2-11), respectively. This is possibly due to the fact that some inter-tidal areas were purposely neglected in the modeling domain. The expansion of the model grid to include inter-tidal areas can increase the tidal prism within the bays, which will in turn improve the model predictions for current velocity.

II-4-3 Salinity calibration

The comparison between model-predicted salinity and field measurements by MDNR in 2004 is given in Fig. 2-12. Although the freshwater input was calculated using a simple area-weighted method based on USGS daily measurements, the model reasonably reproduced field observations throughout the domain. For stations closest to the inlets, the salinity was mainly controlled by ocean water and did not exhibit much fluctuation. In contrast, the upstream stations were much more sensitive to freshwater input and responded quickly to freshwater pulses. For example, there were approximately four major rainfall events that occurred in 2004 (Fig. 2-4). Following each rainfall event
(e.g., Day 103), salinity dropped sharply and gradually recovered at the two upstream stations, XDN4312 and TUV0011, in the northern bays. Although the total freshwater discharge into the entire system is very limited, episodic rainfall events can still have substantial impacts on upper bays and especially tributary creeks.

II-5 Conclusion

A high-resolution, 3-D hydrodynamic model has been successfully set up and calibrated for the MVCBs. Model calculations of surface water level, current velocity, and salinity are in good agreement with field measurements. As the first comprehensive hydrodynamic model specially developed for studying hydrodynamic processes in the MVCBs, it can serve as an important tool to acquire fundamental information on hydrodynamics for any other studies conducted in the system.
Table 2-1. Field stations used for hydrodynamic model calibration (station information was obtained from MDNR, NOAA and XTIDE websites).

<table>
<thead>
<tr>
<th>Station ID</th>
<th>Name</th>
<th>Type</th>
<th>Source</th>
<th>Latitude</th>
<th>Longitude</th>
</tr>
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<tr>
<td>C1</td>
<td>Isle of Wight Bay Channel</td>
<td>Current</td>
<td>MDNR</td>
<td>38.3311</td>
<td>-75.0920</td>
</tr>
<tr>
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<td>Sinepuxent Bay Channel</td>
<td>Current</td>
<td>MDNR</td>
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<td>-75.1001</td>
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<td>C3</td>
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<td>Current</td>
<td>MDNR</td>
<td>37.8826</td>
<td>-75.4142</td>
</tr>
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<td>Water Level</td>
<td>XTIDE</td>
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<td>-75.0833</td>
</tr>
<tr>
<td>W2</td>
<td>Ocean City Inlet</td>
<td>Water Level</td>
<td>XTIDE, NOAA</td>
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<td>-75.0917</td>
</tr>
<tr>
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<td>Water Level</td>
<td>XTIDE</td>
<td>38.3317</td>
<td>-75.0900</td>
</tr>
<tr>
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</tr>
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</tr>
<tr>
<td>W6</td>
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<td>-75.4917</td>
</tr>
<tr>
<td>W7</td>
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<td>Water Level</td>
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<tr>
<td>W9</td>
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<td>Water Level</td>
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<tr>
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<td>MGS</td>
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</tr>
<tr>
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<tr>
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</tr>
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<td>Salinity</td>
<td>MDNR</td>
<td>38.2457</td>
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</tr>
<tr>
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<td>XCM0159</td>
<td>Salinity</td>
<td>MDNR</td>
<td>38.1682</td>
<td>-75.2369</td>
</tr>
<tr>
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<td>Salinity</td>
<td>MDNR</td>
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<td>-75.3332</td>
</tr>
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Fig. 2-1. Hydrodynamic model grid of the Maryland and Virginia Coastal Bays (MVCBs).
Fig. 2-2. Comparisons between different versions of shoreline used for model grid generation for the MVCBs (see text for data sources).
Fig. 2-3. Map showing the subwatershed boundary, hydrodynamic model grid, NOAA weather stations, and USGS flow gages (station information were obtained from USGS and NOAA websites).
Fig. 2-4. An example plot of the daily freshwater discharge calculated from two USGS flow gages. The flow rate is for per unit square mile drainage area (raw flow data were downloaded from USGS website).
Fig. 2-5. Non-tidal water level fluctuations extracted from two NOAA field monitoring stations located in Lewes, DE and Chesapeake Bay Bridge Tunnel (CBBT), DE, respectively (data were downloaded from NOAA websites).
Fig. 2-6. The field stations used for tide, salinity, and current calibrations in the MVCBs (station information is given in Table 2-1).
Fig. 2-7(a). Tidal calibrations in the northern bays.
Fig. 2-7(b). Tidal calibrations in the southern bays.
Fig. 2-7(c). Tidal calibrations in the middle and southern bays.
Fig. 2-8. Along-bay tidal profiles (left panel: $M_2$ amplitude; right panel: $M_2$ phase).
Fig. 2-9. Water level verification at four water level field monitoring stations in the MVCBs (A: Ocean City Inlet, field data were downloaded from NOAA; B: South Point, field data were provided by MGS; C: Harbor of Refuge, field data provided by MGS; D: Turville Creek, field data were downloaded from MDNR website). Model – red solid line; Field – blue dotted line. See Table 2-1 for corresponding station information.
Fig. 2-10. An example plot of the wind data during the one-month period of current calibration in the MVCBs (data were downloaded from NOAA website).
Fig. 2-11. Current calibration results at three stations in the MVCBs (A: Isle of Wight Bay Channel; B: Sinepuxent Bay Channel; C: Chincoteague Channel). Model – red solid line; Field – blue dash line. Current measurements were provided by MDNR.
Fig. 2-12(a). Salinity calibration results in the northern MVCBs (salinity observations were provided by MDNR, see Table 2-1 for station information).
Fig. 2-12(b). Salinity calibration results in the northern MVCBs (salinity observations were provided by MDNR, see Table 2-1 for station information).
Fig. 2-12(c). Salinity calibration results in the southern MVCBs (salinity observations were provided by MDNR, see Table 2-1 for station information).
CHAPTER III DETERMINATION OF HYDRODYNAMIC TRANSPORT TIME SCALES FOR THE MARYLAND AND VIRGINIA COASTAL BAYS

III-1 Introduction

In shallow coastal bays and lagoons, the health of the ecosystem is determined by the interactions between physical, chemical, and biological processes. If exchange between bay and ocean, and inter-basins is limited, the rate of water transport is likely an important physical process affecting water quality. Transport time scales, such as flushing time and residence time, the measures of the rate of water transport, have been widely used to quantify hydrodynamic effects on biogeochemical processes in coastal ecosystems. The importance of physical transport to water quality was first recognized by Vollenweider (1976) in his classic empirical model of lake eutrophication, which describes the average concentration of chlorophyll-a as a function of the phosphorus loading rate scaled by water residence time. It has been argued that residence time is such an important attribute that it should be the basis for comparative analysis of ecosystem-scale nutrient budgets (Boynton et al., 1995). For example, Nixon et al. (1996) showed that the fraction of nitrogen inputs subsequently exported from an estuary decreases as residence time increases. In Waquoit Bay, Valiela et al. (1997) indicated that water residence time together with nutrient loading can control phytoplankton uptake and growth rate and, in turn, affect macroalgae blooms in the shallow water environment. In the Danshuei River estuary of Taiwan, short residence time resulted in low phytoplankton biomass despite extremely high nutrient concentrations in the water column (Wang et al., 2004). Hence, it is widely believed that short residence times in many estuaries may
modify and sometimes alleviate the effects of eutrophication resulting from nutrient enrichment (e.g., Monbet, 1992; Balls et al., 1995; Kelly, 1997; Cloern, 2001).

The MVCBs are representative of shallow coastal bays and lagoons that have limited exchange with the Atlantic Ocean. In general, the restricted bay-ocean exchange results in a poor flushing capability, and thus favors the accumulation of pollutants inside the system. To better study the eutrophication dynamics of the MVCBs, there is a pressing need for understanding the hydrodynamic circulation patterns in the system. The physical transport time scales, which integrate physical transport in terms of rate of renewal, are quantities very useful yet straightforward and can be easily determined with a hydrodynamic model. In this chapter, the calibrated hydrodynamic model was applied to calculate two representative transport time scales, flushing time and residence time, for the MVCBs. Results demonstrate that physical transport time scales do play a key role in regulating biogeochemical features in the MVCBs and should be carefully considered in studying ecological phenomena in the system.

III-2 Concept of different transport time scales

In marine science, three transport time scales, flushing time, residence time, and age, are most commonly used (e.g., Alber and Sheldon, 1999; Deleersnijder et al., 2001; Dettmann, 2001). Although these concepts are essentially similar quantitative parameters characterizing the flushing capability of an aquatic system, they are different from each other in terms of definitions and calculation methods partly due to: (1) unsteadiness imbedded in tidal, wind, and river-driven circulation and (2) spatial variation that
inherently exists in bathymetry, mixing, and circulation patterns. Therefore, one needs to be especially careful in applying them to a system. A detailed review of these concepts is given by Monsen et al. (2002). The following sections summarize their definitions and calculation methods.

III-2-1 Definition of flushing time, age, and residence time

Flushing time

Flushing time (FT) was originally defined as the “time to replace the freshwater volume of the estuary by the total freshwater input flux” (Dyer, 1973; Officer, 1976) or, more generally, as “the ratio of the mass of a scalar in a reservoir to the rate of renewal of the scalar” (Geyer et al., 2000). It is equivalent to both turnover time and hydraulic residence time (Bolin and Rodhe, 1973; Prandle, 1984). While the latter is more commonly used in the engineering fields, its application can also be occasionally found in estuarine studies (e.g., Hagy et al., 2000; Sheldon and Alber, 2002). Obviously, flushing time is generally regarded as a bulk or integrative property that describes the general exchange/renewal capability of a water body. Based on its definition, several standard calculation methods have been proposed. For instance, these methods include the classical tidal prism method, modified tidal prism method, fraction of freshwater method, and continuously stirred tank reactor (CSTR) method (Dyer, 1973; Officer, 1976; Sanford et al., 1992; Alber and Sheldon, 1999; Guo and Lordi, 2000). In reality, however, a single number for the entire system is not enough, especially when one is more concerned about the flushing capability of different sub-regions. To accommodate this,
some researchers have proposed the local flushing time concept for individual segments of a water body (e.g., Choi and Lee, 2004).

Age

Unlike flushing time, age is unique to each water parcel that enters the domain of interest. The concept of age is defined as “the time elapsed since the contaminant entered the system” (Bolin and Rodhe, 1973) or “the time a water parcel has spent since entering the estuary through one of the boundaries” (Zimmerman, 1988).

Because water parcels at different locations within a water body will have different ages, age is spatially variable and is especially useful in quantifying the spatially variable flushing capability for complex coastal systems. For example, the age concept has been applied to the Chesapeake Bay (Shen and Wang, 2007), as well as its tributaries of the York River (Shen and Haas, 2004), and the Lynnhaven Bay (Li, 2006). In these applications, three-dimensional hydrodynamic models were typically used as a major tool.

Residence time

Compared with the aforementioned “bulk” flushing time and “spatially variable” age concepts, residence time (RT) is probably the most widely used transport time scale in marine science. The residence time of a water element is defined as “the time it takes to leave the lagoon through its outlet to the sea” (e.g., Zimmerman, 1976). Based on its definition, residence time can be treated as the complement to age (Monsen et al., 2002;
Shen and Haas, 2004), and both of these metrics depend on the specification of the location of the boundary and the point of measurement within the domain. Thus, the specific way to define “the time to leave the system and the boundary” can also lead to different ways of defining residence time. For example, residence time can be defined as “the time for a water parcel to leave the system once” (once-through residence time, Oliveira and Baptista (1997)), which is useful to characterize the flushing of pollutants that are significantly altered once outside the system. It can also be defined as “the time for a water parcel to leave the system without returning at a later tidal cycle” (named re-entrant residence time in Oliveira and Baptista (1997)). This definition is suitable for the analysis of the retention of more conservative tracers in a system. Moreover, residence time can also be defined as “the time spent in the domain of interest”, which is particularly useful in coastal pollution since it quantifies the time of exposure of a specific system to a specific contaminant. Consequently, this has led to the definitions of “global residence time (GRT)” and “local residence time (LRT)” depending on specific domains and boundaries of interest. On the other hand, flushing time has been widely used as a substitute for residence time under special conditions (e.g., Rasmussen and Josefson, 2002; Sheldon and Alber, 2002; Gomez-Gesteira et al., 2003; Liu et al., 2004).

III-2-2 Selection of transport time scales in MVCBs

Flushing time (or hydraulic residence time) provides an integrative time scale of the flushing capability for a water body. It is simple to calculate, yet particularly useful if one wants to know how long on average the water and its associated pollutants can stay
inside a system. If one wants to obtain a detailed understanding of how spatially variable flushing capability affects the water quality gradients inside a system, the concepts of age and residence time are more appropriate. Since age refers to the elapsed time from a specific time and a specific location, it is more suitable for tracking individual point source discharges into a water body where river discharge plays a dominant role; for example, the calculation of travel time of Susquehanna River discharge within the Chesapeake Bay (Shen and Wang, 2007). In comparison, residence time can provide a spatial distribution of the time needed for any water parcel to leave the system without posing any prerequisite on freshwater input or other conditions.

In the MVCBs, the Saint Martin River is the largest source of freshwater discharge in the northern bays. If one is especially concerned about the travel time after a water parcel is released from the head of the Saint Martin River, age is the most appropriate time scale. As depicted in Fig. 3-1, the time it takes for a water parcel to travel from location A (the discharge point at Saint Martin River) to location B (a position inside the system before it leaves) is defined as its "age". For non-conservative dissolved substances such as nutrients, if age at location B is long enough, we can expect that most of the nutrients that are discharged at location A will be consumed before they can reach location B. Correspondingly, the travel time between locations B and C is called residence time for the parcel that initially remained at location B, if we assume that the parcel will not return once it is transported out of the Bay. For this case, because Ocean City Inlet is referred as the boundary for the domain of interest (Northern Coastal Bays), this type of residence time is called global residence time (GRT). Obviously, we
can easily conclude that, for a water parcel inside the Bay, if it is further away from the inlet, it tends to have a longer GRT. This may partially explain the commonly observed along-bay water quality gradient – poor water quality in the upper bays that improves moving downstream.

In certain situations, however, there is often concern about how effective physical circulation can be in alleviating a locally occurring water quality problem. For example, in the case of chemicals spilled into the Northern Coastal Bays (i.e., the target cell in Fig. 3-1), it is advantageous to know how long it will take for the chemicals to be flushed out of that specific area. Or similarly, if there is a severe harmful algal bloom occurring at the target area, it is important to know how the bloom can be diluted by the physical circulation. Apparently, for these two cases, GRT is not a suitable time scale for quantifying the effect of physical exchanges. Hence, the local residence time (LRT) concept, which focuses on the residence time for individual sub-domains surrounded by their own boundaries, is more meaningful, since the freshwater inputs in the MVCBs are limited, small, and enter the system from multiple sources such as stream discharge, direct surface runoff, and groundwater seepage. Regarding the bay in its entirety, there is not a major discharge point for either freshwater or pollutants. Thus, the age concept is not a suitable transport time scale from the whole bay perspective. Therefore, the rest of the chapter will mainly focus on flushing time and residence time calculations.
III-3 Application of flushing and residence time scales in MVCBs using a numerical model

In the previous section, the definition and selection of different transport time scales in the MVCBs were discussed on a conceptual level. If the objective is to produce a realistic and accurate depiction of transport time scales in the MVCBs and attempt to relate these time scales to the biogeochemical features, an implementation using the MVCBs hydrodynamic model will be required.

III-3-1 Flushing time

Based on original definition of flushing time, the following two equations both apply:

$$\text{Flushing Time} = \frac{V_f}{Q_{in}} \quad (3-1)$$

where $FT =$ flushing time for the target water body or its segment; $V_f =$ volume of fresh water within the target water body or its segment; and $Q_{in} =$ total freshwater inflow rate for the water body or its segment.

$$\text{Flushing Time} = \frac{M_{\text{tracer}}}{J_{in}} \quad (3-2)$$

where $FT =$ flushing time for the target water body or its segment; $M_{\text{tracer}} =$ mass of tracer within the target water body or its segment; and $J =$ total tracer inflow flux for the target water body or its segment.
The hydrodynamic model can be easily configured to calculate flushing time based on either of the two equations. Four numerical experiments were conducted using high (90th percentile, 0.0317 m$^3$ s$^{-1}$ km$^{-2}$), mean (76th percentile, 0.0170 m$^3$ s$^{-1}$ km$^{-2}$), median (50th percentile, 0.0089 m$^3$ s$^{-1}$ km$^{-2}$), and low (10th percentile, 0.0019 m$^3$ s$^{-1}$ km$^{-2}$) freshwater flows based on a 3-year record (2004-2006) of USGS observations. A conservative tracer with a constant concentration of 1 mg/L was discharged into the system together with freshwater input. At the open boundary, the tidal boundary condition was applied and the tracer concentration was set to zero for the incoming flow during the flood stage. No wind forcing was applied. For each experiment, the model was run for 3 years to allow the system to reach a dynamic steady state. The flushing times for the entire system and individual bay-segments (Fig. 3-2) were then calculated based on the model results for both the freshwater volume (Eq. 3-1) and tracer mass (Eq. 3-2).

Calculations of flushing time were performed for high, mean, median, and low flow conditions for each of the 7 embayments that comprise the MVCBs, as well as for the entire MVCBs, as shown in Table 3-1. The results show two expected trends: 1) decreasing flushing time with increasing flow and 2) decreasing flushing time with proximity to the tidal inlets. The longest flushing times in the entire MVCBs system (i.e., 92 – 96 days for low flow conditions) exist in portions of Chincoteague Bay and Newport Bay, both of which are quite distant from either tidal inlet. The shortest flushing times in the system (i.e., 6 - 10 days for low flow conditions) are in Isle of Wight Bay (immediately north of the Ocean City Inlet) and Sinepuxent Bay (immediately south of...
Intermediate values of flushing times (i.e., 26 – 61 days for low flow conditions) are found in Turville Creek, Assawoman Bay, and Saint Martin River, which are 3 small embayments located in the northern portion of the MVCBs and are separated from the Ocean City Inlet by Isle of Wight Bay.

As mentioned earlier, freshwater inflow is an important factor affecting the flushing capability of a water body. Higher freshwater flow increases gravitational circulation and results in a shorter flushing time (e.g., Choi and Lee, 2004; Shen and Haas, 2004; Huang, 2007; Shen and Wang, 2007). As can be seen in Fig. 3-3, a strong correlation was found between flushing time and freshwater discharge rate. If the linear regression equation is extrapolated to near zero freshwater flow, it ends up with a flushing time of about 96 days, which is similar to the flushing time calculated directly under a low flow condition. The implication is that the flushing time contributed by tides is about 96 days for the entire MVCBs. However, this value is significantly higher than that estimated by the classical tidal prism method. The mean water depth for the MVCBs is assumed to be less than 2 meters and the tidal range varies from as little as 0.1 m to as large as 2 m. The most conservative flushing time calculated from the classical tidal prism method (2 m mean water depth vs. 0.1 m tidal range) will be on the order of 10 – 20 days, which is much shorter than that estimated using the hydrodynamic model. It suggests that, in most situations, the traditional tidal prism method is not appropriate for flushing time estimations (Wang et al., 2004; Fugate et al., 2006) because unsteady flow allows the water to flow back. A modified tidal prism method, which accounts for the return ratio (i.e., the portion of water that re-enters the domain of interest after it was
flushed out during the previous ebb tide), is preferred and capable of generating more reasonable results.

III-3-2 Residence time

Two fundamentally different numerical approaches exist for calculating residence time: the Lagrangian particle tracking approach (Bilgili et al., 2005; Orfila et al., 2005; Smith et al., 2005) and the Eulerian passive tracer approach (Gillibrand, 2001; Shen and Haas, 2004; Wang et al., 2004).

Lagrangian particle tracking approach

The Lagrangian particle tracking method estimates residence time based on the Lagrangian trajectory of individual particles calculated from the velocity field. Numerically, a fourth-order Runge-Kutta integration scheme is employed to obtain the particle position based on the calculated advection from the computation grid of the hydrodynamic model (e.g., Dias et al., 2001). A visual example is shown in Fig. 3-4 to demonstrate the Lagrangian tracking method. Two particles were initially released from Isle of Wight Bay and Newport Bay, respectively. It can be easily seen that the particle initially released in Isle of Wight Bay was flushed out of the system after a few tidal cycles. In comparison, the Newport Bay particle was moved back and forth by tidal currents surrounding its original location. This demonstrates the spatial variability of residence time in the MVCBs using the Lagrangian tracking approach. However, in most situations, the substances of interest, e.g., nutrients and other dissolved materials, are not particles; they experience diffusion while they are advected by currents. To account for
diffusion, the random walk component of motion needs to be added. There are other
difficulties associated with the particle tracking method in that it requires a rather
complicated 2-D or 3-D interpolation and integration over a computational grid and needs
special treatment for both closed and open boundary conditions. Therefore, this method
was not selected as the major approach in this study.

Eulerian passive tracer approach

Takeoka (1984) proposed a remnant function that can be used to calculate
residence time based on the Eulerian passive tracer approach. Assuming the initial
amount of material in a water body at $t = 0$ is $R_0$, and the amount of the material that still
remains in the system at time $t$ is $R(t)$, $R(t)$ denotes the amount of the material whose
residence time is larger than $t$. The residence time distribution function can be defined as:

$$\phi = -\frac{1}{R_0} \frac{dR(t)}{dt} \quad (3-3)$$

It can be further assumed that all the material will be eventually flushed out of the
system such that:

$$\lim_{t \to \infty} R(t) = 0 \quad (3-4)$$

The averaged residence time $RT$ of the material is defined as:

$$RT = \int_0^\infty t \phi(t) dt \quad (3-5)$$

Integrating the above equation by parts gives:

$$RT = \int_0^\infty \frac{R(t)}{R_0} dt = \int_0^\infty r(t) dt \quad (3-6)$$
where \( r(t) = \frac{R(t)}{R_0} \) is called the remnant function (Takeoka, 1984). It can be easily solved with a hydrodynamic model and the result of RT gives the average residence time for a water body.

In this chapter, the remnant function was solved with the calibrated hydrodynamic model to obtain local residence time (LRT) distributions in the MVCBs. Because wind is a highly variable factor and the major focus of this study is to obtain the base residence time distribution as affected by freshwater and tides, the wind was not included in the calculations. The calibrated hydrodynamic model was first set to run continuously for three years to reach a dynamic equilibrium under each freshwater inflow condition. Then a conservative tracer with neutral buoyancy was released at each grid cell throughout the entire MVCBs except the ocean domain at a time of mean tidal level (slack before ebb). Meanwhile, a slightly modified form of the remnant equation (in Eq. 3-6, tracer mass was replaced with cell-averaged tracer concentration) was solved for RT continuously with time. Once the daily incremental rate of RT for all the cells fell below the criterion of 1% (i.e., RT increases 1 day during the 100-day integration), the model was stopped and the results were output for further analysis.

The map of spatial distribution of local residence time in the MVCBs under different flow conditions was thus generated, as shown in Fig. 3-5. This map shows that the residence time can range from a few days to more than 200 days, depending on the flow conditions and the location. During the high flow condition, the maximum local residence time is about 160 days; it increases to 180 days for the mean flow condition and
to 200 days in the low flow condition. Spatially, the northern Chincoteague Bay has consistently the highest local residence time regardless of the flow conditions, whereas Sinepuxent Bay and Isle of Wight Bay near the Ocean City Inlet and southern Chincoteague Bay inlet near Chincoteague Bay all have the shortest local residence times (i.e., less than 10 days). For other embayments located between the two inlets, such as Little Assawoman Bay, Assawoman Bay, Saint Martin River, and Turville Creek, the local resident time values lie between the two extremes and exhibit a spatial gradient. The spatial gradient occupies a vast area shown as yellow and green colors in Figure 3-5. In a general sense, spatial patterns of residence time are similar to those of flushing time because tides and freshwater are the two major driving forces responsible for flushing the conservative tracer out of the system. Thus, we can see that the shortest residence times mostly occur in regions that are either near the two inlets or located at the heads of bays receiving direct freshwater input (Figs. 3-5 and 3-6). However, there are fundamental differences between flushing time and residence time. Unlike flushing time as a bulk integral time scale, local residence time considers the transport time scales consisting of many different individual time scales as a continuous distribution function in space. Thus, it provides a much more detailed spatial distribution map for transport time over the entire MVCBs. This will be useful for making comparison with spatially inhomogeneous and sometime patchy biogeochemical features.

III-3-3 Biogeochemical feature and residence time in MVCBs

Transport time scales have been widely used to correlate with biological and chemical processes in aquatic ecosystems (e.g., Nixon, 1996; Boynton et al., 1996; Wang
et al., 2004). Typical biogeochemical processes, such as phytoplankton growth and nutrient uptake, require hours to a few days. Under normal flow conditions, the flushing time in the MVCBs is on the order of 2 – 3 months, which is much longer than those time scales for biogeochemical process. Thus, it is reasonable to conclude that most nutrients and organic matters (allochthonous origins) associated with freshwater input have been transformed into other forms through a series of biogeochemical processes inside the system. In addition, we may expect that any pollutants discharged into the bay can potentially exert their impact on the system before they are flushed out.

One of the most striking features that can be seen in the MVBCs is the brown tide, a type of harmful algal bloom caused by *Aureococcus anophagefferens*, which occurs most severely near Newport Bay and the Public Landing area (Fig. 3-7, Wazniak et al., 2004b). A multi-year survey revealed that the brown tide is most likely to occur in Northern Chincoteague Bay, which is the area with the longest local residence time. This clearly indicates that the Northern Chincoteague Bay has the strongest potential to accumulate pollutants due to low physical transport. The long residence time not only favors the growth of phytoplankton populations, but also promotes the accumulation and regeneration of dissolved organic nitrogen (DON) species (e.g., Gobler et al., 2005), which may support growth of harmful algal blooms. This is consistent with studies indicating that *Aureococcus anophagefferens* has a strong preference for regenerated DON forms including urea (Glibert et al., 2001, 2005, and 2007). The comparison between biogeochemical features and transport time scales has also been made using a water quality index and local residence time in the MVCBs, as shown in Fig. 3-8. The
water quality index consists of 5 ratings: excellent, good, fair, poor, and very poor. As one can readily recognize, the “very poor” ratings are located primarily in the mid- and northern Chincoteague Bay. This is the area corresponding to high local residence time. In contrast, areas having “excellent” ratings are located in Sinepuxent Bay, Isle of Wight Bay near Ocean City Inlet, and southern Chincoteague near Chincoteague Inlet. The “fair” water quality rating areas are in regions having spatial gradient values of local residence time.

**III-4 Discussion and conclusions**

Regarding flushing time, if the model is executed long enough to reach dynamic equilibrium, both methods (Eq. 3-1 and Eq. 3-2) should give the same result theoretically. As expected, the flushing time results calculated separately from Eqs. 3-1 and 3-2 matched extremely well. The averaged flushing times are provided in Table 3-1. Our results are also consistent with previous studies by Pritchard (1960) and Lung (1994) for the MVCBs, and are also within reasonable agreement with that of the Indian River-Rehoboth Bay, DE (another Delmarva Coastal Bay). The latter has a mean flushing time of approximately 90 days (Cerco and Seitzinger, 1997; Nixon et al., 2001). When compared with the shallow coastal ecosystems world-wide, the MVCBs have a longer flushing time compared to most others reported and reviewed by Nixon et al. (2001). A long flushing time suggests that the MVCBs could be more susceptible to pollutant input.

As for the local residence times, they vary substantially under different flow conditions. A high flow normally corresponds to a short residence time for all the bays.
In terms of spatial variability, the bays closer to the two inlets (i.e., Isle of Wight Bay and Sinepuxent Bay) tend to have a shorter flushing time, which is mainly controlled by bay-ocean exchange through tidal flushing. Consequently, these individual bays are not as sensitive to freshwater input as those in the upstream segments (e.g., Saint Martin River and Newport Bay), which are much more sensitive to freshwater inflow and also have a longer residence time.

It is noteworthy that, although all the hydrodynamic simulations were conducted in a 3-D mode, the final results have been vertically averaged before they were presented in this chapter. In addition, to simplify the problem, the wind forcing was neglected and a constant freshwater discharge rate was used for each flow condition. However, in reality, wind and freshwater discharge are both highly variable and play an important role in affecting circulation and mixing patterns (e.g., Shen and Wang, 2007). For example, the wind can increase the mixing and thus improves the flushing condition in general. In addition, wind can substantially change water circulation patterns in the MVCBs, depends on wind speed, direction, and duration. Hence, the real transport time scales can vary substantially from their ideal values as estimated in this study. The wind effect will be included into the future work.

In conclusion, a calibrated 3-D hydrodynamic model has been applied for estimating two typical transport time scales, flushing time and residence time, in the MVCBs. The results suggest that the system is characterized by a poor flushing capability despite its shallowness. The correspondence between residence time and the water quality
index indicates that physical forcing does play a crucial role in regulating biogeochemical processes in the system. For instance, the flushing capability of a system can directly affect the competition between different primary producers such as phytoplankton and macroalgae. The importance of transport time scales will be further addressed in later chapters.
Table 3-1. Flushing times for the MVCBs.

<table>
<thead>
<tr>
<th>Bay</th>
<th>Flushing Time (days)</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>High flow</td>
<td>Mean flow</td>
<td>Median flow</td>
<td>Low flow</td>
</tr>
<tr>
<td>Little Assawoman Bay</td>
<td>24.0</td>
<td>32.4</td>
<td>40.2</td>
<td>50.8</td>
</tr>
<tr>
<td>Assawoman Bay</td>
<td>37.4</td>
<td>43.4</td>
<td>47.7</td>
<td>52.4</td>
</tr>
<tr>
<td>Saint Martin River</td>
<td>19.6</td>
<td>28.3</td>
<td>38.7</td>
<td>61.0</td>
</tr>
<tr>
<td>Turville Creek</td>
<td>13.5</td>
<td>17.5</td>
<td>21.1</td>
<td>25.8</td>
</tr>
<tr>
<td>Isle of Wight Bay</td>
<td>5.1</td>
<td>5.4</td>
<td>5.6</td>
<td>5.9</td>
</tr>
<tr>
<td>Sinepuxent Bay</td>
<td>9.2</td>
<td>9.6</td>
<td>9.9</td>
<td>10.4</td>
</tr>
<tr>
<td>Newport Bay</td>
<td>47.2</td>
<td>60.0</td>
<td>71.8</td>
<td>92.1</td>
</tr>
<tr>
<td>Chincoteague Bay</td>
<td>83.0</td>
<td>89.7</td>
<td>93.7</td>
<td>96.6</td>
</tr>
<tr>
<td><strong>The entire MVCBs</strong></td>
<td><strong>71.7</strong></td>
<td><strong>80.4</strong></td>
<td><strong>87.0</strong></td>
<td><strong>96.2</strong></td>
</tr>
</tbody>
</table>
Fig. 3-1. A diagram explaining the definitions of age and residence time.
Fig. 3-2. Coastal Bays segmentation for flushing time calculation.
Fig. 3-3. The relationship between flushing time for the entire MVCBs and freshwater discharge rate. Black solid line denotes linear regression fit.

$y = -790.41x + 95.547$

$R^2 = 0.9611$, $P = 0.02$
Fig. 3-4. An example plot showing the track of two particles released in Isle of Wight Bay (top) and Newport Bay (bottom). Green dots denote particle initial release locations. The whole simulation lasts about 10 days.
Fig. 3-5. Local residence time distributions in the MVCBs under four different flow conditions (unit for the color map is day).
Fig. 3-6. An example plot of the along-bay local residence time (LRT) profile under the mean flow condition.
Brown Tide Distribution in the Coastal Bays

Average Peak Concentrations
(1999-2001)

- > 250 cells/ml.
- 25-250 cells/ml.
- 10-25 cells/ml.
- < 10 cells/ml.

Fig. 3-7. Average peak concentration of brown tide at each Coastal Bays sample station between 1999 and 2001. The figure taken from Wazniak et al. (2004b).
Fig. 3-8. Water Quality Index for the MVCBs (Jones et al., 2004).
CHAPTER IV ANALYSIS OF WATER QUALITY MONITORING DATA IN THE MVCBS

IV-1 Introduction

In the 1970s and early 1990s, the University of Maryland (UMD) (Boynton, 1973; Boynton et al., 1993) and Virginia Institute of Marine Science (VIMS) (Fang et al., 1977a, b; Cerco et al., 1978) conducted a series of field surveys in the MVCBs. These surveys included studies of physical, chemical, and biological properties in MVCBs waters as well as the compilation of information on land, including land use and nutrient loadings to the Bays (Boynton et al., 1996). The data have been synthesized by Boynton et al. (1996) to produce the first thorough assessment of eutrophication patterns in the MVCBs. Since the late 1990s, more intensive and systematic monitoring activities have been undertaken by state governments. For example, the Maryland Department of Natural Resources (MDNR) has been routinely monitoring water quality year-round in the MVCBs since 1999 (www.eyesonthebay.net). The water quality data are collected monthly from more than 40 monitoring stations spanning regions from non-tidal tributaries to open bays. The sampled parameters cover major water quality indicators, such as nutrients, chlorophyll, DO, and water clarity. These data have been analyzed and incorporated into a series of publications (e.g., MDNR, 2004; Wazniak et al., 2004b and 2007).

In addition to the aforementioned monthly monitoring program, MDNR also has maintained in recent years a real-time, fixed station, high-frequency shallow water
monitoring program (http://mddnr.chesapeakebay.net/newmontech/contmon/index.cfm) in order to monitor shallow water habitat for seagrass and nursery areas for juvenile fishes. The automatic data loggers of Yellow Springs Instrument Company (YSI™) were deployed at each shallow monitoring site, similar to those used by the National Estuarine Research Reserve's (NERR) System-wide Monitoring Program (SWMP) (Wenner and Geist, 2001; Kennish, 2004). Basic water quality parameters including temperature, salinity, DO, pH, turbidity, and chlorophyll a fluorescence were simultaneously measured at 15-minute intervals year-round. This high-frequency monitoring provides an unparalleled temporal coverage for tracking high frequency variability in the shallow water ecosystem at several representative sites in the MVCBs. For instance, by using NERR’s high-frequency monitoring data, Caffrey (2003 and 2004) was able to calculate net ecosystem metabolism (NEM) rates and concluded that most sites were net heterotrophic with respiration exceeding gross primary production on an annual basis.

In this chapter, a field data analysis was conducted based on the water quality monitoring data collected by MDNR. The analysis results not only described the general water quality pattern in the system, but also provided important guidance for subsequent eutrophication modeling studies.

IV-2 Field data collection

Two types of water quality data were used: (1) the traditional, monthly monitoring survey data and (2) high-frequency, fixed station in situ measurements. The monthly monitoring survey data, collected from 2000 – 2005, which have undergone extensive
QA/QC, were provided by MDNR (courtesy of Ms. Cathy Wazniak). Dissolved oxygen (DO) and salinity measurements were made at multiple depths; however, nutrients and chlorophyll a were sampled only in the surface layer (0.3 m below surface). The high-frequency monitoring data were directly downloaded from MDNR website (http://mddnr.chesapeakebay.net/newmontech/contmon/index.cfm). A detailed description of data collection methods and QA/QC procedures can be obtained from MDNR website and related publications (e.g., MDNR, 2004). The map of the monthly monitoring stations used for data analysis is shown in Figure 4-1. Most of the stations are located in the tidal portions of the MVCBs except for Station 16 (see Figure 4-2), which is located in the headwaters of Turville Creek separated from tidal portions of Turville Creek by a dam-like structure. Because of its special location, this station serves as a reference site for the remaining stations located in the tidal MVCBs. A high-frequency monitoring station recording water quality parameters continuously at a shallow site at a mean depth of 0.8 m (MLW) was also maintained in the upstream portion of Turville Creek. In conjunction with VIMS' benthic macroalgae survey (Hardison, 2009) in 2006 (Fig. 4-2), special attention was paid to the relationship between water quality and macroalgae along the Turville Creek - Isle of Wight Bay transect. Turville Creek and Isle of Wight Bay were reported to be hot spots for benthic macroalgae (McGinty et al., 2004), one of the main themes of this dissertation.
IV-3 Results and discussion

IV-3-1 Spatial water quality gradient in the MVCBs

The averaged water quality parameter values over the 6-year period from 2000 to 2006 are plotted in Figs. 4-3 (a-d). As can be easily seen, water quality parameters are highly variable over spatial scales. Judging from the mean values of nutrients, chlorophyll $a$, and Secchi depth, water quality generally improves towards the Ocean. For instance, in Fig. 4-3(a), water clarity increased towards the Inlets, as revealed by Secchi depth profiles in both the St. Martin River and Turville Creek. In Fig. 4-3(b), chlorophyll $a$ exhibits a strong longitudinal gradient especially in tributaries receiving high nutrient inputs. For example, the mean chlorophyll $a$ concentrations in the St. Martin River decreased from as high of 60 $\mu$g L$^{-1}$ in the upstream to less than 20 $\mu$g L$^{-1}$ at the river mouth. The same pattern is also found in Turville Creek, except the magnitude of chlorophyll $a$ is smaller than that in the St. Martin River. This difference is possibly caused by different nutrient loading rates for the two systems, as the St. Martin River receives a higher areal rate than does Turville Creek (Boynton et al., 1996). In addition, the abundant benthic macroalgal biomass in Turville Creek can potentially further reduce phytoplankton levels.

Like most temperate marine ecosystems, primary production in the MVCBs is generally limited by nitrogen instead of phosphorus (Boynton et al., 1996). Apparently, nitrogen concentrations are especially variable throughout the Bays (Fig. 4-3(c)). For example, despite its abundance in headwaters (e.g., Stations 6 and 16), NO$_x^-$ is quickly consumed or diluted downstream. In the southern bays (Stations 22 – 28), NO$_x^-$ is almost
absent from the water column. In contrast, NH$_4^+$ and DON concentrations are comparable for most stations (Figs. 4-3 (c-d)). This suggests that NO$_x^-$ serves as an important nitrogen source only in the areas receiving direct watershed inputs such as the upstream portion of the St. Martin River. As reviewed by Glibert et al. (2007), primary production in the MVCBs is mainly fueled by regenerated nitrogen species instead of NO$_x^-$. This conclusion is likely to be true for the southern bays.

In terms of DO, except for Station 14, which is located in the deep hole (water depth > 6 m) at Manklin Creek, there was not much difference among the remaining stations (Fig. 4-3 (b)). The averaged DO concentrations do not reveal any persistent low DO (or persistent hypoxia) problems in the system. However, because DO in eutrophic shallow waters can be heavily mediated by biological activities, these data may not reflect the true DO status in the system as they were normally collected during daytime (MDNR, 2004).

The spatial gradients of nutrients can be better elucidated using principal component analysis (PCA). A bi-plot of the two largest principal components (contribute to 65.5% and 26.5% of the sum of the total eigenvalues, respectively), which were calculated from the averaged 6-year MDNR monthly measurements of NH$_4^+$, NO$_x^-$, DON, PO$_4^{3-}$, DOP, and DOC, is given in Fig. 4-4(a). The corresponding loadings from the each water quality variable on the two principal components are given in Fig. 4-4(b). As can be seen, the 28 water quality stations are distributed reasonably corresponding to their relative locations in the MVCBs (Fig. 4-1). For instance, Station 16, located in the
nontidal headwaters of Turville Creek, has a distinct water quality profile from other stations in the MVCBs, and is visually isolated from all the other stations in Fig. 4-4(a). Similarly, Station 6 is separated from other stations because it is located in the upstream of St. Martin River and is characterized by high nutrient concentrations as well. In comparison, the remaining stations tend to accumulate into individual subgroups. For example, Stations 23 – 26 (Fig. 4-4(a)), which are all located in Northern Chincoteague Bay, exhibit very similar water quality patterns, as can be easily seen from Fig. 4-3. It is thus clear that spatial water quality gradients exist throughout the bays, and are potentially controlled by interactions between watershed loading rates and local physical characteristics. This justifies that a systematic numerical modeling approach is warranted to address the spatial variability of water quality within the same framework.

IV-3-2 Water quality profiles along Turville Creek – Isle of Wight Bay transect

Turville Creek is a small tributary of Isle of Wight Bay (Fig. 4-2). Both of these water bodies were reported to be hot spots for benthic macroalgae (McGinty et al., 2004). In this section, water quality monitoring data for stations along the transect of Turville Creek – Isle of Wight Bay (Fig. 4-2) were further analyzed for temporal and spatial characteristics. The results are presented in Figs. 4-5 and 4-6.

First of all, the results suggest that strong seasonality exists for all the stations. For Station 1 in Fig. 4-2, which corresponds to nontidal headwater Station 16 in Fig. 4-1, the chlorophyll \(a\) concentrations exhibit a bimodal distribution which peaks in spring and fall (Figs. 4-5(a) and 4-6(a)). However, the chlorophyll \(a\) levels at Station 1 are much
lower (less than 10 μg L⁻¹) compared with others, though this station shows the highest nutrient levels. In contrast, the two downstream Stations 2 and 3 show a very distinct pattern from Station 1, with chlorophyll a peaks in summer (July-August). Further downstream, summer chlorophyll a peaks still remain at Stations 4-6, but the magnitude decreases downstream. Meanwhile, the winter (January) peak of chlorophyll a becomes increasingly dominant. This may be directly affected by signals from the coastal ocean. Overall, the commonly observed spring and fall phytoplankton blooms in temperate, deep marine waters are not evident along the transect of Turville Creek – Isle of Wight Bay. This is also consistent with other studies by Boynton et al. (1996) in the MVCBs and Li (2006) in Lynnhaven Bay, VA, in large part due to the mediation effect of benthic communities.

For nutrients, the seasonality varies for individual parameters. For example, NH₄⁺ tends to reach its peak in the fall (October) at Stations 3-6, lagging behind the summer chlorophyll a peak by approximately two months (Fig. 4-6(a)). The same trend is also found for PO₄³⁻ (Fig. 4-6(b)). The fall peaks of NH₄⁺ and PO₄³⁻ suggest that sediment could be the major source of NH₄⁺ and PO₄³⁻ for these downstream stations. Phytoplankton and benthic macroalgae tend to bloom in the early summer and die off from mid-summer to early fall (Tyler, 2002). Therefore, the mismatch between primary producers and benthic nutrient flux resulting from summer deposition subsequently leads to the fall peaks of NH₄⁺ and PO₄³⁻ in the water column. As for NO₃⁻, which is mainly regulated by watershed input and algal uptake, a more complex pattern is shown. NO₃⁻ normally remains low in summer and reaches a maximum in winter for Stations 2-5.
However, this general pattern is often interrupted by watershed inputs and thereby does not show the same consistency as NH$_4^+$ and PO$_4^{3-}$. In addition, the winter peak of NO$_3^-$ normally lags 1-2 months behind that of NH$_4^+$ and PO$_4^{3-}$. As expected, among all the parameters, DO concentrations exhibit the strongest seasonality for all 6 stations (Fig. 4-5(b)), as they are largely controlled by seasonal temperature variations and dominant primary producers. Low DO concentrations (< 5 mg L$^{-1}$) during the summer can be frequently found, especially for stations located in the upstream (e.g., Stations 1-3).

Second, in terms of the spatial variability, as can be seen from Figs. 4-5(a) and 4-6(a), chlorophyll $a$ concentrations exhibit a strong longitudinal gradient along the Turville Creek – Isle of Wight Bay transect. Station 1, which is located in the nontidal, freshwater headwater of Turville Creek, reflects the changes of water quality in the freshwater stream as directly affected by watershed nutrient inputs. Despite having the highest nutrient concentrations among all the stations, the chlorophyll $a$ levels at Station 1 were much lower than at other stations. The low chlorophyll $a$ concentrations could be caused by high turbidity and short residence time. Chlorophyll $a$ concentrations were highest at Station 2, and gradually decreased downstream. The longitudinal chlorophyll $a$ gradient was mainly controlled by the combination of nutrient loading and tidal flushing. Correspondingly, NO$_x^-$ decreased sharply moving downstream as it was quickly used up within the system, as shown in Fig. 4-6(b). In contrast, the same pattern was not found for NH$_4^+$ and PO$_4^{3-}$ (Fig. 4-6(a-b)). This disparity suggests that additional sources of NH$_4^+$ and PO$_4^{3-}$, such as benthic flux and water column regeneration, play a substantial role in the system.
IV-3-3 High frequency continuous measurements in Turville Creek

The monthly DO records indicate that low DO (<5 mg L\(^{-1}\)) events occurred in summer months, as shown in Fig. 4-5(b). However, the sparse, daytime measurements are not sufficient to fully characterize DO variability in eutrophic shallow water. Specifically, DO in the shallow water can exhibit strong diel fluctuations due to its response to photosynthesis and respiration. In this vein, the high-frequency measurements collected at the continuous monitoring station in Fig. 4-2 can provide a much more detailed temporal coverage for the high frequency variation of DO. For example, Fig. 4-7 shows 1-year records (March 2004 to December 2004) of continuous measurements for temperature, salinity, turbidity, pH, DO, DO saturation, and chlorophyll \(a\). The data clearly indicate that DO frequently dropped below 5 mg L\(^{-1}\) from late spring to early fall. The high-frequency chlorophyll \(a\) measurements also confirm previous findings that phytoplankton tend to reach their seasonal abundance in summer instead of spring and fall. Occasionally, phytoplankton blooms could raise chlorophyll \(a\) over 100 \(\mu g\) L\(^{-1}\), which is rarely observed in the monthly monitoring survey data.

To analyze the temporal characteristics imbedded in the high-frequency measurements, a spectral analysis method was used to reveal dominant periodicities. Fig. 4-8 shows the 1-month summer period water quality measurements and the corresponding spectral analysis results. As one can see, the diurnal constituent (period \(\approx 24\) hours) is strongest for all the water quality parameters except salinity, which is dominated by the semi-diurnal (period \(\approx 12\) hours) constituent. The short-term (hours)
fluctuation of temperature in shallow waters is more affected by daily light cycle than tidal pumping, which has a dominant frequency $\approx 12$ hours. For salinity, as expected, its short-term fluctuations are almost completely controlled by tides, which mainly consist of both semi-diurnal (major) and diurnal (minor) constituents. However, the rest of the water quality parameters are more affected by biological activities than by physical processes. For example, during daytime, algae increase $\text{DO}$ and $\text{pH}$ through photosynthesis. At night, $\text{DO}$ is consumed and DIC (dissolve inorganic carbon) is increased through respiration. Consequently, $\text{pH}$ decreases. In addition, the daily variations in turbidity could attribute to the diel cycle of phytoplankton, as reflected by chlorophyll $a$ concentrations shown in Fig. 4-8. In summary, these data clearly suggest that during the highest biological activities in summertime of the year, water quality in shallow waters is more controlled by biological activities rather than physical processes.

Based on high-frequency $\text{DO}$ records, net ecosystem metabolism (NEM) can be calculated using simple mass-balance equations (e.g., Chapra, 1997; Caffrey, 2003 and 2004). The typical mass-balance equation for $\text{DO}$ can be written as follows when physical transport is neglected:

$$\frac{dC}{dt} = P - R + k_a (C_s - C)$$

(4 -1)

where:

$C =$ $\text{DO}$ concentration in the water column, mg L$^{-1}$

$P =$ Gross primary production rate, g O$_2$ m$^{-3}$ d$^{-1}$

$R =$ Gross/community respiration rate, g O$_2$ m$^{-3}$ d$^{-1}$

$k_a =$ surface reaeration rate coefficient, d$^{-1}$

83
Cs = DO saturation concentration, mg L\(^{-1}\)

As net ecosystem metabolism (g O\(_2\) m\(^{-3}\) d\(^{-1}\)) equals the sum of gross primary production and community respiration, i.e. NEM = P - R, Eq. 4-1 can be written as:

\[
NEM = \frac{dC}{dt} - k_a(Cs - C)
\]  \(4-2\)

which can be written as the following finite difference form:

\[
NEM_{t+1} = \frac{C_{t+1} - C_t}{\Delta t} - k_a\left(\frac{(Cs_{t+1} - C_{t+1}) + (Cs_t - C_t)}{2}\right)
\]  \(4-3\)

where:

\(NEM_{t+1}\) = net ecosystem metabolism rate calculated at time step \(t+1\), g O\(_2\) m\(^{-3}\) d\(^{-1}\)

\(\Delta t\) = time step, 15 minutes, or 0.0104 d

\(C_{t+1}\) = observed DO concentration at time step \(t+1\), mg L\(^{-1}\)

\(C_t\) = observed DO concentration at time step \(t\), mg L\(^{-1}\)

\(Cs_{t+1}\) = observed DO saturation concentration at time step \(t+1\), mg L\(^{-1}\)

\(Cs_t\) = observed DO saturation concentration at time step \(t\), mg L\(^{-1}\)

The surface reaeration rate \(k_a\) is a function of wind speed, current velocity, water depth, and temperature (Chapra, 1997), and varies in both time and space. For narrow and shallow estuaries (e.g., Turville Creek) with limited tidal effects, \(k_a\) is very small in general compared with open bays (e.g., Chapra, 1997; Caffrey, 2004). In this study, constant typical \(k_a\) values were used to obtain a first-order estimation of the daily NEM based on the 15-min continuous DO records in Fig. 4-8. The estimated daily NEM rates calculated using four constant \(k_a\) rates are presented in Fig. 4-9. Apparently, daily NEM...
rates varied from day to day. During the 1-month period, the NEM rates were usually negative. This suggests that the continuous monitoring site was mostly heterotrophic with community respiration exceeding gross primary production during the 1-month monitoring period. This is also consistent with previous findings for U.S. shallow estuaries based on NERR’s high-frequency data (Caffrey, 2003 and 2004). The results also demonstrate that $k_a$ is a crucial parameter for NEM estimation. In Eq. 4-2, as both $C_s$ and $C$ are directly measured by instruments, the value of $k_a$ determines the magnitude of surface reaeration term, $k_a(C_s - C)$. In Fig. 4-10, the estimated monthly averaged NEM rates are strongly affected by $k_a$ ($R^2 = 1$). Obviously, one needs to be especially careful in choosing proper $k_a$ values for the NEM calculation. High uncertainty is often associated with NEM results calculated from in situ continuous DO records.

**IV-4 Summary**

This chapter summarizes the general water quality characteristics in the MVCBs with special emphasis on its spatial water quality gradient from the watershed toward inlets. The field monitoring data demonstrate that water quality varies both temporally and spatially corresponding to both physical and biological forcings such as temperature, physical transport, nutrient loadings, and phytoplankton dynamics. Such complex interactions justify the need for an integrated numerical modeling approach; specifically, a modeling system that has enough resolution in both temporal and spatial scales to address the variability associated with the eutrophication of the biochemical system.
Fig. 4-1. A map showing MDNR monthly water quality monitoring stations in the MVCBs.
Fig. 4-2. A map showing field monitoring stations along Turville Creek – Isle of Wight Bay – Ocean City Inlet transect.
Fig. 4-3 (a). Average monthly monitoring water quality parameter values in the MVCBs (top panel – salinity; bottom panel – Secchi depth). Error bars represent one standard deviation. Raw data were collected by MDNR.
Fig. 4-3 (b). Average monthly monitoring water quality parameter values in the MVCBs (top panel – DO; bottom panel – chlorophyll a). Error bars represent one standard deviation. Raw data were collected by MDNR.
Fig. 4-3 (c). Average monthly monitoring water quality data in the MVCBs (top panel – NH$_4^+$-N; center panel - NO$_x^-$-N; bottom panel – PO$_4^{3-}$-P). Error bars represent one standard deviation. Raw data were collected by MDNR.
Fig. 4-3 (d). Average monthly monitoring water quality data in the MVCBs (top panel – DOC; middle panel – DON; bottom panel – DOP). Error bars represent one standard deviation. Raw data were collected by MDNR.
Fig. 4-4 (a). A bi-plot of the principal component analysis (PCA) result (x-axis – PC1 (65.5%); y-axis – PC2 (26.5%)) in the MVCBs. Data labels denote water quality monitoring stations in Fig. 4-1. Raw data were collected by MDNR.
Fig. 4-4 (b). Loadings of the 6 water quality variables on PC1 and PC2.
Fig. 4-5 (a). Time series plot of 6-year (2000-2005) monthly chlorophyll a concentrations along the transect of Turville Creek – Isle of Wight Bay (from top to bottom are monthly monitoring Stations 1 – 6 in Fig. 4-2). Raw data were collected by MDNR.
Fig. 4-5 (b). Time series plot of 6-year (2000-2005) monthly DO concentrations along the transect of Turville Creek – Isle of Wight Bay (from top to bottom are monthly monitoring Stations 1 – 6 in Fig. 4-2). Raw data were collected by MDNR.
Fig. 4-6 (a). Monthly averaged chlorophyll a and NH₄⁺ profiles along the transect of Turville Creek – Isle of Wight Bay (error bars represent one standard deviation). From top to bottom are Stations 1-6 in Fig. 4-2. Raw data were collected by MDNR.
Fig. 4-6 (b). Monthly averaged NO$_x$ and PO$_4^{3-}$ profiles along the transect of Turville Creek – Isle of Wight Bay (error bars represent one standard deviation). From top to bottom are Stations 1-6 in Fig. 4-2. Raw data were collected by MDNR.
Fig. 4-7 (a). Time series plot of high-frequency water quality data in the upstream of Turville Creek. Raw data were collected by MDNR.
Fig. 4-7 (b). Time series plot of high-frequency water quality data in the upstream of Turville Creek. Raw data were collected by MDNR.
Fig. 4-8. Time series plot of summer high-frequency water quality data (left panel) and corresponding periodicity profiles (right panel) in the upstream of Turville Creek.
Fig. 4-9. Calculated daily net ecosystem metabolism (NEM) rates with four constant surface reaeration rates. Legend denotes the surface reaeration rate $k_a$. 
Fig. 4-10. Calculated monthly mean net ecosystem metabolism rates vs. surface reaeration rates. The squares are monthly mean net ecosystem metabolism rate calculated under four constant $k_a$ (error bars represent ± one standard deviation), and the straight line denotes the best-fit linear regression line.

$NEM = -0.9739 \times K_r - 0.0773$

$R^2 = 1$
CHAPTER V DEVELOPMENT OF A BENTHIC MACROALGAL MODULE WITHIN THE CE-QUAL-ICM WATER QUALITY MODEL FRAMEWORK

V-1 Introduction

The occurrence of macroalgae in shallow coastal waters has been of interest and increasing concern worldwide (Valiela et al., 1997; Curiel et al., 2004; Brush, 2002). The proliferation of macroalgae in coastal waters is commonly regarded as an indicator of coastal eutrophication (Josefson and Rasmussen, 2000; Sundbäck et al., 2003; Schaffelke et al., 2006). In Waquoit Bay, MA, for example, benthic macroalgae have been increasingly dominant and have progressively replaced the historically abundant eelgrass since the 1950s as a result of increasing nitrogen loading from septic systems (Valiela et al., 1992; Hauxwell et al., 2001). In the Lagoon of Venice, macroalgae have been replacing seagrass beds in the 1970s (Runca et al., 1996). Macroalgae were also reported to be especially abundant throughout the MVCBs, with a maximum biomass of 444 g L⁻¹ (Goshorn et al., 2001).

Macroalgae are important benthic primary producers in shallow coastal ecosystems. According to Valiela et al. (1997), the ecological significance of macroalgae in a typical shallow estuary can be described by a conceptual model as shown in Fig. 5-1. With increased nitrogen loading, slow-growing seagrass is replaced by fast-growing macroalgae and phytoplankton. Macroalgae can co-exist with seagrass and phytoplankton, and at the same time compete for light and nutrients. Apparently, macroalgae can play a dominant role in shallow ecosystems characterized by high nutrient loading and short
residence time. A similar conceptual model was also proposed by Dahlgren and Kautsky (2004) to explain the relationship between different vegetative states and external nutrient loads in shallow coastal bays of the Baltic Sea.

The proliferation of macroalgae in shallow ecosystems has many ecosystem-level implications. For instance, macroalgae can play a key role in regulating carbon and nitrogen cycling (Valiela et al., 1997; McGlathery et al., 2001; Tyler et al., 2001). Macroalgae, often characterized with “luxury uptake” capability and high biomass, can uptake and store a significant portion of nutrients from the system. In Waquoit Bay, the stored N by macroalgae was approximately of the same magnitude as the annual N loading from the watershed (Valiela et al., 1997). In a study conducted by Sfriso et al. (1989) in the central part of the Venice Lagoon, it was estimated that in spring-summer, macroalgae recycled 78–104% and 38–51% of the total annual nitrogen and phosphorus that entered the central lagoon, while the phytoplankton standing crop appeared negligible in most of the studied area with macroalgae present. Thus, it is not uncommon that eutrophic shallow ecosystems can support large macroalgal populations with low water column nutrient concentrations and phytoplankton biomass during much of the growing season despite high nutrient loading rates (e.g., Sfriso et al., 1989 and 1992; Fong et al., 1993; Nixon et al., 2001; McGlathery et al., 2007).

In addition, benthic macroalgae are especially effective in disrupting benthic-pelagic coupling by intercepting nutrient flux from the sediment to the water column due to their unique position at the water-sediment interface (Valiela et al., 1997).
McGlathery et al. (1997) found that actively-growing macroalgal mats can efficiently sequester benthic nutrient (ammonium) inputs to the overlying water column and reduce nutrient availability to a level that may limit phytoplankton production. Tyler et al. (2001 and 2003) also reported that macroalgae were shown to play a key role in the uptake of dissolved inorganic nitrogen (DIN) from the water column and urea from the sediment, as well as other dissolved organic nitrogen (DON) compounds released to the water column during their active growth. The extremely dynamic DO fluctuations observed in shallow ecosystems may be related to the abundance of macroalgae. For example, D’Avanzo and Kremer (1994), Peckol and Rivers (1996), and Park et al. (2003) indicated that large diurnal variations of DO and transient hypoxia that normally lasted for a few hours before dawn are commonly observed in macroalgae-dominated coastal bays. Moreover, frequent episodes of prolonged DO depletion (hypoxia or anoxia occurring for several days) throughout the water body following the characteristic collapse of macroalgal blooms will inevitably have profound ecosystem-level effects (Valiela et al., 1997; Vahteri et al., 2000; McGlathery et al., 2001; Thomsen et al., 2006). Dalsgaard (2003) concluded that ephemeral macroalgal populations can significantly lower denitrification rates and thereby retain more N as macroalgal biomass in the system. On the other hand, ephemeral macroalgae are not long-lived, and thus can not serve as a permanent reservoir for C, N, and P. McGlathery et al. (2007) stated that, as eutrophication proceeds, biotic factors in shallow coastal bays (e.g., the dominance of macroalgae) will result in a positive feedback to eutrophication. In this context, it is of particular interest to investigate how macroalgae can affect the basic “filter” function in shallow coastal bays.
There is no doubt that benthic macroalgae play a unique role in regulating nutrient recycling and ecosystem metabolism and are indispensable for our understanding of the biogeochemical processes related to eutrophication in shallow coastal bays such as the MVCBs. The goal of this chapter is to report on the development of a benthic macroalgal module within a well-established water quality model framework (CE-QUAL-ICM). The macroalgae kinetics are built with proper formulations and the parameters drawn from both literature and recent laboratory studies. The macroalgal module was further examined with a simple box model containing one water column and two sediment layers before it was applied to the MVCBs. Section V-2 describes basic assumptions, the detailed macroalga formulation, and the parameters used. Section V-3 analyzes the simulation results of basic properties of macroalgae using a box model.

V-2 Model development

V-2-1 Description of the general water quality model framework

The 3-D, time-variable eutrophication model, CE-QUAL-ICM (ICM), originally developed for deep water ecosystems like Chesapeake Bay (Cerco and Cole, 1993), was selected to investigate the eutrophication dynamics of the MVCBs. As an advanced water quality modeling package, ICM includes both the water column process model (see Table 5-1 for model state variables) and a predictive sediment diagenesis model (DiToro and Fitzpatrick, 1993). Besides its extensive applications in deep marine ecosystems like Chesapeake Bay, ICM has also been applied to a number of shallow coastal ecosystems including Indian River-Rehoboth Bay, DE (Cerco and Seitzinger, 1997) and Lynnhaven Bay, VA (Li, 2006). The model has been under continuous expansion and improvement.
For instance, a benthic microalgae module was added to its sediment diagenesis model to account for the contribution by benthic microalgae in shallow waters (Cerco and Seitzinger, 1997; Li, 2006). To support SAV restoration in shallow regions of Chesapeake Bay, a predictive submerged aquatic vegetation (SAV) module was also incorporated into ICM (Cerco and Moore, 2001). In this study, a benthic macroalgal module was developed within the existing ICM framework to address the unique role played by benthic macroalgae in shallow coastal ecosystems.

Two macroalgae species, *Ulva lactuca* and *Gracilaria vermiculophylla*, which are the two most representative benthic macroalgae species in coastal bays on the Maryland and Virginia Peninsula (e.g., Goshorn et al., 2001; Thomsen et al., 2006), were included into the current benthic macroalgal module. These two species share the same formulations as presented above, except that they use different model parameters. In ICM, macroalgae are modeled at the bottom layer of the model grid. They, however, do not directly uptake nutrients from the sediment. Instead, macroalgae interact with the water column via processes of uptake and release of inorganic and organic matters. The two macroalgal species are assumed to coexist in the same grid cell, and compete against each other for nutrients and light etc. The interactions between macroalgae and the remaining water quality state variables are formulated in a similar way as phytoplankton and SAV in ICM. Hence, the mass conservation is strictly satisfied.

A detailed description of CE-QUAL-ICM and its modules for SAV and benthic microalgae can be found elsewhere (Cerco and Cole, 1993; Cerco and Seitzinger, 1997;
This chapter focuses on those processes related to the benthic macroalgal module.

V-2-2 Major assumptions for the benthic macroalgal module

The following assumptions were made for the benthic macroalgal module:

1) The modeled macroalgae are strictly bottom-attached species (benthic macroalgae) and thereby not subject to physical transport during their active growing stage. Macroalgae can grow in several ways: free-floating, bottom-attached, or both. In this study, only the bottom-attached species were addressed.

2) Macroalgae directly exchange nutrients and organic matter within the water column and are linked to the sediment diagenesis model via settling of detritus. Although benthic macroalgae stay on the sediment surface, they are commonly thought to only uptake nutrients from the water column (Lobban and Harrison, 1994). In this study, benthic macroalgae are configured to stay at the bottom of the water column layer and are linked to the sediment flux model. Consequently, they have the function of intercepting and mediating benthic nutrient flux as the result of the settling of detritus and sediment biogeochemical processes.

3) The detachment of benthic macroalgae from sediment surface and the breakage of macroalgae thallus by physical forces are not addressed. Strong currents and waves can erode benthic macroalgae away from the sediment surface and also cause direct physical damages (Thomsen, 2004). Thus, physical forces may directly limit macroalgal growth and re-distribute macroalgal biomass in a system through strong advection and settling (Biber, 2007; Flindt et al., 2007).
erosion/sloughing of benthic macroalgae from bottom attachment has been considered in a few benthic macroalgae models (Salomonsen et al., 1999; Trancoso et al., 2005) using the Partheniades’s approach for sediment erosion (Partheniades, 1965). In shallow ecosystems like the MVCBs, the areas affected by strong currents and waves are mostly around deep channels, where macroalgal growth is naturally restricted by nutrients and light. Therefore, in a certain sense, the erosion of benthic macroalgae directly by currents and waves can be considered secondary as far as the total macroalgal biomass is concerned.

V-2-3 Formulations of the benthic macroalgal module

The major kinetic processes of benthic macroalgae are shown in Fig. 5-2. The change of benthic macroalgal biomass with time is described by the following governing equation:

$$\frac{\partial B}{\partial t} = (P(1 - \beta) - R - M - Gr)B$$ (5-1)

Where:

- $B =$ benthic macroalgal biomass, g C m\(^{-2}\) (to be consistent with ICM, carbon unit is used here)
- $P =$ growth rate, day\(^{-1}\)
- $\beta =$ fraction of growth-related respiration
- $R =$ basal metabolic rate, day\(^{-1}\)
- $M =$ natural (nonpredatory) mortality, day\(^{-1}\)
- $Gr =$ grazing/predation by benthic grazers, day\(^{-1}\)
As portrayed in the governing equation, the change of benthic macroalgal biomass is determined by four major processes: growth, respiration, mortality, and grazing. The growth term is formulated as a first-order process limited by environmental factors including light, nutrients, and temperature. The respiration term combines both growth-related respiration (which is treated as a portion of growth) and the basal metabolism. Because benthic grazers were not explicitly modeled as a state variable in the model, the grazing term is treated in a simple way as a first- or second-order reaction process. Lastly, the mortality term accounts for the loss of macroalgal biomass intensified by unfavorable environmental conditions, including high temperature and low DO. Detailed formulations on individual processes are described below.

A. Growth Rate

The growth of benthic macroalgae depends on light intensity, nutrient availability, and temperature. The effects of these processes are considered to be multiplicative:

\[
P = P_m \cdot f(I) \cdot f(N) \cdot f(T)
\]

(5-2)

where:

\(P_m\) = maximum growth rate under optimum conditions (d\(^{-1}\))

\(f(I)\) = light limitation function, \((0 \leq f(I) \leq 1)\)

\(f(N)\) = nutrient limitation function, \((0 \leq f(N) \leq 1)\)

\(f(T)\) = temperature limitation function, \((0 \leq f(T) \leq 1)\)
Light limitation function formulation

In general, macroalgae increase their photosynthetic activity as light intensifies. Above a certain threshold, photoinhibition is expected to occur and photosynthetic activity is reduced. The relationship between photosynthetic rate and irradiance can be determined by the Steele photoinhibition law (Steele, 1962). However, in turbid, shallow coastal waters, irradiance seldom reaches a value high enough to incur inhibition (Solidoro et al., 1997b; Wong and Chang, 2000). In addition, based on our previous experience, Steele’s photoinhibition function could cause unrealistic behavior (i.e., produces double peaks of DO concentration during the daytime) when applied to shallow coastal waters. Therefore, photoinhibition is seldom considered in coastal eutrophication models (e.g., Brush, 2002). In the macroalgal module, the existing light limitation function used by ICM for phytoplankton was adopted (Jassby and Platt, 1976):

\[ P = P_m \frac{I}{\sqrt{I^2 + IK^2}} \]  \hfill (5-3)

where:

\( P \) = growth rate \( (d^{-1}) \)

\( I \) = irradiance \( (E \text{ m}^{-2} \text{ d}^{-1}) \)

The parameter \( IK \) is defined as the irradiance at which the initial slope of the production vs. irradiance relationship intersects the value of \( P_m \):

\[ IK = \frac{P_m}{\alpha} \]  \hfill (5-4)

where:

\( \alpha \) = initial slope of production vs. irradiance relationship \( ((E \text{ m}^{-2} \text{ d}^{-1})^{-1} \text{ d}^{-1}) \)
Light extinction formulation

The commonly adopted Lambert-Beer law for light extinction was used to define the extinction of light with depth:

$$I(z) = I_0 e^{-k_e z}$$  \hspace{1cm} (5-5)

where:

$I(z)$ = irradiance (E m$^{-2}$ d$^{-1}$) at a given depth $z$ (m)

$I_0$ = irradiance at the surface (E m$^{-2}$ d$^{-1}$)

$k_e$ = light extinction coefficient (m$^{-1}$), which is commonly formulated using a multiple linear regression formula

Above the benthic macroalgal canopy, the extinction of light in the water column can be affected by several water quality variables, including water itself, chlorophyll, organic matter (both dissolved and particulate), and total suspended solids (TSS). However, these variables normally overlap and interact with each other. For example, chlorophyll is a measure of phytoplankton, which in fact is part of the particulate organic matter pool. Additionally, particulate organic matter is part of TSS. Although inorganic suspend solids (ISS) are often used to exclude the overlap between particulate organic matter and TSS, they are not practically available in water quality models. Therefore, in order to properly formulate the light extinction coefficient $k_e$, one needs to decide the dependent variables on the basis of both field measurements and the predictive capability of the water quality model.
In the MVCBs, the MDNR have collected underwater light irradiance data since 2004. These data have a broad coverage along both temporal and spatial scales. In this study, the 2004 data were complied to generate a best-fit multiple linear regression relationship between the light extinction coefficient $k_e$ and selected water quality variables, such as chlorophyll $a$, TSS, POC, and DOC. The statistically significant, best-fit relationship is ($R^2 = 0.8$ and $P = 0.000$):

$$k_e = 0.796 + 0.036 \cdot \text{Chlorophyll } a + 0.0397 \cdot \text{TSS}$$

(5-6)

The comparison between model predicted $k_e$ based on Eq. 5-6 and the field measurements is given in Fig. 5-3. As can be seen from Fig. 5-3, the model predictions agree well with field measurements. More importantly, this relationship is also consistent with that being used by the ICM.

Within the benthic macroalgal mat, light is further attenuated by self-shading. This part of the light extinction coefficient is calculated as:

$$k_m = a \cdot B/h_m$$

(5-7)

where:

$k_m =$ light attenuation coefficient contributed from benthic macroalgae (m$^{-1}$)

$a =$ self-shading coefficient (g C m$^{-2}$)$^{-1}$

$B =$ macroalgal biomass (g C m$^{-2}$)

$h_m =$ benthic macroalgal layer thickness (m)
Thus, the total light extinction coefficient within the benthic macroalgal layer is defined as the sum of Eqs. 5-6 and 5-7:

\[ k_t = k_e + k_m = 0.796 + 0.036 \times \text{Chlorophyll a} + 0.0397 \times \text{TSS} + a \times \text{B/h}_m \] (5-8)

Assuming that the incident radiation at the water surface is \( I_0 \), the irradiance at the top of the benthic macroalgal layer is:

\[ I_{\text{top}} = I_0 e^{k_t z} \] (5-9)

where:

\( I_{\text{top}} = \) irradiance at the top of benthic macroalgal canopy (\( \text{E m}^{-2} \text{ d}^{-1} \))

\( z = \) distance between the top of benthic macroalgal canopy and the water surface (m)

The irradiance at the bottom of benthic macroalgal layer is defined as:

\[ I_{\text{bot}} = I_{\text{top}} e^{-k_t h_m} \] (5-10)

where:

\( I_{\text{bot}} = \) irradiance at the bottom of benthic macroalgal layer (\( \text{E m}^{-2} \text{ d}^{-1} \))

If the benthic microalgae module is activated as well, \( I_{\text{bot}} \) will be used as the incident irradiance above the benthic microalgae mat. Thus, the shading effect of macroalgae on benthic microalgae is properly addressed here.

Thus, the average irradiance within the macroalgal mat is calculated as:
where \( I_{avg} = \frac{I_{top} - I_{bot}}{k_i h_m} \) (5-11)

where \( I_{avg} \) = averaged irradiance within the benthic macroalgal layer (\( E \ m^{-2} \ d^{-1} \)), which is used as irradiance \( I \) in Eq. 5-3 for calculating light limitation.

The effect of nutrients on growth

Formulations of nutrient limitation on algal growth can be divided into two types: fixed stoichiometry models and variable stoichiometry models. The majority of water quality models are of the fixed stoichiometry type. These models are generally based on the conventional Monod or Michaelis-Menten kinetics formulation, which assumes that algae uptake nutrients (e.g., N and P) concurrently with their growth. In other words, algal growth is directly limited by external nutrient concentrations in the water column instead of intracellular nutrient contents. Thus, this approach assumes nutrient contents are always fixed, e.g., the Redfield ratio (C:N:P = 106:16:1) for phytoplankton.

ICM uses the fixed stoichiometry approach for phytoplankton and the approach generally works well because phytoplankton are fast-growing and capable of efficiently converting assimilated nutrients into new biomass. In contrast, macroalgae are known to perform luxury uptake and potentially uncouple nutrient uptake from growth. Luxury uptake can, for example, allows macroalgae to uptake and store a significant amount of nutrients (especially N) compared to what they actually need for growth (Tyler et al., 2002). Conversely, macroalgae can maintain growth in the absence of ambient nutrients by using internally stored nutrients. Therefore, the commonly used fixed stoichiometry approach, which assumes growth and uptakes rates are closely related, is obviously not
suitable for macroalgae. Consequently, the variable stoichiometry approach, which was first proposed by Droop (1973 and 1977) and has been subsequently used by others (Solidoro et al., 1995 and 1997a, b; Coffaro and Bocci, 1997; Oberg, 2005) for modeling macroalgae, was adopted for this study. The dependence of macroalgal growth on internal nitrogen is formulated as follows (Solidoro et al., 1997b):

\[
f(Q) = \frac{Q - Q_{\text{min}}}{Q - Q_c}
\]

(5-12)

where:

- \( f(Q) \) = internal nitrogen limiting factor for macroalgal growth (0 \( \leq f(Q) \leq 1 \))
- Q = intracellular quota for nitrogen (g N g\(^{-1}\) C)
- Q\(_{\text{min}}\) = minimum intracellular quota for nitrogen (g N g\(^{-1}\) C)
- Q\(_c\) = critical intracellular quota for nitrogen (g N g\(^{-1}\) C)

The dependence of macroalgal growth on phosphorus is based on the Monod kinetics, as macroalgal growth is commonly assumed to depend on external phosphorus concentrations (Solidoro et al., 1995 and 1997b; Coffaro and Bocci, 1997; Oberg, 2005). The phosphorus limitation function is formulated as:

\[
f(P) = \frac{PO_4^{3-}}{KH_P + PO_4^{3-}}
\]

(5-13)

where:

- \( f(P) \) = limiting factor by phosphorus (0 \( \leq f(P) \leq 1 \))
- KH\(_P\) = half-saturation constant for algal P uptake (g P m\(^{-3}\))
- PO\(_4^{3-}\) = phosphate concentration in the water column (g P m\(^{-3}\))
Based on Liebig's "law of the minimum", the nutrient limiting function \( f(N) \) in Eq. 5-2 can be defined as:

\[
f(N) = \text{minimum} \{f(Q), f(P)\} \quad (5-14)
\]

Change in the intracellular quota of nitrogen \( Q \) is defined as follows (Solidoro et al., 1997b):

\[
\frac{dQ}{dt} = \left( V_{mNH} \frac{NH_4^+}{K_{NH} + NH_4^+} + V_{mNO} \frac{NO_x^-}{K_{NO} + NO_x^-} \right) \times \left( \frac{Q_{\text{max}} - Q}{Q_{\text{max}} - Q_{\text{min}}} \right)
\]

\[
- P_m f(I) f(N) f(T) \times \left( \frac{Q - Q_{\text{min}}}{Q - Q_c} \right) Q
\]

Where:

- \( V_{mNH} \) = maximum ammonium N uptake rate (g N g\(^{-1}\) C d\(^{-1}\))
- \( V_{mNO} \) = maximum uptake rate for nitrite-nitrate N (g N g\(^{-1}\) C d\(^{-1}\))
- \( NH_4^+ \) = ammonium N concentration in the water column (g N m\(^{-3}\))
- \( NO_x^- \) = nitrite-nitrate N concentration in the water column (g N m\(^{-3}\))
- \( K_{NH} \) = half-saturation constant for ammonium N uptake (g N m\(^{-3}\))
- \( K_{NO} \) = half-saturation constant for nitrite-nitrate N uptake (g N m\(^{-3}\))
- \( Q_{\text{max}} \) = maximum intracellular N quota (g N g\(^{-1}\) C)

In Eq. 5-15, the increment of \( Q \) is contributed by the sum of the two uptake terms,

\[
V_{mNH} \frac{NH_4^+}{K_{NH} + NH_4^+} \text{ and } V_{mNO} \frac{NO_x^-}{K_{NO} + NO_x^-}.
\]

The uptake rate is further regulated by the internal nitrogen quota \( Q \) through a feedback mechanism \( \frac{Q_{\text{max}} - Q}{Q_{\text{max}} - Q_{\text{min}}} \). Obviously, if the internal N quota \( Q \) is high enough, i.e., \( Q \) approaches \( Q_{\text{max}} \), the feedback
term $\frac{Q_{\text{max}} - Q}{Q_{\text{max}} - Q_{\text{min}}}$ tends to approach 0. Thus, low uptake rates are expected. On the other hand, if $Q$ is as low as $Q_{\text{min}}$, the uptake rate approaches its maximum value. Macroalgal growth utilizes the internal nitrogen to produce new biomass and reduces nitrogen quota $Q$. Hence, the actual growth rate is represented as $P_{\text{mf}} f(I) f(N) f(T) \times \left( \frac{Q - Q_{\text{min}}}{Q - Q_{c}} \right)$, which accounts for limitation by light, nutrients, and temperature. Consequently, the decreased rate of $Q$ is defined as $P_{\text{mf}} f(I) f(N) f(T) \times \left( \frac{Q - Q_{\text{min}}}{Q - Q_{c}} \right) Q$.

The variable stoichiometry approach is more complicated than traditional, fixed stoichiometry models; e.g., it involves more parameters and variables. However, the variable stoichiometry approach is especially warranted if one wants to accurately simulate macroalgal distributions in the MVCBs. For example, in Hog Island Bay, VA, the internal N contents of the two representative benthic macroalgal species were found to be especially variable in both temporal and spatial scales, reasonably reflecting the ambient N availability in the system (Fig. 5-4) (Tyler et al., 2001; Tyler and McGlathery, 2006).

**The effect of temperature on growth**

In ICM, the effect of temperature on phytoplankton growth is represented by a function similar to the Gaussian probability curve:
\[ f(T) = e^{(KTG_1(T - TM)^2)} \quad \text{when } T \leq TM \\
= e^{(KTG_2(TM - T)^2)} \quad \text{when } T > TM \]  

(5-16)

where:

\[ TM = \text{optimal temperature for algal growth (°C)} \]

\[ KTG_1 = \text{effect of temperature below TM on algal growth (°C}^2) \]

\[ KTG_2 = \text{effect of temperature above TM on algal growth (°C}^2) \]

Based on a recent laboratory experiment (Fig. 5-5) performed at VIMS on *Gracilaria vermiculophylla*, an invasive species in the MVCBs, our assessment is that its temperature-dependent optimum curve more resembles that developed by Thornton and Lessem (1978) than the Gaussian curve formulation; thus we adopted the Thornton and Lessem formulation for the benthic macroalgal module:

\[ f(T) = K_A(T)K_B(T) \]  

(5-17)

\[ K_A(T) = \frac{K_1 e^{\gamma_1(T - T_{\min})}}{1 + K_1 e^{\gamma_1(T - T_{\min}) - 1}} \]

\[ \gamma_1 = \frac{1}{(T_{\min}^{opt} - T_{\min})} \ln \left[ \frac{K_2(1 - K_1)}{K_1(1 - K_2)} \right] \]

\[ K_B(T) = \frac{K_4 e^{\gamma_2(T_{\max}^{opt} - T)}}{1 + K_4 e^{\gamma_2(T_{\max}^{opt} - T) - 1}} \]

\[ \gamma_2 = \frac{1}{(T_{\max} - T_{\max}^{opt})} \ln \left[ \frac{K_3(1 - K_4)}{K_4(1 - K_3)} \right] \]

where:
\( T_{\text{min}} \) = minimum tolerance temperature for macroalgal growth (°C)

\( T_{\text{max}} \) = maximum tolerance temperature for macroalgal growth (°C)

\( T_{\text{min opt}} \) = minimum optimal temperature for macroalgal growth (°C)

\( T_{\text{max opt}} \) = maximum optimal temperature for macroalgal growth (°C)

\( K_1, K_2, K_3, \) and \( K_4 \) = empirical coefficients, which control the shape of the temperature response curve

This equation was used for phytoplankton and macroalgae modeling by Coffaro and Bocci (1997) and Trancoso et al. (2005). In fact, the previous Gaussian curve can be regarded as a special case of the Thornton and Lessem curve when \( T_{\text{min opt}} = T_{\text{max opt}} \).

**B. Respiration**

Similar to the formulation for phytoplankton respiration used in ICM, macroalgal respiration includes two processes: growth-related respiration and basal metabolism. The growth-related respiration term assumes that a certain portion of the carbon fixed by gross production is respired to maintain normal biological activities. Hence, this term partially mimics the photo-respiration process. In Eq. 5-1, a fixed fraction \( (\beta) \) of the gross production term \( P \) is counted as growth-related respiration and subtracted from the gross production. The basal metabolism term \( R \) is commonly considered to be an exponential function of temperature:

\[
R = R_{\text{ref}} \times e^{K(T-TR)}
\]

(5-18)

where:

\( R_{\text{ref}} \) = base metabolic rate at reference temperature \( TR \) (day \(^{-1}\))
KTR = effect of temperature on metabolism (°C⁻¹)

TR = reference temperature for metabolism (°C)

T = water temperature (°C)

C. Mortality

The nonpredatory mortality term includes all algal losses that are not explicitly accounted for by the grazing term or other loss processes. It includes processes such as senescence, parasitism, and stress-induced mortality due to severe environmental conditions (Bowie et al., 1985). The nonpredatory mortality term for phytoplankton is often simply neglected, or implicitly modeled as a fraction of respiration. However, for benthic macroalgae, nonpredatory mortality can be a crucial process. It is sometimes the leading cause for the characteristic summer crash of the dense macroalgal mat (Solidoro et al., 1997a, b). The product of mortality is treated as nonliving particulate organic matter, which is subjected to physical transport (advection, diffusion, and settling) and a series of biogeochemical processes (e.g., decomposition in the water column and diagenesis in the sediment).

It is well-known fact that macroalgae undergo a boom-and-bust life cycle; it often crashes in the later summer (e.g., Tyler, 2002). However, a proper formulation for the nonpredatory mortality is still lacking due to the fact that the mechanism of macroalgal mortality is not well understood. This remains as a challenge for modelers. Some studies used a constant rate for mortality (Aveytua-Alcazar et al., 2008), while others formulated mortality as a function of temperature and DO (Coffaro and Bocci, 1997; Solidoro et al.,
1997b; Giusti and Marsili-Libelli, 2005; Trancoso et al., 2005). Obviously, temperature is an important factor contributing to mortality and needs to be considered. For example, Coffaro and Bocci (1997) employed a formula similar to the basal metabolism function. In their formulation, if macroalgal biomass and water temperature both increase above certain thresholds, the mortality term starts to take effect. In terms of the toxic effect induced by low DO, as argued by Solidoro et al. (1997a), the lack of enough oxygen within the macroalgal mat has a feedback effect on mortality. Once DO levels drop below the level that is sufficient for basal metabolism, the mortality rate increases. The increased mortality of macroalgae in turn stimulates the DO consumption process and, as a consequence, the macroalgal population may suddenly collapse. Similar phenomena have been observed in the field as well as the laboratory experiments (e.g., Solidoro et al., 1997a; Brush, 2002; Tyler, 2002). However, as mentioned earlier, the exact mechanism of the mortality term has not been clearly quantified; hence, the mortality formulations are essentially empirically based. Consequently, the parameters have to be calibrated for individual systems.

In this study, the formula proposed by Solidoro et al. (1997a) and Coffaro and Bocci (1997) was adopted:

$$M = M_{DO} \frac{\max\left(\frac{AOCR \cdot R \cdot B - DO}{DO} \right) 0}{AOCR \cdot R \cdot B} + M_{ref} e^{KTM(T-MR)}$$  \hspace{1cm} (5-19)

where:

$$M_{DO} = \text{base mortality rate induced by low DO (d}^{-1})$$
$M_{\text{ref}} =$ background mortality rate (d$^{-1}$)

$\text{DO} =$ dissolved oxygen concentration in the water column (mg L$^{-1}$)

$\text{AOCR} =$ oxygen:carbon mass ratio = 2.67 g O$_2$ g$^{-1}$ C

$\text{KTM} =$ effect of temperature on mortality (°C$^{-1}$)

$\text{TMR} =$ reference temperature for mortality (°C)

Additionally, it is well-established that elevated H$_2$S can have detrimental effects on macrophyte growth (Koch et al., 1990; Erskine and Koch, 2000). The following equation can be used to account for the mortality rate induced by H$_2$S:

$$M_s = M_{s0} \times e^{(KSM[H_2S-H_{2SR}])}$$  \hspace{1cm} (5-20)

where:

$M_s =$ mortality rate induced by H$_2$S (d$^{-1}$)

$M_{s0} =$ base mortality rate induced by H$_2$S (d$^{-1}$)

$KSM =$ effect of H$_2$S on mortality (mg L$^{-1}$)$^{-1}$

$H_2S =$ H$_2$S concentration in the water column (mg L$^{-1}$)

$H_{2SR} =$ reference H$_2$S concentration in the water column (mg L$^{-1}$)

Eq. 5-20 has a similar form similar to that of temperature-induced mortality. It states that as H$_2$S concentration in the water column rises above a certain threshold, the H$_2$S toxicity can sharply increase the mortality rate of benthic macroalgae. As a positive feedback, increased macroalgal mortality in turn accelerates H$_2$S production in both the sediment and water column. However, this equation is not used in the model due to the fact that no parameter values can be obtained from the literature. Additionally, the
mortality effect of $H_2S$ has been partially included into the DO-induced mortality term, as there is a certain correlation between low DO and the formation of $H_2S$.

**D. Grazing**

In temperate estuaries, benthic grazers may exert a significant "top-down" control on macroalgal biomass (Valiela et al., 1997; Giannotti and McGlathery, 2001). It was found that in Hog Island Bay, VA, grazing could remove up to 88% of new macroalgal growth at a low N supply site. In the current benthic macroalgal module, grazing is treated as the predatory mortality process, which is formulated in a manner similar to the basal metabolism process:

$$Gr = Gr_{ref} \times e^{(KTGr[T-TGr])}$$  \hspace{1cm} (5-21)

where:

- $Gr_{ref}$ = base grazing rate at reference temperature $T_{Gr}$ (day$^{-1}$)
- $KTGr$ = effect of temperature on metabolism ($°C^{-1}$)
- $T_{Gr}$ = reference temperature for metabolism ($°C$)

**V-2-4 Parameter evaluation**

The selection of proper model parameters is performed in several ways, which include literature values, observational data from both laboratory and field studies, and model calibrations. Because ICM is a carbon-based water quality model, all parameters obtained from the literature and observations were converted to carbon-based units from their original units. Based on the literature (Brush, 2002) and field data collected by
Hardison (2009) in the MVCBs (Figs. 5-6 and 5-7), the dry weight/wet weight ratios (dw:ww) were determined as 0.25 and 0.30 g dw g⁻¹ ww for Ulva lactuca and Gracilaria vermiculophylla, respectively. The carbon/dry weight (C:dw) ratios were determined as 0.28 g C g⁻¹ dw and 0.30 g C g⁻¹ dw for Ulva lactuca and Gracilaria vermiculophylla, respectively. These numbers were used universally for unit conversion throughout this study.

A. Growth related parameters

The growth rate is probably the most important parameter for algae-based eutrophication models. The maximum growth rate $P_m$ varies significantly for different algal species. In water quality models, the maximum growth rate for the same algal species is commonly assumed to be a fixed value that does not vary in time and space. In this study, the measured maximum growth rate by Giordano (2009) in Isle of Wight Bay and Hog Island Bay was used as an important reference (Fig. 5-8). The final parameter values are listed in Tables 5-2 and 5-3.

B. Respiration, mortality, and grazing related parameters

In temperate estuaries, episodic crashes of dense macroalgal mats were frequently observed. For example, in Hog Island Bay, VA, dense macroalgal mat often crashes right after reaching their peak biomass every summer at the most abundant site (e.g., Tyler et al., 2002), probably as a result of high temperature and self-shading within the macroalgal mat (Tyler, 2002). High temperature leads to a high respiration rate, which accounts for the basic loss process of macroalgae. The positive correlation between
temperature and respiration rate was also observed for both macroalgal samples taken from Hog Island Bay and Isle of Wight Bay (Fig. 5-8, Giordano, 2009). In our opinion, however, macroalgal respiration is a process that can only be performed by “living” macroalgae and cannot by itself explain the sudden and massive collapse of the entire macroalgal population. Based on the current respiration-temperature relationship, the model results also suggest that benthic macroalgae tend to form a much higher fall-winter peak as temperature decreases. However, it is not true as suggested by field observations (e.g., Tyler, 2002). Grazing is sometimes an important loss process for macroalgae; however, it can be inhibited by hypoxia at the onset of the crash (Sfriso and Marcomini, 1996). Hence, the mortality term, which directly converts active macroalgae into nonliving particulate organic matter, is a logical choice as a major process which is responsible for the dysfunction and subsequent crash of the macroalgal population.

The respiration rate is readily available from both field measurements and literature. The grazing rate is a parameter that is highly variable and needs to be calibrated in the course of model simulations. Parameters for the mortality term were first obtained from literature, and finally tuned through calibrations. All the parameter values and their literature sources are given in Tables 5-2 and 5-3.

V-3 Simulating benthic macroalgae kinetics using a box-model

After the benthic macroalgal module was built into the ICM water quality model, our first task was to conduct a series of numerical experiments using a simple box model to examine the basic properties and functions of the macroalgae-included water quality
model. The box model consists of a well-mixed water column as well as two sediment layers: an oxic and an anoxic layer, as shown in Fig. 5-9. The water column has a fixed volume of 1 m$^3$ and its flushing time is regulated by adjusting the inflow rates. The inflow is assumed to be "clean" and saturated with DO. Thus, this box can be thought to represent a well-mixed shallow coastal bay, which is connected to an ideal "clean" ocean without nutrients and organisms. The scenarios conducted include:

(1) Experiment #1: The effect of flushing time on algal species interaction

(2) Experiment #2: The seasonal pattern of benthic macroalgae

(3) Experiment #3: A comparison between Droop and Monod kinetics

V-3-1 The effect of flushing time on algal species competition

As hypothesized by Valiela et al. (1997), transport time scales can regulate species competition between benthic macroalgae and phytoplankton in shallow estuaries. In well-flushed estuaries (e.g., Waquoit Bay, MA), benthic macroalgae can out-compete phytoplankton and be the dominant primary producer. The first numerical experiment was designed to investigate the competition under four flushing regimes (Table 5-4). To simplify the problem, the box model only simulated one macroalgal species and one phytoplankton species. The model was first configured to simulate the conditions when benthic macroalgae and phytoplankton were individually present in the system. All the runs were carried out under a constant temperature (20 °C), an optimal temperature for algal growth. In addition, nitrate was continuously added to the water column at a constant loading rate (0.05 g N m$^{-3}$ day$^{-1}$) that is within the range of nitrogen loading rates for the MVCBs (Boynton et al., 1996). Phosphate was added to the water column at 0.1 g
P m$^{-3}$ day$^{-1}$, to avoid any possible phosphorus limitation for algal growth. The total daily solar radiation was set as constant (60 E m$^{-2}$ day$^{-1}$) and the change of light intensity in a day was modeled using a sinusoidal function (assuming a 12-hour photoperiod). In each simulation, the box model was continuously run for 10 years to guarantee that a dynamic equilibrium was reached. The model results for algal biomass and other state variables are provided in Tables 5-5, 5-6, and 5-7. These variables include water column concentrations for NH$_4^+$, NO$_x^-$, DON, and DOC, as well as benthic fluxes for NH$_4^+$ and SOD (sediment oxygen demand).

As shown in Tables 5-5 and 5-6, the equilibrium biomass of both benthic macroalgae and phytoplankton increases with flushing time when these two species are present in the system individually. However, benthic macroalgae reach a much higher biomass than phytoplankton and retain more nitrogen internally under all flushing conditions. In addition, for the case of benthic macroalgae only, the corresponding water column concentrations of NH$_4^+$ and NO$_x^-$ (Table 5-6) are approximately one magnitude lower than those when phytoplankton are present (Table 5-5). This does suggest that benthic macroalgae are extremely efficient in sequestering inorganic nitrogen from the water column.

When benthic macroalgae and phytoplankton are both present in the system, the model results are much different from previous reference runs in which they are present separately. As expected, benthic macroalgae outcompete phytoplankton under better flushing conditions (i.e., flushing time = 1 and 10 days). Moreover, benthic macroalgae
are still able to dominate phytoplankton as flushing time increases to 100 days. This implies that, if under optimal growth conditions (e.g., temperature and light), benthic macroalgae can potentially outcompete phytoplankton regardless of flushing time.

V-3-2 Seasonal patterns of benthic macroalgae

In temperate shallow estuaries, benthic macroalgal biomass is well-known to have a distinct seasonal pattern. Thus, the second experiment was designed to examine if the model can successfully simulate the seasonal variation of benthic macroalgae. To account for the seasonality, both water temperature and solar radiation were forced by sinusoidal functions (Fig. 5-10), similar to observational data in the MVCBs. The remaining settings were the same as Run # 2 in Experiment 1, with a flushing time of 10 days. The model was run continuously for 10 years and the results for the last two years were presented in Figs. 5-11.

As one can see from Fig. 5-11(a), benthic macroalgae are the dominant primary producers during most of the year whereas phytoplankton concentrations remain extremely low most of the time. Following the summer crash of benthic macroalgae, however, phytoplankton starts to proliferate immediately and becomes the dominant feature in the fall. In this simulation, the whole crash process takes about one to two weeks. Keep in mind that the nutrient input here is constant throughout the experiment rather than the familiar pattern of high input during spring and low in the summer in the region. In that case, a small spring bloom of phytoplankton combined with a fall peak is possible. The remaining water quality variables also exhibit reasonable responses to the
seasonality of benthic macroalgal biomass (Figs. 5-11(b-d)). For example, hypoxia occurs concurrently with the summer crash of the macroalgal population (Fig. 5-11(b)). Large amounts of organic matter are released into the water column and sediment following the macroalgal die-off (Figs. 5-11(b-c)). Phytoplankton starts to take up the nutrients and bloom. In addition, increased deposition of organic matter into the sediment results in a sharp increase of the benthic flux of NH$_4^+$, SOD, and COD (chemical oxygen demand) (Fig. 5-11(d)). As a positive feedback, this exacerbates water column hypoxia, which further promotes macroalgal die-off. In general, the model is able to capture the major seasonal patterns of benthic macroalgae and phytoplankton in an idealized temperate shallow water ecosystem. This is important for understanding the role played by benthic macroalgae in shallow coastal waters on an annual basis.

V-3-3 A comparison between Droop and Monod kinetics

In the benthic macroalgal module, both Droop and Monod formulations can be used for simulating uptake kinetics. The third box-model experiment was designed to compare results using Droop versus Monod formulations for representing the benthic macroalgae–nitrogen relationship. The model setup is basically the same as Run # 2 in Experiment 1 with benthic macroalgae present only. However, nitrate loading was added to the water column as pulses instead of at a constant rate (Fig. 5-12). The model was configured with the same initial conditions and parameter sets for both the Droop and Monod kinetics simulations.
The model was run for 180 days and the results are shown in Fig. 5-12. As can be seen, both benthic macroalgal biomass and water column NO$_3^-$ concentrations respond differently when Monod and Droop formulations are used. Following each NO$_3^-$ loading pulse, a sharp increase of water column NO$_3^-$ is predicted if the Monod formulation is used; In contrast, there is little increase in NO$_3^-$ concentrations if Droop kinetics are used. It is apparent that the NO$_3^-$ loading pulse was immediately taken up by benthic macroalgae and stored internally for subsequent growth; this can be seen in the sharp increase in intracellular N quota using the Droop formulation. Furthermore, macroalgae can still maintain net growth when the external NO$_3^-$ loading is diminished (e.g., from Day 110 to 120). The Droop equation can describe the internal N storage capability and thus, the luxury uptake by benthic macroalgae, which is crucial for survival in variable nutrient loading environments. The model results using the Droop formulation may also partially explain why inorganic nitrogen (DIN) concentrations remain low in the water column when macroalgae are present.

V-4 Summary

In this chapter, we described how a benthic macroalgal module has been developed within the CE-QUAL-ICM model framework. For the module, we adopted the Droop formulation for nutrient uptake kinetics and drew parameters from both the literature and recent laboratory studies. The macroalgal module-included modeling framework was tested by conducting a series of numerical experiments using a simple box model. It examined (1) the effects of flushing time on algal species competition, (2) the seasonal pattern for benthic macroalgae abundance, and (3) compared uptake kinetics
when using the Droop and Monod formulations. Results suggest that the model can successfully capture the key characteristics of benthic macroalgae in shallow coastal bays. In addition, the box-model experiments also provide useful guidance for subsequent model applications to the MVCBs.
Table 5-1. Water column state variables in CE-QUAL-ICM

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>T</td>
</tr>
<tr>
<td>Salinity</td>
<td>S</td>
</tr>
<tr>
<td>Fixed Suspended Solids</td>
<td>FSS</td>
</tr>
<tr>
<td>Cyanobacteria</td>
<td>Be</td>
</tr>
<tr>
<td>Diatoms</td>
<td>Bd</td>
</tr>
<tr>
<td>Green Algae/Dinoflagelette</td>
<td>Bg</td>
</tr>
<tr>
<td>Microzooplankton</td>
<td>SZ</td>
</tr>
<tr>
<td>Mesozooplankton</td>
<td>Lz</td>
</tr>
<tr>
<td>Refractory Particulate Organic Carbon</td>
<td>RPOC</td>
</tr>
<tr>
<td>Labile Particulate Organic Carbon</td>
<td>LPOC</td>
</tr>
<tr>
<td>Dissolved Organic Carbon</td>
<td>DOC</td>
</tr>
<tr>
<td>Refractory Particulate Organic Nitrogen</td>
<td>RPON</td>
</tr>
<tr>
<td>Labile Particulate Organic Nitrogen</td>
<td>LPON</td>
</tr>
<tr>
<td>Dissolved Organic Nitrogen</td>
<td>DON</td>
</tr>
<tr>
<td>Ammonium/Urea Nitrogen</td>
<td>NH₄⁺</td>
</tr>
<tr>
<td>Nitrate+Nitrite Nitrogen</td>
<td>NO₂⁻</td>
</tr>
<tr>
<td>Refractory Particulate Organic Phosphorus</td>
<td>RPOP</td>
</tr>
<tr>
<td>Labile Particulate Organic Phosphorus</td>
<td>LPOP</td>
</tr>
<tr>
<td>Dissolved Organic Phosphorus</td>
<td>DOP</td>
</tr>
<tr>
<td>Total Phosphate</td>
<td>PO₄³⁻</td>
</tr>
<tr>
<td>Particulate Biogenic Silica</td>
<td>SU</td>
</tr>
<tr>
<td>Available Silica</td>
<td>SA</td>
</tr>
<tr>
<td>Chemical Oxygen Demand</td>
<td>COD</td>
</tr>
<tr>
<td>Dissolved Oxygen</td>
<td>DO</td>
</tr>
</tbody>
</table>
Table 5-2. Benthic macroalgal module parameters  – Ulva lactuca

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Units</th>
<th>Value</th>
<th>Sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_m$</td>
<td>Maximum growth rate</td>
<td>$d^{-1}$</td>
<td>0.50</td>
<td>Coffaro and Bocci, 1997; Solidoro et al., 1997; Guimaraens et al., 2005; Brush and Nixon, 2003; Giordano, 2009</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Fraction of growth-related respiration</td>
<td>-</td>
<td>0.25</td>
<td>Cerco and Noel, 2002; Calibrated</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Initial slope of the P-I curve</td>
<td>$(\mu E : m^2 : s^{-1})^{-1} : d^{-1}$</td>
<td>0.004</td>
<td>Brush, 2002; Coffaro and Sfriso, 1997; Sand-Jensen, 1988</td>
</tr>
<tr>
<td>$a$</td>
<td>self-shading coefficient</td>
<td>$(g : C : m^{-2})^{-1}$</td>
<td>0.10</td>
<td>Brush, 2002; Calibrated</td>
</tr>
<tr>
<td>$Q_{min}$</td>
<td>Minimum N quota</td>
<td>$g : N : g^{-1} : C$</td>
<td>0.036</td>
<td>Coffaro and Bocci, 1997; Solidoro et al., 1995, 1997; Oberg, 2005; Hardison, 2009</td>
</tr>
<tr>
<td>$Q_{max}$</td>
<td>Maximum N quota</td>
<td>$g : N : g^{-1} : C$</td>
<td>0.15</td>
<td>Coffaro and Bocci, 1997; Solidoro et al., 1995, 1997; Oberg, 2005; Hardison, 2009</td>
</tr>
<tr>
<td>$Q_c$</td>
<td>Critical N quota</td>
<td>$g : N : g^{-1} : C$</td>
<td>0.029</td>
<td>Solidoro et al., 1997</td>
</tr>
<tr>
<td>$K_{NP}$</td>
<td>half-saturation constant for P uptake</td>
<td>$g : N : g^{-1} : C : m^{-3}$</td>
<td>0.01</td>
<td>Solidoro et al., 1997</td>
</tr>
<tr>
<td>$V_{mNH}$</td>
<td>maximum ammonium N uptake rate</td>
<td>$g : N : g^{-1} : C : d^{-1}$</td>
<td>0.45</td>
<td>Solidoro et al., 1995, 1997</td>
</tr>
<tr>
<td>$V_{mNO}$</td>
<td>maximum nitrite-nitrate N uptake rate</td>
<td>$g : N : g^{-1} : C : d^{-1}$</td>
<td>0.07</td>
<td>Solidoro et al., 1995, 1997; Coffaro and Bocci, 1997</td>
</tr>
<tr>
<td>$K_{NH}$</td>
<td>half-saturation constant for ammonium N uptake</td>
<td>$g : N : m^{-3}$</td>
<td>0.66</td>
<td>Solidoro et al., 1997; Gownaris and Brush, 2008</td>
</tr>
<tr>
<td>$K_{NO}$</td>
<td>half-saturation constant for nitrite-nitrate N uptake</td>
<td>$g : N : m^{-3}$</td>
<td>0.25</td>
<td>Lavery and McComb, 1991</td>
</tr>
</tbody>
</table>
Table 5-2 (Cont’d). Benthic macroalgal module parameters – Ulva lactuca

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Units</th>
<th>Value</th>
<th>Sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tmin</td>
<td>minimum tolerance temperature for macroalgal growth</td>
<td>°C</td>
<td>5</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>Tmax</td>
<td>maximum tolerance temperature for macroalgal growth</td>
<td>°C</td>
<td>35</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>T_{min}^{opt}</td>
<td>minimum optimal temperature for macroalgal growth</td>
<td>°C</td>
<td>15</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>T_{max}^{opt}</td>
<td>maximum optimal temperature for macroalgal growth</td>
<td>°C</td>
<td>25</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>K_1</td>
<td>empirical coefficient for temperature function</td>
<td>-</td>
<td>0.05</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>K_2</td>
<td>empirical coefficient for temperature function</td>
<td>-</td>
<td>0.98</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>K_3</td>
<td>empirical coefficient for temperature function</td>
<td>-</td>
<td>0.98</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>K_4</td>
<td>empirical coefficient for temperature function</td>
<td>-</td>
<td>0.02</td>
<td>Coffaro and Boci, 1997; Trancoso et al., 2005; Calibrated</td>
</tr>
<tr>
<td>R_{ref}</td>
<td>base metabolic rate at reference temperature TR</td>
<td>d^{-1}</td>
<td>0.02</td>
<td>Peckol and Rivers, 1996; Solidoro et al., 1997; Giordano, 2009; Calibrated</td>
</tr>
<tr>
<td>KTB</td>
<td>effect of temperature on metabolism</td>
<td>°C^{-1}</td>
<td>0.069</td>
<td>Cerco and Noel, 2002; Calibrated</td>
</tr>
<tr>
<td>TR</td>
<td>reference temperature for metabolism</td>
<td>°C</td>
<td>20.0</td>
<td>Cerco and Noel, 2002; Calibrated</td>
</tr>
<tr>
<td>KTM</td>
<td>effect of temperature on mortality</td>
<td>°C^{-1}</td>
<td>0.7</td>
<td>Coffaro and Boci, 1997; Calibrated</td>
</tr>
<tr>
<td>TMR</td>
<td>reference temperature for mortality</td>
<td>°C</td>
<td>30.0</td>
<td>Coffaro and Boci, 1997; Calibrated</td>
</tr>
<tr>
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<td>Solidoro et al., 1997; Calibrated</td>
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<tr>
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<td>Flindt et al., 1997; Giannotti and McGlathery, 2001; Calibrated</td>
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<tr>
<td>KTGr</td>
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<td>°C^{-1}</td>
<td>0.069</td>
<td>Cerco and Noel, 2002</td>
</tr>
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<td>TGr</td>
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<td>°C</td>
<td>20</td>
<td>Cerco and Noel, 2002</td>
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Table 5-3. Benthic macroalgal module parameters – Gracilaria vermiculophylla

<table>
<thead>
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<th>Parameter</th>
<th>Definition</th>
<th>Units</th>
<th>Value</th>
<th>Sources</th>
</tr>
</thead>
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<tr>
<td>$P_m$</td>
<td>Maximum growth rate</td>
<td>d$^{-1}$</td>
<td>0.30</td>
<td>Brush, 2002; Giordano, 2009</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Fraction of growth-related respiration</td>
<td>-</td>
<td>0.25</td>
<td>Cerco and Noel, 2002; Calibrated</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Initial slope of the P-I curve</td>
<td>($\mu$E m$^{-2}$ s$^{-1}$)$^{-1}$ d$^{-1}$</td>
<td>0.01</td>
<td>Brush, 2002; Wong and Chang, 2000; Giordano, 2009</td>
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<tr>
<td>$\alpha$</td>
<td>self-shading coefficient</td>
<td>(g C m$^{-3}$)$^{-1}$</td>
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<td>$Q_{min}$</td>
<td>Minimum N quota</td>
<td>g N g$^{-1}$ C</td>
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<td>Coffaro and Bocci, 1997; Solidoro et al., 1995, 1997; Oberg, 2005; Hardison, 2009</td>
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<td>$Q_{max}$</td>
<td>Maximum N quota</td>
<td>g N g$^{-1}$ C</td>
<td>0.12</td>
<td>Coffaro and Bocci, 1997; Solidoro et al., 1995, 1997; Oberg, 2005; Hardison, 2009</td>
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<tr>
<td>$Q_c$</td>
<td>Critical N quota</td>
<td>g N g$^{-1}$ C</td>
<td>0.033</td>
<td>Solidoro et al., 1997</td>
</tr>
<tr>
<td>$K_{H_2}$</td>
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<td>g N g$^{-1}$ C</td>
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<td>Solidoro et al., 1997</td>
</tr>
<tr>
<td>$V_{mNH}$</td>
<td>maximum ammonium N uptake rate</td>
<td>g N g$^{-1}$ C d$^{-1}$</td>
<td>0.22</td>
<td>Solidoro et al., 1995, 1997; Gownaris and Brush, 2008</td>
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<td>$V_{mNO}$</td>
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<td>$K_{NO}$</td>
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<td>g N m$^{-3}$</td>
<td>0.12</td>
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Table 5-3 (Cont’d). Benthic macroalgal module parameters – *Gracilaria vermiculophylla*

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<th>Parameter</th>
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<th>Units</th>
<th>Value</th>
<th>Sources</th>
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<tr>
<td>(T_{\text{min}})</td>
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<td>°C</td>
<td>4</td>
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<td>(T_{\text{max}})</td>
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<td>(T_{\text{max}}^{\text{opt}})</td>
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<td>°C</td>
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<td>(K_1)</td>
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<td>(K_2)</td>
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<td>0.98</td>
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<td>(K_3)</td>
<td>empirical coefficient for temperature function</td>
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<td>(K_4)</td>
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<td>(R_{\text{ref}})</td>
<td>base metabolic rate at reference temperature (TR)</td>
<td>(\text{d}^{-1})</td>
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<td>(K_{TB})</td>
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<td>°C(^{-1})</td>
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<td>Cerco and Noel, 2002</td>
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<td>Cerco and Noel, 2002</td>
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<td>(K_{TM})</td>
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<td>(^{\circ}\text{C}^{-1})</td>
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<td>(T_{MR})</td>
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<td>(M_{\text{ref}})</td>
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<td>Calibrated</td>
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<td>(K_{TGr})</td>
<td>effect of temperature on metabolism</td>
<td>°C(^{-1})</td>
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<td>Cerco and Noel, 2002</td>
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<tr>
<td>(T_{Gr})</td>
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Table 5-4. Box model configurations for Experiment 1

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<tr>
<th>Run #</th>
<th>Flushing Time (days)</th>
<th>NO₃⁻ Loading Rate (g N m⁻³ day⁻¹)</th>
<th>Normalized NO₃⁻ Loading Rate (g N m⁻³ day⁻¹)</th>
<th>Conservative Tracer Concentration (mg L⁻¹)</th>
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Table 5-5. Model results for Experiment 1 – phytoplankton only

<table>
<thead>
<tr>
<th>Run #</th>
<th>Phytoplankton (Chl-a, μg L⁻¹)</th>
<th>Nitrogen Retained by phytoplankton (g N)</th>
<th>NH₄⁺ (mg N L⁻¹)</th>
<th>NO₃⁻ (mg N L⁻¹)</th>
<th>DON (mg N L⁻¹)</th>
<th>DOC (mg C L⁻¹)</th>
<th>Sediment NH₄⁺ flux (g N m⁻² day⁻¹)</th>
<th>SOD (g O₂ m⁻² day⁻¹)</th>
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<tr>
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<td>0.0000</td>
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<td>4.692</td>
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Table 5-6. Model results for Experiment 1 – benthic macroalgae only

<table>
<thead>
<tr>
<th>Run #</th>
<th>Benthic Macroalgal (g C m&lt;sup&gt;-2&lt;/sup&gt;)</th>
<th>Benthic Macroalgal N Quota (g N g&lt;sup&gt;-1&lt;/sup&gt; C)</th>
<th>Nitrogen Retained by Benthic Macroalga (g N)</th>
<th>NH&lt;sub&gt;4&lt;/sub&gt;&lt;sup&gt;+&lt;/sup&gt; (mg N l&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>NO&lt;sub&gt;3&lt;/sub&gt;&lt;sup&gt;-&lt;/sup&gt; (mg N l&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>DON (mg N l&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>DOC (mg C l&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>Sediment NH&lt;sub&gt;4&lt;/sub&gt;&lt;sup&gt;+&lt;/sup&gt; flux (g N m&lt;sup&gt;-2&lt;/sup&gt; day&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>SOD (g O&lt;sub&gt;2&lt;/sub&gt; m&lt;sup&gt;-2&lt;/sup&gt; day&lt;sup&gt;-1&lt;/sup&gt;)</th>
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<td>3.06</td>
<td>0.0006</td>
<td>0.0007</td>
<td>0.013</td>
<td>0.081</td>
<td>0.004</td>
<td>0.21</td>
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<td>0.0005</td>
<td>0.247</td>
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<td>2.395</td>
<td>11.946</td>
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Table 5-7. Model results for Experiment 1 – both phytoplankton and benthic macroalgae present

<table>
<thead>
<tr>
<th>Run #</th>
<th>Phytoplankton (Chl-a, μg L(^{-1}))</th>
<th>Nitrogen Retained by phytoplankton (g N)</th>
<th>Benthic Macroalgal Nitrogen Quota (g N g(^{-1}) C)</th>
<th>Benthic Macroalgae Nitrogen Retained by Sediment (g N)</th>
<th>NH(_4^+) (mg N L(^{-1}))</th>
<th>NO(_3^-) (mg N L(^{-1}))</th>
<th>DON (mg C L(^{-1}))</th>
<th>DOC (mg C L(^{-1}))</th>
<th>Sediment NH(_4^+) flux (g N m(^{-2}) day(^{-1}))</th>
<th>SOD (g O(_2) m(^{-2}) day(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.00</td>
<td>78.0</td>
<td>0.039</td>
<td>0.001</td>
<td>0.0007</td>
<td>0.013</td>
<td>0.081</td>
<td>0.004</td>
<td>0.21</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
<td>0.00</td>
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<td>0.043</td>
<td>0.001</td>
<td>0.0005</td>
<td>0.247</td>
<td>1.396</td>
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<td>0.0004</td>
<td>1.986</td>
<td>11.416</td>
<td>0.114</td>
<td>2.79</td>
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</table>
Fig. 5-1. Conceptual diagram showing hypothetical pattern of change in the relative contribution by three major groups of primary producers (phytoplankton - P; macroalgae - M; seagrass - S) in response to changes in nitrogen loading rate and residence time in shallow temperate estuaries (adopted from Valiela et al., 1997).
Fig. 5-2. Kinetic processes to be incorporated into the proposed benthic macroalgal module (BMAC – benthic macroalgae; DOM – dissolved organic matter; POM – particulate organic matter; DO – dissolved oxygen).
Fig. 5-3. Predicted light attenuation coefficient $k_e$ vs. measured values. Black solid line denotes the linear regression fit, and the pink dotted line denotes the 1:1 relationship.

\[ y = 0.804x + 0.437 \]

\[ R^2 = 0.8043 \]
Fig. 5-4. Temporally and spatially variable macroalgal N content as found in Hog Island Bay, VA. (Top panel: Ulva lactuca, Tyler et al., 2001; Bottom panel: Gracilaria vermiculophylla, Tyler and McGlathery, 2006).
Fig. 5-5. Net growth (biomass increment) of Gracilaria vermiculophylla under different temperature conditions after a 12-day incubation experiment (error bar stands for ± SE). Top panel – Experiment conducted in April, 2009; Bottom panel – Experiment conducted in May, 2009.
Fig. 5-6. Observed benthic macroalgal characteristics in Isle of Wight Bay, MD (data courtesy of Amber Hardison, VIMS).
Fig. 5-7. Observed macroalgal biomass at three monitoring stations in the MVCBs. Stations M-1 and M-2 were located in Turville Creek, and station M-3 was in Isle of Wight Bay. Data courtesy of Amber Hardison. (Legend: G – Gracilaria vermiculophylla; U – Ulva lactuca; O – other macroalgae).
Fig. 5-8(a). Maximum photosynthesis rates $P_m$ (top panel) and respiration rates $R$ (bottom panel) measured for macroalgal samples taken in different months from Hog Island Bay, VA. Data courtesy of Juliette Giordano.
Fig. 5-8(b). Maximum photosynthesis rates $P_m$ (top panel) and respiration rates $R$ (bottom panel) measured for macroalgal samples taken in different months from Isle of Wight Bay, MD. Data courtesy of Juliette Giordano.
Fig. 5-9. Diagram showing box model configurations. The water column has a fixed volume = $1 \times 1 \times 1$ m$^3$. The bottom sediment layer consists of two sublayers (upper oxic layer (brown color in the figure) thickness = ~ 0.1 cm and lower anoxic layer (grey color in the figure) thickness = ~ 0.1 m; thus, the total sediment layer thickness $\approx 0.1$ m).
Fig. 5-10. Solar radiation (top panel) and temperature (bottom panel) forcing for the 2nd numerical experiment.
Fig. 5-11(a). Seasonal variations of benthic macroalgal biomass, intracellular N:C mass ratio, and phytoplankton concentrations during a 2-year model simulation period.
Fig. 5-11(b). Seasonal variations of DO, DOC, and POC concentrations in the water column during a 2-year model simulation period.
Fig. 5-11(c). Seasonal variations of DIN, DON, and PON concentrations in the water column during a 2-year model simulation period.
Fig. 5-11(d). Seasonal variations of sediment fluxes of NH$_4^+$, COD (chemical oxygen demand in the form of H$_2$S), and SOD during a 2-year model simulation period.
Fig. 5-12. Comparisons between Droop and Monod kinetics in the 3rd box-model experiment.
CHAPTER VI CALIBRATION OF WATER QUALITY MODEL IN THE MARYLAND AND VIRGINIA COASTAL BAYS

VI-1 Introduction

Numerical water quality models have been extensively used for investigating water quality issues in coastal ecosystems (e.g., Cerco and Cole, 1993). However, for shallow coastal ecosystems like the MVCBs, the complicated geometry and highly diverse biogeochemical processes impose many challenges for modeling practices. For example, the tight interconnection between watersheds, individual bays, and the coastal ocean calls for an integrated approach, which includes modeling studies on watershed characterization, hydrodynamics, and water quality processes. Besides, variable grid sizes from as small as 10 m to as large as 1000 m are needed to represent tributaries to ocean boundaries. Lastly, the water quality model should include benthic autotrophs that are indispensable and unique to shallow ecosystems.

Previous water quality modeling studies of the MVCBs treated the system as individual tributaries and bays instead of an interconnected system (Lung, 1994). In addition, the models did not predict the low DO concentrations that are likely to be caused by benthic algae in the system (Tango et al., 2004). As a matter of fact, benthic macroalgae are so abundant in the MVCBs (e.g., Goshorn et al., 2001; McGinty et al., 2004) that they warrant a careful treatment in the water quality models. In this chapter, the previously expanded CE-QUAL-ICM water quality model (Chapter V) was linked to the high-resolution hydrodynamic model (Chapter II) to study the eutrophication dynamics in the MVCBs. The
model was first calibrated against comprehensive field monitoring data collected in the system, and was further used to address those scientific questions proposed in Chapter I.

VI-2 Model setup

As described by Cerco and Cole (1993) and Li (2006), ICM is driven by the physical transport field provided by independent hydrodynamic models such as CH3D and UnTRIM. Therefore, ICM uses the same model grid and physical transport information as the previously calibrated hydrodynamic model. Because detailed description and verification processes of the linkage between ICM and UnTRIM have been provided by Li (2006), this chapter only focuses on the applications of the modeling system to the MVCBs.

VI-2-1 External nutrient loadings

Nutrient loadings for the MVCBs come from a variety of sources, including nonpoint source inputs (e.g., surface runoff, groundwater seepage, and shoreline erosion) from various land uses of the watershed, direct point source discharges, and atmospheric deposition onto the bay water surface. Among all the origins, nonpoint source inputs from the watershed are the most important (Boynton et al., 1996; Wazniak et al., 2004c). It was also estimated that one-half to two-thirds of nutrients entering the bays come from agricultural sources (Bohlen et al., 1997). Similar to many other coastal ecosystems, the MVCBs are believed to be generally limited by nitrogen rather than phosphorus (Boynton et al., 1996).
A watershed model using HSPF (Hydrological Simulation Program - FORTRAN) has been developed for the entire MVCBs by the University of Maryland (Gutierrez-Magness, personal communication, 2008) (Fig. 6-1). The model is under continuous refinement with updated information on the watershed. Thus, the current water quality modeling study used the best available watershed model results to date. Since point sources are heavily regulated in the MCVBs, their estimated contribution of nutrients is very small compared with other sources. For example, Boynton et al. (1996) estimated that point sources of nitrogen represent only 3% of the total loading. In addition, many of these point sources are located in the upper portions of the watershed and discharge into nontidal streams. Hence, their impact on tidal portions of the MCVBs could be much alleviated, because they may have been consumed partially in the nontidal streams. However, if the current water quality model is to be used for TMDL studies, the contribution of point sources has to be carefully considered. Fig. 6-2 summarizes the annual nonpoint source loading rates for the entire MCVBs as provided by the watershed model. The atmospheric loading rates for nitrogen are fairly similar (the difference is less than 10%) to those estimated by Boynton et al. (1996). Direct atmospheric deposition of nutrients onto the bay water surface is another important source for the MCVBs. The loading rates for nitrogen and phosphorus were determined as 3.54 kg N km\(^{-2}\) day\(^{-1}\) and 0.22 kg P km\(^{-2}\) day\(^{-1}\) respectively, based on published literature values for the mid-Atlantic region (Norton et al., 2000; Castro et al., 2001).

VI-2-2 Initial conditions

For short-term simulations, it is crucial to start the model with a set of reasonable and accurate initial conditions for both the water column and sediment. However, for complicated
systems like the MVCBs, it is extremely difficult to specify spatially variable initial conditions for all the model grid cells on the basis of observational data. As discussed in previous chapters, the MDNR’s monitoring program has a broad coverage in the MVCBs. However, considering the high resolution of the model grid, the MDNR’s monthly water quality monitoring data are too coarse to generate a spatially variable initial condition for the entire system. Because of the relatively longer time scales involved in kinetic processes occurring in benthic sediments, the effects of initial conditions in the sediment diagenesis model persist even longer for sediment state variables than for water column state variables. In theory, the initial conditions should reflect the past history of the depositional fluxes as well as the overlying water column conditions (Liu, 2002). However, in reality, no such data are available throughout the model domain.

The watershed model generates freshwater flow and nutrient loadings from January 1998 through August 2005. They have been compared to available USGS gauge data using the automatic calibration tool PEST (Parameter Estimation with HSPF). This is a new technology that has a great potential to eliminate the trial-and-error procedure of tuning the parameter. A comparison between modeled and measured flows is shown in Fig. 6-3. As suggested by DiToro and Fitzpatrick (1993), initial conditions for the sediments can be obtained by repeatedly running the model under historical loading conditions until the model reaches a dynamic steady state. Hence, in this study, this strategy was used to generate the initial conditions for both the water column and sediments with given nutrient loadings during 1998 – 2003. The final concentration field at the end of 2003 was used as the initial condition for the calibration year of 2004 when observational solar radiation data became
available for the MVCBs. The solar radiation data were provided by the National Park Service at the Assateague Island National Seashore weather station.

For the benthic macroalgal module, the initial distribution of macroalgal biomass was specified for individual grid cells on the basis of field observations. Specifically, the macroalgal survey data collected during 1998 – 1999 (Goshorn et al., 2001) were used as the guideline for model initialization. However, the occurrence of benthic macroalgae in the MVCBs is highly variable along both temporal and spatial scales. There is also the issue of patchiness. It is the hope that, after many repeated runs, the model results should be close to the temporal and spatial variability with the given set of initial conditions through self-adjustment. Fig. 6-4 shows the spatial distribution of benthic macroalgae at the end of 2003. As can be seen, benthic macroalgae mainly occur in shallow areas characterized by high availability of light.

VI-2-3 Boundary conditions

Since the model grid extends out into the coastal ocean, there are no regular field observational data available at the open boundary. However, because water quality inside the MVCBs is mainly controlled by nutrient loadings from the watershed, the incorporation of a substantial area of the coastal ocean as part of the model domain not only can incorporate bay-ocean exchange processes, but also reasonably assures a long-term average value for the open boundary conditions without a detailed prescription in time. For instance, as can be seen from the salinity calibration results in Chapter II, a constant salinity boundary condition of 33 ppt is sufficient for a reasonable comparison between model predictions and field
observations. Therefore, the open boundary conditions for water quality variables were specified using all available long-term averaged monitoring data in the coastal ocean (Dr. Anderson, personal communication). In addition, the seasonality was derived from the MDNR’s monthly observational data at the two stations (Stations 21 and 28 in Fig. 4-1) closest to the Ocean.

VI-2-4 Parameter determination

A typical set of model parameters, which originated from the Chesapeake Bay Eutrophication Model (Cerco and Noel, 2002) and was later adopted by Li (2006) for the Lynnhaven Bay, was initially used for model setup. Most of these kinetic parameters were used without any modification except a few, which were further adjusted during model calibration. Specifically, the surface reaeration rate, \( k_r \), was modified from function of wind speed, temperature, and salinity (as ICM’s default formulation) to include a higher surface reaeration rate during the supersaturation condition (e.g., Merlivat and Memery, 1983; Farmer et al., 1993; McNeil et al., 2006; Marks, 2008), the following equation was used to calculate \( k_r \) under the super-saturation conditions:

\[
  k_{rs} = k_{r0} \times \left( \frac{DO}{DO_s} \right)^2 \quad \text{when } DO > DO_s \quad (6-1) 
\]

where \( k_{rs} \) = surface reaeration rate under supersaturation, m d\(^{-1}\); \( k_{r0} \) = default surface reaeration rate calculated by the model, m d\(^{-1}\); \( DO \) = dissolved oxygen concentration in the water column, mg L\(^{-1}\); \( DO_s \) = DO saturation concentration, mg L\(^{-1}\). Regarding to the parameters used for the benthic macroalgal module that was newly developed in this study,

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1 In Table V-3 (Li, 2006), the value of \( TM_d \) was changed from 16 to 20 based on Park et al. (1995); the value of \( W_{S_d} \) was changed from 0.2 to 0.35 based on Park et al. (1995). In Table V-8 (Li, 2006), \( K_{RDO} \) was not a constant in this study.
the values from the literature were used and finalized through subsequent model calibration. The final parameter values are listed in Tables 5-2 and 5-3.

VI-3 Results of benthic macroalgae simulation

The benthic macroalgal module was activated throughout the water quality model calibration process. The model predicted benthic macroalgal distribution along both temporal and spatial scales for the calibration year of 2004 is summarized in this section.

VI-3-1 Turville Creek – Isle of Wight Bay profile

The model predicted spatial distribution of the maximum benthic macroalgal biomass (more specifically, the biomass for *Gracilaria vermiculophylla*, the dominant species in this region) along the transect of Turville Creek – Isle of Wight Bay, and this distribution is compared with MDNR’s field survey results (Fig. 6-5). The MDNR’s spatial distribution map was generated based on a series of intensive surveys during 1998 – 1999 (Goshorn et al., 2001). Whereas benthic macroalgae are extremely variable both temporally and spatially, their general patterns should not change significantly in the system. Furthermore, this is the only dataset that contains information on the spatial distribution of benthic macroalgae in the MVCBs. Hence, it was adopted here to evaluate model performance. The comparison was made using 1998 – 1999 observation data against the model simulation in 2004.

As one can see from Fig. 6-5, there is an overall good agreement in the spatial pattern between model prediction and field survey. Both the model prediction and field survey
suggest that *Gracilaria vermiculophylla* is most abundant in the shallow areas, e.g., along the shorelines and in the shallow tributaries. In contrast, in the central area of Isle of Wight Bay and around the Ocean City Inlet, *Gracilaria vermiculophylla* is almost absent. This indicates that light availability is important in determining the establishment and subsequent accumulation of *Gracilaria vermiculophylla* in the MVCBs. In addition, the model successfully captures several hot spots in the field survey map, i.e., those sites where the maximum *Gracilaria* biomass exceeds 100 g/L (Fig. 6-5).

Three macroalgal survey stations by Hardison (2009) (Stations M-1, M-2, and M-3 in Fig. 4-2 of Chapter IV), are overlaid on the model predicted *Gracilaria vermiculophylla* distribution map as well (Fig. 6-5). Interestingly, all the stations fall into the grid cells with abundant benthic macroalgae. In addition, the model predicted temporal variations of the two benthic macroalgal species, *Gracilaria vermiculophylla* and *Ulva lactuca*, as modeled by the benthic macroalgal module, are presented in Fig. 6-6(a). Meanwhile, the corresponding water column profiles of phytoplankton (represented by chlorophyll a) and DO are given in Fig. 6-6(b). As one can see from Fig. 6-6(a), both macroalgal biomass and intracellular N:C ratio exhibits strong seasonality at all three stations. For instance, *Gracilaria vermiculophylla* and *Ulva lactuca* both peak in late spring (May) and dieback in summer. This should be controlled by temperature and nutrient (especially N) availability, as reflected in corresponding intracellular N:C profiles (Fig. 6-6(a)). With increasing water temperature and high nutrient availability from early spring, macroalgae start to grow and accumulate at all stations. As nitrogen becomes limiting in the water column, macroalgae manage to grow using internal N. However, with continuously decreasing N availability in both the water column and
macroalgal tissue, macroalgal growth is eventually limited by N. Meanwhile, high temperature increases the loss rate through respiration, grazing, and mortality, which subsequently reduce macroalgal biomass in summer. Consequently, the combination of decreasing growth and increasing loss leads to a temporal increase of the internal N content in late summer. In the fall, macroalgae start to recover from the summer biomass decrease as temperature drops. When temperature becomes low enough to inhibit growth, the macroalgal biomass gradually decreases. Meanwhile, the intracellular N:C ratio increases, resulting from decreasing macroalgal growth and increasing nutrient availability in the water column. In addition, *Gracilaria vermiculophylla* dominate *Ulva lactuca* at all three stations. This is consistent with the few field observations available (e.g., Goshorn et al., 2001; McGinty et al., 2004).

In comparison, phytoplankton (represented by chlorophyll \(a\)) shows a different seasonal pattern from that of benthic macroalgae (Fig. 6-6(b)). For instance, chlorophyll \(a\) levels reach annual maxima in late summer immediately following the summer decline of benthic macroalgae. In addition, water column DO exhibits strong diurnal oscillations (Fig. 6-6(b)) at all three stations. Transient hypoxia (DO < 5 mg L\(^{-1}\)), which normally lasts for several hours at night, can be readily seen at the two stations located in Turville Creek (Stations M-1 and M-2). Apparently, they are largely controlled by macroalgal activities. However, hypoxia is rarely seen at Station M-3, which is close to Ocean City Inlet. Obviously, a better flushing capability at Station M-3 accounts for much of the spatial variability.
VI-3-2 Bay-wide benthic macroalgal distributions

The model predicted bay-wide macroalgal characteristics are summarized in Fig. 6-7(a-d). The spatial distribution maps cover the typical seasonal cycle of benthic macroalgae as demonstrated in Fig. 6-6(a). More specifically, the maps span four major temporal stages: A – initial condition at the beginning of 2004; B – annual abundance in May; C – summer decline; and D – final condition at the end of 2004. The results clearly indicate that benthic macroalgae are extremely variable in time and space.

As one can easily see, benthic macroalgae are mostly distributed in the shallow regions with favorable light availability. They rarely exist in the deep channels and the middle portions of the MVCBs (e.g., central Chincoteague Bay), where water depths are generally greater than 1.5 m. In addition to aforementioned regions of Turville Creek and Isle of Wight Bay, the model predicts that benthic macroalgae can extensively occur along the east side (ocean side of the MVCBs) of the Bays. As a matter of fact, these regions are also the prior sites for seagrass (Orth et al., 2006). Obviously, if the sites are good for seagrass, they are likely to be suitable for benthic macroalgal establishment as well.

Besides the effect of light, the availability of nutrients (especially N) also plays a role in determining the spatial variability of benthic macroalgae. In general, as far as the light condition has been satisfied, high nutrient availability normally results in a high density of benthic macroalgal biomass. As can be seen from Fig. 6-7(a, c), the abundant macroalgae sites are mostly located in nutrient-enriched northern bays, e.g., Turville Creek and Isle of Wight Bay. In Chincoteague Bay, nutrients are generally more abundant on the west side
(land side) than the east side (ocean side). This type of nutrient gradient is also reflected in the spatial maps of intracellular N:C ratios (Fig. 6-7 (b and d)). The model results may suggest that, in order to maintain high biomass under a nutrient-limited environment (e.g., east side), benthic macroalgae manage to grow using a smaller amount of nitrogen than that needed in a nutrient-enriched environment (e.g., west side).

Similar seasonal patterns were also found at three macroalgal survey stations by Hardison (2009) in the northern bay (Fig. 6-7). Throughout the system, benthic macroalgae proliferate in May and decline in summer. As expected, internal N:C ratios exhibited an opposite temporal pattern from that of biomass.

VI-4 Results of water quality model calibration

For the full calibration of ICM, the year of 2004 was selected as the calibration period in this study, because it is the only year that has a complete set of model input for both nutrient loadings and solar radiation (Wazniak et al., personal communication). The model results of major water quality variables were subsequently compared with MDNR’s field monitoring data inside the MVCBs. Unfortunately, for benthic macroalgae, there are no survey data available in 2004 to simultaneously compare with model predictions (the earliest benthic macroalgal survey data collection started from 2006).
The model predicted water quality variables in 2004 for the five stations along the transect of Turville Creek – Isle of Wight Bay (Stations 2-6 in Fig. 4-2) are compared against MDNR monthly observations (Fig. 6-8). Station 1 is not included here due to its position in the nontidal headwaters (and thus it is not included in the water quality model grid). These stations are selected for comparison because they are located in the areas characterized with abundant benthic macroalgae (Goshorn et al., 2001; McGinty et al., 2004). In addition, there are macroalgal biomass survey data available in 2006 collected by Hardison (2009) along the Turville Creek – Isle of Wight Bay transect (Figs. 4-2 and 5-6). The 2006 macroalgal data are qualitatively compared with model predictions in 2004; they provide guiding information (e.g., magnitude and seasonality of macroalgal biomass) for calibrating the benthic macroalgal module.

Overall, the model results agree very well with observational data for most stations presented in Fig. 6-8. For example, in Fig. 6-8(a), the model captures both temporal and spatial features of chlorophyll a along the transect of Turville Creek – Isle of Wight Bay. As shown in Chapter IV (Fig. 4-6(a)), chlorophyll a exhibits a strong longitudinal gradient from Station 2 to Station 6. The same spatial variability can be clearly seen from the model results (Fig. 6-8(a)), e.g., chlorophyll a decreases from ~ 40 µg L\(^{-1}\) at Station 2 (upper Turville Creek) to less than 10 µg L\(^{-1}\) at Station 6 (lower Isle of Wight Bay). The model also captures the seasonality well. For instance, at Station 2, the chlorophyll a levels remain low in winter and reach maximum in late summer. This general pattern has been well reproduced in the model. Additionally, the model also catches the spring phytoplankton bloom event around
Day 110, when chlorophyll $a$ suddenly jumps above 40 µg L$^{-1}$. As expected, the same event has been recorded at MDNR's continuous monitoring site (Figs. 4-2 and 4-7(b)) as well. This phytoplankton bloom event should be fueled by a large freshwater pulse (Fig. 2-4), the effect of which can also be seen from the sharp salinity drop shown in Fig. 4-7(a).

Dissolved oxygen is a water quality variable warranting special attention. The comparisons also indicate that the model is capable of simulating the temporal and spatial variability of DO. As discussed in Chapter IV, DO meets the water quality standard of 5 mg L$^{-1}$ in most areas along the Turville Creek – Isle of Wight Bay transect. However, transient, diurnal (~hours) hypoxia and episodic, prolonged (~days) low DO events can occur in upper portions, as driven by high respiration and decomposition. This general pattern has been well described by the model. First, the model results exhibit substantial high-frequency oscillations at Stations 2 and 3 (Fig. 6-8(b)), especially in warm months. As expected, diurnal hypoxia occurs concurrently with DO diurnal swings. Second, the model is capable of capturing several episodic hypoxic events. For example, at Station 2, the monitoring data reveal a DO drop around Day 210. This event is also reasonably captured by the model. Lastly, along with field measurements, the model results reasonably reflect DO seasonality (i.e., daily mean DO follows the seasonal trend of temperature) and the longitudinal gradient (e.g., low DO rarely occurs at Stations 4-6 closer to the Ocean City Inlet).

In terms of simulating major nutrient variables, the model also performs satisfactorily in general. First of all, the model captures the typical seasonality of nutrients in the system. For instance, NO$_3^-$, the most important land-originated N source for most coastal ecosystems,
has a distinct seasonal pattern that normally becomes abundant in winter-spring (due to watershed inputs) and depleted in summer (due to rapid uptake by autotrophs, etc.). This temporal variability is well produced by the model (Fig. 6-8(d)). While NH$_4^+$, which mainly relies on in situ recycling/regeneration processes in both the sediment and water column, often exhibits typical summer-fall abundance (e.g., Fig. 4-6(a) in Chapter IV). The model successfully captures this temporal trend (Fig. 6-8(c)). For PO$_4^{3-}$, which shows seasonality somewhat similar to that of NH$_4^+$ (Fig. 4-6(b) in Chapter IV), this parameter might be potentially more dominated by the remineralization processes (especially in the sediment) in addition to watershed sources. The model’s performance is still acceptable. Lastly, dissolved organic nutrients (e.g., DON and DOP), are heavily regulated by the balance between in situ production (source) and decomposition (sink) processes. However, due to the relatively slow rates associated with the decomposition processes, DON and DOP are capable of maintaining more stable and abundant levels than inorganic nutrients in both temporal and spatial scales. This is partially reflected in Fig. 4-7(d) of Chapter IV. As one can easily see from Fig. 6-8(f-g), both DON and DOP do not exhibit substantial variations (e.g., over several orders of magnitude) in either temporal (seasonal) or spatial (at difference stations) scales. However, there does exist a clear seasonal trend (i.e., both DON and DOP show abundance in warmer months, presumably fueled by high primary production and respiration in the system). The model results agree well with field observations.

To summarize, the model is capable of capturing both the temporal and spatial variability of major water quality variables along the transect of Turville Creek – Isle of Wight Bay. Due to the lack of macroalgal survey data for directly calibrating the benthic
macroalgal module, a good agreement between model predictions and field observations could serve as an alternative to justify that the model can perform well with the addition of a benthic macroalgal module.

VI-4-2 Bay-wide comparisons

To ensure the model also has the capability of capturing bay-wide water quality distributions, the calibration results for an additional five stations throughout the MVCBs (Stations A-E in Fig. 6-9) are presented in Fig. 6-10. These stations span broad areas of the MVCBs, including Assawoman Bay, St. Martin River, and Chincoteague Bay. Due to the huge spatial variability (e.g., watershed characteristics, as well as physical and biological properties of individual bays) across the MVCBs, it is especially challenging for a water quality model to characterize the system-wide water quality properties within the same framework.

In general, the model’s performance is encouraging. For example, the model results capture the spatial variability of chlorophyll $a$ very well (Fig. 6-10(a)), e.g., chlorophyll $a$ is generally more abundant in the northern bays (Stations A and B) than in the southern bays (Stations C, D, and E), largely determined by spatially varying nutrient loading rates. In addition, there is also an apparent longitudinal gradient along the axis of Stations C, D, and E in Chincoteague Bay. Similar to the water quality gradient observed along the transect of Turville Creek – Isle of Wight Bay in the northern bays, this type of chlorophyll $a$ gradient must be controlled by both nutrient loadings (which mostly discharge into the upper bays) and spatially varying flushing properties (e.g., local residence time distribution in Chapter
However, a closer look at the comparisons between predicted and observed chlorophyll $a$ suggests that the model frequently misses the episodic high/low chlorophyll $a$ measurements, e.g., the chlorophyll $a$ maxima around Day 205 at Stations B and C (Fig. 6-10(a)). Similar mismatches also can be found for other water quality variables, e.g., DO, NH$_4^+$, and NO$_3^-$. In reality, these episodic events can potentially be triggered by a combination of many factors, such as meteorological forcing and watershed inputs. For example, within a very short period of time, a heavy storm can discharge a large amount of nutrients into the bay through both watershed runoff and direct wet atmospheric deposition. In addition, high winds associated with the storm event not only mix the water column but also resuspend nutrients and particulates into the water from the sediment. Consequently, a sharp increase in water column nutrients is expected following a storm event. Elevated nutrient levels can subsequently stimulate an algal bloom under clear conditions, which further raises DO in the daytime. Besides, many other biotic factors (e.g., crash of algal blooms) can further complicate the problem. Hence, due to the uncertainty associated with model inputs (e.g., meteorological forcing, watershed loadings, and open boundary conditions), it is often more important to focus on the general patterns. Based on the comparisons (Fig. 6-10(a-g)), it is fair to conclude that the model has reasonably captured the basic water quality characteristics for stations shown in Fig. 6-9.

Additionally, as can be seen from Fig. 6-10, most time series of water quality variables show a somewhat reduced amplitude of short-term (~hours) fluctuations at Stations C, D, and E in Chincoteague Bay, as compared to those at Stations A and B, which are located in Assawoman Bay and the St. Martin River, respectively (Fig. 6-9). These
short-term fluctuations consist of two major frequencies, i.e., diurnal and semi-diurnal, corresponding to the daily light cycle and the semi-diurnal tidal cycle, respectively. If the station is located in an area characterized by high productivity, strong diurnal oscillations are expected to occur for its water quality variables. On the other hand, for stations located inside the bays that are characterized by small tidal amplitudes, its water quality variables will not exhibit strong tidal signals. In summary, the combination of both biological activities (e.g., diurnal cycle of autotrophs as regulated by daily light cycle) and physical forcing (tides) controls the short-term fluctuations. Stations A and B are located in the northern bays characterized by high productivity and relatively strong tides; thus, the water quality variables demonstrate pronounced fluctuations. In contrast, for Stations C, D, and E, they are characterized either by extremely weak tidal signals and high productivity (Station C), or by weak tides and reduced productivity (Station D), or by increased tidal impact and extremely low productivity (Station E). As a result, these three stations show dampened short-term fluctuations in general.
Fig. 6-1. Map showing watershed model configurations and the linkage between watershed and the hydrodynamic model grid. The raw ArcView shape files of outfalls, streams, and watershed were provided by Dr. Angelica Gutierrez-Magness (UMD).
Fig. 6-2. Total annual nonpoint source loading rates calculated by the watershed model for the entire MVCBs (top panel – total nitrogen; bottom panel – total phosphorus). The raw data were provided by Dr. Angelica Gutierrez-Magness (UMD).
Fig. 6-3: A comparison between HSPF predicted daily flow vs. USGS measurements (top panel – USGS1148471320; bottom panel - USGS01484719. See Fig. 2-3 for station locations). The model results were provided by Dr. Angelica Gutierrez-Magness (UMD).
Fig. 6-4. The spatial pattern comparisons between model predicted benthic macroalgal distribution at the end of 2003 (green color denotes the occurrence of benthic macroalgae) vs. MDNR field survey data (McGinty et al., 2004).
Fig. 6-5. A spatial pattern comparison between MDNR survey data (left panel, McGinty et al, 2004) and model predicted maximum Gracilaria biomass (right panel, unit in g C m$^{-2}$) in Turville Creek and Isle of Wight Bay.
Fig. 6-6(a). Model predicted temporal variations of benthic macroalgal biomass and intracellular N:C mass ratio at three macroalgal survey stations in Fig. 6-9.
Fig. 6-6(b). Model predicted temporal variations of water column chlorophyll a and DO at three macroalgal survey stations in Fig. 6-9.
Fig. 6-7(a). Model predicted seasonal (2004) variations of Ulva lactuca biomass (unit: g C m$^2$) in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution).
Fig. 6-7(b). Model predicted seasonal (2004) variations of Ulva lactuca intracellular N:C mass ratio in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution).
Fig. 6-7(c). Model predicted seasonal (2004) variations of Gracilaria vermiculophylla biomass (unit: g C m$^{-2}$) in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution).
Fig. 6-7(d). Model predicted seasonal (2004) variations of Gracilaria vermiculophylla intracellular N:C mass ratio in the MVCBs (A – initial distribution; B – bloom in May; C – dieback in August; D – final distribution).
Fig. 6-8(a). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV). All the filed data were collected by MDNR.
Fig. 6-8(b). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV).
Fig. 6-8(c). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV).
Fig. 6-8(d). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV).
Fig. 6-8(e). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV).
Fig. 6-8(f). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV).
Fig. 6-8(g). Water quality model calibration – comparisons between model predictions and field observations. Stations IDs correspond to those shown in Fig. 4-2 (Chapter IV).
Fig. 6-9. Map showing additional water quality model calibration stations in the MVCBs.
Fig. 6-10(a). Water quality model calibration for selected stations in the MVCBs (Fig. 6-3) – comparisons between model predictions and field observations.
Fig. 6-10(b). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions and field observations.
Fig. 6-10(c). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions and field observations.
Fig. 6-10(d). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions and field observations.
Fig. 6-10(e). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions and field observations.
Fig. 6-10(f). Water quality model calibration for selected stations in the MVCBs – comparisons between model predictions and field observations.
Fig. 6-10(g). Water quality model calibration for selected stations in the MVCBs.
CHAPTER VII THE EFFECT OF MACROALGAE ON EUTROPHICATION DYNAMICS

In the last chapter, a water quality model with a newly developed benthic macroalgal module applied to the entire MVCBs was discussed. The model calibration results suggest that the model is capable of simulating the general water quality characteristics of the entire system well. In addition, the model also successfully captured both the temporal and spatial patterns of benthic macroalgae in the system. The unique role played by benthic macroalgae has also been discussed. In this chapter, the role of macroalgae is further investigated: Section VII-1 describes species interactions with the focus on phytoplankton dynamics in the presence of macroalgae. Section VII-2 discusses the nutrient dynamics in the presence of benthic macroalgae and Section VII-3 describes the role of benthic macroalgae on enhancing diurnal oscillations of dissolved oxygen.

VII-1 Species interaction and phytoplankton dynamics in the presence of benthic macroalgae

Two common species of macroalgae, Gracilaria vermiculophylla and Ulva lactuca, were included in the model. The model results indicate that Gracilaria vermiculophylla generally outcompete Ulva lactuca in the system (Figs. 6-6(a) and 6-7). This general pattern also agrees well with field observations (Goshorn et al., 2001; McGinty et al., 2004). This may be explained by two major mechanisms. First, Ulva lactuca tends to have higher half-saturation constants for nutrients (Ks) than Gracilaria vermiculophylla (e.g., laboratory studies conducted by Gownaris and Brush (2008)) and thus prefers a nutrient-enriched environment. Hence, the environment conditions of the MVCBs
normally favor *Gracilaria vermiculophylla* over *Ulva lactuca*. Second, *Gracilaria vermiculophylla* can tolerate a wide range of temperatures (e.g., Freshwater et al., 2006). This has been also observed in our recent laboratory studies. For example, *Gracilaria vermiculophylla* can survive and even manage to grow under 35 °C during a 12-day incubation period. The robustness of *Gracilaria vermiculophylla* makes it more adaptable to the MVCBs in which water temperature varies from ~0 – 35 °C within an annual cycle.

In the current benthic macroalgal module, *Ulva lactuca* can be thought to represent a more ephemeral, fast-growing, and nutrient-responsive species in the MVCBs. In comparison, *Gracilaria vermiculophylla* represents a more slow-growing and stable species. Hence, their relative abundance as predicted by the model may reflect the nutrient conditions in the MVCBs. The overall dominance of *Gracilaria vermiculophylla* over *Ulva lactuca* indicates that nutrients are still the major limiting factor for algal growth. In fact, the same pattern has been observed in Hog Island, VA, where *Gracilaria vermiculophylla* is the most abundant (constitutes 74% of the total macroalgal biomass) species in all seasons and locations (Thomsen et al., 2006).

The interactions between phytoplankton and macroalgae are of particular interest in this study. Apparently, at hot spots of benthic macroalgae, e.g., Turville Creek and Isle of Wight Bay, benthic macroalgae show an exclusive dominance over phytoplankton. This dominance can be easily seen from a comparison of the relative abundance of phytoplankton vs. macroalgal carbon in the MVCBs. For example, chlorophyll *a* levels generally range from 10 to 50 μg L⁻¹ in most areas, except the very upstream sites (e.g.,
field data presented in Chapter IV), which corresponds to <3 mg C L\(^{-1}\) in terms of carbon (assuming the mass ratio between carbon and chlorophyll \(a\) equals 60, Park et al., 1995).

In contrast, the benthic macroalgal biomass ranges from 10 – 100 g C m\(^{-2}\), which is equivalent to 10 – 100 mg C L\(^{-1}\), assuming a 1-m water depth. Throughout the MVCBs, the standing stock of benthic macroalgae is within the range of \(1 \times 10^6 - 5 \times 10^6\) kg C (Fig. 7-1). In comparison, the maximum standing stock of phytoplankton is about \(1 \times 10^6\) kg C as calculated by the model. Thus, from the entire bay perspective, benthic macroalgae maintain a substantially higher biomass than phytoplankton.

As hypothesized by Valiela et al. (1997), phytoplankton tends to outcompete benthic macroalgae in systems characterized by both high nutrient availability and long residence time. In the model, benthic macroalgae are forced to stay at the sediment surface and are subjected to light limitation due to both water depth and the shading effect resulting from water column substances. Therefore, phytoplankton has the advantage over benthic macroalgae concerning light availability. For instance, benthic macroalgal biomass is generally very low in the main stem of the St. Martin River (Fig. 6-9), consistent with field surveys (McGinty et al., 2004). High nutrient availability, long residence time, and relatively deep water depths favor the growth of phytoplankton, which may subsequently shade out benthic macroalgae. Interestingly, Turville Creek, receives smaller amounts of nutrient loading, and yet is one of the hot spots for benthic macroalgae. It is suspected that the combination of a shorter flushing time and the shallower water depths in Turville Creek may account for the difference.
Species interactions were further investigated through model sensitivity runs. The results for the first sensitivity run are presented in Fig. 7-2. Basically, this run was conducted by turning off the benthic macroalgal module ("No MA" in Fig. 7-2). Thus, similar to deep waters, only phytoplankton were activated in the model. As one can see from Fig. 7-2, benthic macroalgae are efficient in suppressing the spring phytoplankton bloom. When benthic macroalgae are present (base scenario “with MA”), water column chlorophyll $a$ concentrations are reduced substantially at all three macroalgae survey stations, as compared with those in the sensitivity run. Specifically, the phytoplankton blooms in spring and fall are largely inhibited in the presence of benthic macroalgae. This type of species interaction is more remarkable at Stations M-1 and M-2, both located in nutrient-enriched Turville Creek. It basically suggests that actively growing benthic macroalgae can modify the phytoplankton seasonal cycle by competing for nutrients. In turn, phytoplankton may contribute to summer decline of benthic macroalgae by shading them out. However, this effect has not been confirmed in this study.

As mentioned earlier, benthic microalgae are reported to be abundant in the MVCBs, especially in areas characterized with high light availability, such as Isle of Wight Bay and Sinepuxent Bay (Wazniak, 2004). Besides, previous studies also suggest that benthic microalgae are extremely effective in intercepting the sediment N flux (e.g., Anderson et al., 2003; Tyler et al., 2003) because of their location within the surface sediment. In addition, benthic microalgal biomass tends to be more stable than both phytoplankton and benthic macroalgae (Anderson et al., in review). Thus, on an annual basis, benthic microalgae can be more important than benthic macroalgae and
phytoplankton in certain areas. The second model sensitivity run was designed to test the possible effects contributed by benthic microalgae. The model results are given in Fig. 7-3. Compared to the base scenario (Fig. 6-6), the existence of benthic microalgae greatly suppresses the biomass of both benthic macroalgae and phytoplankton. Moreover, as reflected in persistently low benthic macroalgae internal N:C ratios, water column inorganic N species could be nearly depleted throughout the warm months. Apparently, the incorporation of benthic microalgae can further complicate species interactions. However, this is beyond the scope of this dissertation and will not be further addressed here.

VII-2 Nutrient dynamics in the presence of benthic macroalgae

Previous studies suggested that benthic macroalgae are extremely effective in retaining nutrients within their body due to high standing stock of the biomass and the “luxury uptake” capability (Sfriso et al., 1989; Valiela et al., 1997; Tyler, 2002). Based on the model simulation results in 2004, the amount of N stored by benthic macroalgae in the entire MVCBs is given in Fig. 7-1. Similar to biomass, the stored N by benthic macroalgae also exhibits strong seasonality with lowest N levels in summer. Compared to the annual nonpoint source N loading rate (Fig. 6-2), benthic macroalgae retained roughly 10% of the total annual loading in 2004. The number, however, is significantly lower than those reported for other shallow ecosystems. For instance, in the central Venice Lagoon, it was estimated that, in spring-summer, macroalgae recycled 78–104% of the total annual nitrogen which entered the central lagoon (Sfriso et al., 1989). Valiela et al. (1997) also reported that, in Waquoit Bay, the N stored by macroalgae was approximately
of the same magnitude as the annual N loading from the watershed. It is suspected that phytoplankton may play a more important role in regulating N cycling in the system. The longer residence time in the MVCBs (especially in nutrient-enriched tributaries such as the St. Martin River and Newport River/Bay) favors the growth of phytoplankton species, which have a higher N:C ratio than macroalgae and thereby could remove the majority of inorganic nitrogen before it can reach benthic macroalgae. As estimated in Chapter III, the residence time in the MVCBs is on the order of months in regions receiving direct watershed loadings. In contrast, residence times in Waquoit Bay and Venice Lagoon are much shorter, and are on the order of several days (Valiela et al., 1997) and less than 10 days (Svensson et al., 2000), respectively. Hence, although phytoplankton maintain a much smaller standing crop than that of benthic macroalgae, they may be more important in removing inorganic N from the water column in nutrient-enriched regions, where benthic macroalgae are normally restricted by poor light availability.

In environments when benthic microalgae are also present, they could be another important N sink. Benthic microalgae have been shown to play a crucial role in regulating nutrient cycling in shallow lagoons (e.g., Anderson et al., 2003). Furthermore, they can effectively inhibit phytoplankton abundance by intercepting nutrient flux at the sediment-water interface (Fong et al., 1993). In their eutrophication modeling studies, Cerco and Seitzinger (1997) and Li (2006) both demonstrated that benthic microalgae had a major influence in the intra-annual cycling of nitrogen and phosphorus, especially in late winter and spring. In fact, their findings have been further examined in this study. As can be seen in the water quality model calibration results for NO\textsubscript{3} (Figs. 6-4(d) and
6-6(d)), the model severely overestimates NO$_3^-$ water column concentrations in late spring and early spring, when benthic macroalgae and phytoplankton are both inhibited by cold temperature. In contrast, benthic microalgae are found to be active throughout the year (Anderson et al., in review); thus, their effect in removing water column NO$_3^-$ can be especially significant in winter/spring but also fall. Because the water quality model was calibrated without the presence of benthic microalgae, as expected, it over predicts NO$_3^-$ concentrations in the water column. In the sensitivity run in which benthic microalgae are activated as well, the model prediction is substantially improved (results not shown). Hence, it is reasonable to conclude that, in the MVCBs, benthic microalgae can be another important sink for N, especially in winter, spring, and fall.

The model results also suggest that benthic macroalgae can generally increase the heterotrophy of sediments by providing more organic carbon to the sediment. As one can see from Fig. 7-4, benthic macroalgae slightly increase sediment oxygen demand (SOD) at all three stations. Rather strikingly, benthic macroalgae substantially enhances the sediment chemical oxygen demand (COD), which is directly released as H$_2$S from the sediment. Apparently, this is largely due to the hypoxic effect induced by the high respiration rate within the macroalgal mat (Fig. 7-2). As a well-known fact, H$_2$S is toxic to most aquatic organisms (e.g., seagrass, Koch et al., 1990; Erskine and Koch, 2000). Thus, an elevated H$_2$S level in the system may have more ecosystem-level consequences, such as initializing the crash of seagrass or even benthic macroalgae themselves. Additionally, the model does capture a characteristic summer crash of benthic macroalgae in 2003 (Fig. 7-5).
VII-3 The role of benthic macroalgae on enhancing diurnal oscillation of dissolved oxygen

Benthic macroalgae are effective in controlling ecosystem metabolism and thus affect the oxygen dynamics. The characteristic large DO swings that have been widely recorded in systems dominated by benthic macroalgae are the most striking feature indicating the importance of benthic macroalgae in controlling ecosystem metabolism (e.g., D'Avanzo and Kremer, 1994). The contribution of benthic macroalgae to enhanced ecosystem metabolism in the MVCBs has been demonstrated in Fig. 7-2. As one can see in Fig. 7-2, the occurrence of benthic macroalgae greatly enhances the diurnal fluctuations of DO in the water column. The amplitude of diurnal DO swings is positively correlated with the magnitude of macroalgal biomass. In a sensitivity run without benthic macroalgae, the effect of phytoplankton on DO was significant only at its most abundant site (Station M-1). However, in the base scenario when macroalgae and phytoplankton were both present in the system, the individual contribution of phytoplankton could be further reduced, simply due to the fact that benthic macroalgae can substantially suppress phytoplankton biomass (Fig. 7-2).

The incorporation of a benthic macroalgal module into ICM can improve its predictive capability in simulating oxygen dynamics in shallow coastal systems. The model results demonstrate that, with the presence of benthic macroalgae, there are now enhanced DO diurnal oscillations. In warmer months, transient (~hours) hypoxia occurs concurrently with strong diurnal DO swings (Stations M-1 and M-2 in Fig. 7-2). As
revealed by MDNR’s monitoring data, episodic low DO events and transient hypoxia can both occur in the system (e.g., Figs. 4-5(b) and 4-7(b)). However, previous water quality modeling studies failed to predict the low DO events that were potentially controlled by benthic autotrophs other than phytoplankton (Tango et al., 2004). From a numerical modeling point of view, one of the keys for successfully simulating diurnal oxygen oscillation in the natural environment is the recognition of large amounts of oxygen were created by intense photosynthesis of autotrophs (macroalgae) during daytime. The oxygen, once generated, can transport through the water column to the surface to form a super-saturation condition near the air-water interface. The reaeration coefficient used under super-saturation condition is known to be different from that in the normal condition (Logan, 1999); a higher reaeration value based on function relationship was used during the supersaturation condition (see equation 6-1 in Chapter VI). As a result, there is more leakage of oxygen from the water into the air under super-saturation conditions during daytime. Consequently, less oxygen is left in the water column such that low DO can occur at night resulting from high respiration and decomposition. The sensitivity test indicates that with proper adjustment of the reaeration coefficient under super-saturation, the DO diel oscillations was better simulated (Fig. 7-6). Without considering the super-saturation condition on surface reaeration rates (“default $k_r$” in Fig. 7-6), the model seems to over-predict DO concentrations especially at Stations M-1 and M-2. In contract, by including the effects super-saturation of oxygen on surface reaeration rates (“increased $k_r$” in Fig. 7-6), the model results are much more reasonable. Therefore, physical process at the air-water combined with macroalgae’s intense photosynthesis and respiration play an important role in shallow water oxygen dynamics.
Fig. 7-1. Model estimated temporal (2004) variations of total benthic macroalgal biomass (top panel) and intracellular nitrogen (bottom panel) retained by benthic macroalgae in the entire MVCBs.
Fig. 7-2. Comparisons of water column profiles for chlorophyll a and DO (base scenario with benthic macroalgae – blue dotted line; sensitivity test scenario without benthic macroalgae – red solid line).
Fig. 7-3(a). With benthic microalgae activated as well, model results for benthic macroalgal biomass and N:C mass ratio.
Fig. 7-3(b). With benthic microalgae module activated as well, model results for water column chlorophyll a, benthic microalgae, and DO.
Fig. 7-4. Model results for sediment oxygen demand (SOD) and chemical oxygen demand (COD) (with MA – blue solid line; no MA – red solid line).
Fig. 7-5(a). Benthic macroalgae simulation results in year 2003, note mortality rate sharply increases at Stations M-1 and M-2.
Fig. 7-5(b). Water column profiles of chlorophyll a and DO in year 2003, note low DO events occurred concurrently with benthic macroalgae dieoff events at Stations M-1 and M-2.
Fig. 7-6. Model sensitivity test results indicating the effect of surface reaeration rates on DO simulations at three benthic macroalgal survey stations. Red line represents the model results with the default surface reaeration rate $k_r$ calculated by ICM; Blue line represents the model results with increased surface reaeration rates under super-saturation conditions. See text for details.
CHAPTER VIII DISCUSSION AND CONCLUSIONS

VIII-1 Discussion

Model predicted water quality variables in general are in good agreement with field observations. Also, the ICM model with included macroalgal module was capable of capturing the basic water quality patterns in the MVCBs. However, the model failed to capture some of the episodic events (e.g., Section VI-4-2 in Chapter VI), which might be caused by wind-induced resuspension. This is partially due to the fact that the current model does not explicitly include the detailed resuspension and deposition processes. However, it is more important for the model to capture the long term water quality pattern instead of individual episodic events. In current model, the water column-sediment exchanges have been described by the net deposition and turbulent diffusion processes.

In addition, there is a large uncertainty associated with benthic macroalgal predictions due to the lack of direct field observations for comparison. In addition, the model seems to simulate the temporal trends reasonably well (Fig. 6-6). In terms of the abundance, the model predicted biomass is within the range of the observational data in 2006 (Fig. 5-7 in Chapter 5, Hardison, 2009). The data show that benthic macroalgal biomass is extremely variable in both time and space, and can span several orders of magnitude, i.e., from 0 to >2000 g dw m\(^{-2}\), roughly equivalent to 0 to >600 g C m\(^{-2}\). However, a closer comparison indicates that the modeled biomass is generally higher than field observations on an annual basis. It is believed that the “over-prediction” of benthic macroalgae by the model should result from the lack of inclusion of other primary producers, such as benthic microalgae and seagrass in the model.
Similar to other shallow coastal bays nearby (e.g., Hog Island Bay, VA, Anderson et al., 2003; Lynnhaven Bay, VA, Li, 2006), benthic microalgae are found to be also abundant in the MVCBs (Wazniak et al., 2004). In the current model simulations, benthic microalgae are deactivated; hence, the role played by them in the real environment has been “replaced” or compensated by benthic macroalgae in the model. Furthermore, there are many other macroalgal species existing in the MVCBs (Goshorn et al., 2001). Thus, due to similar biological properties, these additional species have also been represented by the two modeled macroalgal species, *Gracilaria vermiculophylla* and *Ulva lactuca*. Therefore, all these could contribute to the over-prediction of benthic macroalgal biomass.

Whereas benthic macroalgal biomass could potentially be amplified in the model, it is reasonable to conclude that the overall model performance is encouraging. The calibration run basically serves as the base scenario, which is subsequently used to address the hypotheses proposed in the first chapter. In addition, the calibrated water quality model is a useful tool for diagnosing existing water quality issues and answering research questions that are difficult to study using laboratory experiments.

Another point I would like to discuss is the nonpredatory mortality which plays a crucial role in contributing to the summer crash of dense macroalgal mat. However, in 2004, the model did not show any apparent crash events at all three macroalgal survey stations (Fig. 6-6(a)). In comparison, the model does capture a characteristic summer crash of benthic macroalgae in 2003 (Fig. 7-5). The decline of the benthic macroalgal mat led to a series of ecosystem-level consequences (Valiela et al., 1997). Some major consequences have been
captured by the model. For instance, prolonged hypoxic/anoxic events occurred concurrently with the decline of the benthic macroalgal mat. In addition, the large amount of organic matter released into the water body sharply increased the oxygen demand in both the water column and sediment. However, due to low DO level in the system, the increased oxygen demand was mostly in the form of H$_2$S. Moreover, as can be seen in Fig. 7-5(b), phytoplankton immediately took up the nutrients and bloomed following the macroalgal dieoff. This type of species succession was especially apparent at Station M-2. Lastly, as compared with the 2004 condition (Fig. 6-6), the massive summer crash in 2003 also inhibited the subsequent macroalgal bloom in the fall.

One interesting question is: what causes this intra-annual difference between 2003 and 2004? There are many potential reasons for that. For example, the nonpoint source loading rate in 2003 was much higher than in the other years (Fig. 6-2). High nutrient availability maintained high macroalgal growth from spring till summer (e.g., Station M-1 in Fig. 7-5(a)). Meanwhile, increased water temperature combined with high biomass enhanced the oxygen demand in the system. Consequently, once unfavorable environmental conditions (e.g., rainfall events) occurred, the massive macroalgal crash was initiated.

**VIII-2 Conclusions**

In this dissertation, a hydrodynamic-water quality modeling system has been applied to the Maryland and Virginia Coastal Bays (MVCBs), to understand its eutrophication dynamics and associated physical characteristics. The major findings are summarized as follows:
First of all, the UnTRIM hydrodynamic model, using an unstructured model grid and the finite volume method, is ideally suited for investigating hydrodynamic characteristics in shallow coastal bays. The hydrodynamic model has been verified extensively against observational data collected by the Maryland Department of Natural Resources (MDNR) in the MVCBs, including water level, currents, and salinity. The hydrodynamic model calibration results demonstrate that the model has successfully reproduced the basic hydrodynamic characteristics in the system. Therefore, as a fully calibrated, high-resolution hydrodynamic model, it provides fundamental information on physical circulations for any other studies conducted in the system.

Second, the calibrated hydrodynamic model was further applied to determine the physical transport time scales in the MVCBs. Two commonly used yet conceptually different physical transport time scales, flushing time and residence time, were calculated under four typical freshwater discharge conditions. The results suggest that, in spite of the shallowness, the MVCBs are a poorly flushed system due to restricted bay-ocean exchanges and limited freshwater inputs. In addition, the transport time scales are highly variable in space. For example, flushing time varies for individual bay segments, and is largely determined by segment size (volume), freshwater discharge rate, and distance from the two inlets. In general, the flushing time for the entire system is on the order of 2-3 months, which are sufficiently long when compared with typical time scales required by most biological processes. As a contrast to flushing time, which is an integrative, bulk property in nature, residence time provides a more continuous, spatially varying transport time scale for the MVCBs. The
model results suggest that residence time is highly variable throughout the system. Depending on specific locations, residence time can vary from 0 to more than 200 days. In general, the longest residence time occurs in regions characterized by smallest tidal amplitudes, i.e., northern Chincoteague Bay. In contrast, residence time is much shorter in areas closer to the inlets, e.g., Isle of Wight Bay and southern Chincoteague Bay. The calculated transport time scales were further correlated with spatial water quality distributions in the system. It was found that transport time scales do have a good correlation with some of the water quality phenomena observed in the MVCBs. This demonstrates that physical processes do play an important role in modulating biological processes and thus warrant special attention in understanding water quality issues in the system.

Third, to improve the predictive capability of CE-QUAL-ICM in modeling shallow coastal ecosystems, a benthic macroalgae module, which assimilated benthic macroalgae kinetics from both literature and recent laboratory studies, was incorporated into the existing water quality model framework. The module includes two benthic macroalgal species, *Ulva lactuca* and *Gracilaria vermiculophylla*, and employs the internal nutrient-limited growth kinetics proposed by Droop. It was analyzed using a box model before being applied to the MVCBs. The box model simulation results suggest that the model is capable of capturing the major properties of benthic macroalgae. For instance, benthic macroalgae tend to outcompete phytoplankton in systems characterized with a short flushing time (e.g., several days).

Lastly, the expanded water quality model that included the macroalgae module was applied to the MVCBs to understand the general eutrophication dynamics. Particularly, the
role played by benthic macroalgae in regulating nutrient dynamics and ecosystem metabolism was investigated based on sensitivity analyses. The model was first calibrated against MDNR field monitoring data for major water quality variables, including chlorophyll $a$, DO, and nutrients. The calibration results demonstrate that the model is capable of capturing bay-wide water quality distributions, which are mainly controlled by spatially varying nutrient loading rates from the watershed as well as physical circulations inside the bay. In addition, the model performance justifies that a system-level numerical modeling approach is warranted in understanding spatially varying water quality issues within the same framework. The calibrated water quality model was further used to investigate the unique role played by benthic macroalgae in mediating ecosystem metabolism and nutrient cycling in the MVCBs. It was found that benthic macroalgae play a key role in regulating ecosystem metabolism through high rates of production and respiration in the shallow areas where they are dominant. The incorporation of a benthic macroalgae module improves the predictive capability of CE-QUAL-ICM in simulating the characteristic diurnal DO oscillations and transient hypoxia. In addition, the model estimates that benthic macroalgae retain approximately 10% of annual nitrogen inputs from the watershed in the year of 2004. This is less than the contribution by microalgae, reported by Li (2006) in the Lynnhaven Bay, VA.
REFERENCES


224


Cerco, C.F., C.S. Fang, and A. Rosenbaum. 1978. Intensive hydrographical and water quality survey of the Chincoteague/Sinepuxent/Assawoman Bay systems, Volume III. Non-point source pollution studies in the Chincoteague Bay system. Special
Scientific Report No. 86. Virginia Institute of Marine Science, Gloucester Point, VA.


Gutierrez-Magness, A.L. 2009. Research Associate in Department of Civil and Environmental Engineering, University of Maryland. Personal communication.


Institute of Marine Science, the College of William & Mary, Gloucester Point, VA.


Maryland Department of the Environment (MDE). 2005. Water quality analyses of fecal coliform for eight basins in Maryland: Assawoman Bay, Sinepuxent Bay, Newport Bay, and Chincoteague Bay in Worcester County; Monie Bay in Somerset County; Kent Island Bay in Queen Anne’s County; Rock Creek in Anne Arundel County; and Langford Creek in Kent County. 65pp.

Maryland Department of Natural Resources (MDNR). 2004. Maryland’s Coastal Bays: Ecosystem Health Assessment. DNR-12-1202-0009.

McGinty, M. C. Wazniak, and M. Hall. 2004. Results of recent macroalgae surveys in the Maryland Coastal Bays. Chapter 6.3 in Maryland’s Coastal Bays: Ecosystem Health Assessment. DNR-12-1202-0009.


Wazniak, C. 2004. Benthic chlorophyll measurements in the Maryland Coastal Bays. Chapter 4.5 in Maryland’s Coastal Bays: Ecosystem Health Assessment. DNR-12-1202-0009.


Wazniak, C., D. Wells, and M. Hall. 2004c. The Maryland Coastal Bays ecosystem. Chapter 1.2 in Maryland’s Coastal Bays: Ecosystem Health Assessment. DNR-12-1202-0009.


234


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