Ecohydrodynamic model of the Baltic Sea. Part 2. Validation of the model*

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Abstract

The ecohydrodynamic model for the Baltic Sea consists of two interacting parts: one describes the hydrodynamics of the water (3HD), the other organic matter production and destruction (ProDeMo). The results of the simulation were validated. The modelled processes were compared with direct observations, which demonstrated the recurrence of cycles, from the spring diatom blooms through the summer depletion of nutrient salts and algal blooms, to autumn blooms of diatoms and the subsequent destruction of organic matter, and intensified mineralisation of detritus in winter. Calibration yielded a set of coefficients complementing the algorithm of equations describing the production and destruction of organic matter in the coastal zone. Verification of the model has demonstrated that in multi-year simulations it is stable and also that it follows the laws of conservation of mass and energy. The third procedural stage of the model investigation was validation, in which statistical measures in the form of bias, correlation coefficients and effectiveness between simulations and observations not used in calibration describe the quality of ecohydrodynamic modelling in southern Baltic Sea waters.

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The complete text of the paper is available at http://www.iopan.gda.pl/oceanologia/
1. Introduction

The increasing threat from terrigenous and atmospheric pollutants entering the sea has provided the impetus for intensifying research into marine ecosystems. We need to understand how these function in order to be able to forecast the directions and results of the changes taking place in them. The 1990s saw the publication of numerous papers on North Sea ecosystem modelling (Baretta et al. 1995, Blackford & Radford 1995, Radach & Lenhart 1995, Varela et al. 1995, Moll 1997, 1998, Delhez 1998, Hoch & Garreau 1998). Specifically, they dealt with the dynamics of organisms inhabiting various trophic levels of the food chain, from bacteria to fish, and also the nutrient cycles. The Baltic, a sea particularly exposed to eutrophication, has also been the subject of much work on ecosystem modelling (Elken (ed.) 1996, Fennel & Neumann 1996, Savchuk & Wulff 1996, Suursaar & Astok (eds.) 1996, Tamsalu (ed.) 1996, Jędrasik 1997, Oldakowski & Renk 1997, Mamerfelt et al. 2000, Fennel et al. 2001). Papers have also been published on the functioning of coastal zone ecosystems, that of the Gulf of Gdańsk in particular (Jędrasik & Kowalewski 1993, Oldakowski et al. 1994, Robakiewicz & Karelse 1994, Van der Vat 1994).

The ecohydrodynamic model used in our research into the waters of the southern Baltic consists of two interacting modules: a hydrodynamic module (3HD), and the ProDeMo, which covers the dynamics of organic matter production and destruction, and includes aspects of nutrient circulation. The aim of the present work is to validate the model, so that its effectiveness and utility with regard to the waters of the southern Baltic can be specified.

2. Methodology

Southern Baltic Sea monitoring data (not used previously for calibration), obtained by the Institute of Meteorology and Water Management in Gdynia in 1994–2000, were used for validating the ProDeMo model. The positions of the relevant observation stations in the Gulf of Gdańsk, Gdańsk Deep and Bornholm Deep are shown in Fig. 1. The measured parameters were sea water temperature and salinity, nutrient concentrations (nitrate N-NO$_3$, ammonia N-NH$_4$, total nitrogen N-N$_{tot}$, phosphate P-PO$_4$, total phosphorus P-P$_{tot}$, and silicate Si-SiO$_4$), and dissolved oxygen O-O$_2$. The statistical techniques applied in the validation are discussed in Jędrasik (2005, this volume).
3. Results of validation of the ProDeMo model

The measured and modelled concentrations of nitrate (N-NO$_3$), ammonia (N-NH$_4$), total nitrogen (N-N$_{tot}$), phosphate (P-PO$_4$), total phosphorus (P-P$_{tot}$), silicate (Si-SiO$_4$) and dissolved oxygen (O-O$_2$) were compared at the standard depths at the following stations: P1 in the Gulf of Gdańsk, P140 in the Gdańsk Basin and P5 in the Bornholm Basin. The relations between the observed and modelled nutrient concentrations were presented on scatter plots in the form of ‘clouds of points’ and regression curve slopes (Fig. 2). Positive correlation coefficients were obtained for all variables – the highest values for water temperature (0.88–0.96), dissolved oxygen concentration (0.68–0.93) and phosphate phosphorus (0.75–0.80), lower ones for silicates (0.31–0.84) and nitrate (0.58–0.65), and the lowest ones for ammonia (0.29–0.49).

The measured concentrations of nitrate (Fig. 3), phosphate (Fig. 4) and dissolved oxygen (DOC) (not shown) in the Vistula – Gdańsk Deep (P1) transect were compared with their modelled counterparts. During early spring and summer these transects were very similar with respect to depth-distance distribution. Concentrations were high off the Vistula mouth, decreasing with distance towards station P1 to reach values of 0.1 [g m$^{-3}$]. Local increases were recorded in the near-bottom layer between 30 km and 50 km from the coast. In summer there was a marked local increase in the nitrate concentration in the near-bottom layer off the Vistula
mouth (Fig. 3b). Horizontal diversification was pronounced in spring, likewise vertical stratification in summer. An expected result, this provides further evidence for the regularity already observed in the Gulf of Gdańsk (Trzosińska 1990).

Although vertical phosphate gradients below the halocline were steep, differentiation in the mixing layer off the Vistula mouth was not significant. In spatial distribution, DOC resembled the thermal stratification of the water. In spring, the water layer above the halocline was homogeneous and well-aerated but poorly aerated below it. In summer, thermal stratification produced a thermocline.

Correlation coefficients and the standard deviations of the differences between modelled and observed values were calculated on the basis of measurements available from each station. The highest correlation coefficients

![Graphs showing correlation between observed and modelled values of chemical and physical parameters in the southern Baltic (stations P1, P140, P5) from 1994 to 2000 (R – correlation coefficient, SD – standard deviation, N – number of observations)]
were obtained for dissolved oxygen – from 0.64 at station ZN4 to 0.84 at station NP in the Gulf of Gdańsk, from 0.68 at deep stations P63 and P140 to 0.78 at the coastal station R4 in the Gdańsk Basin, and 0.9 in the Bornholm Basin (Table 1).

The spatial differentiation of the quality of the modelled state variables was analysed according to the location of the observation stations (Table 1) and vertical distributions (Table 2).

Moreover, decreasing standard deviations of the differences between measured and modelled DOC paralleled increasing correlation coefficients. This relationship had been expected and was indeed observed at certain stations (Table 1). However, this relationship did not usually hold in respect of the other variables. The correlations of the silicon compounds, for example, were particularly inconsistent, from 0.77 at station P116 in the Gulf of Gdańsk to no correlation at all at the other stations in that basin, and from 0.47 to 0.81 in the Gdańsk and Bornholm Basins. The results from
the Gulf of Gdańsk suggest that the biogeochemical cycle of silicon compounds at the near-shore stations were inadequately described by the assumed differential equations, or else the estimates of terrigenous silicate inflow were unreliable. At station K off the Vistula mouth, the correlation coefficients for nitrate (0.84), ammonia (0.61) and phosphate (0.77) were relatively high (Table 1).

High correlations were calculated for nitrates and phosphates at station P116. Modelled at stations in the western Gulf of Gdańsk, these parameters highly correlated with observations. Better values were obtained at stations K and ZN4, located respectively on the Vistula Spit and the Hel Peninsula. The correlations of modelled nitrates and phosphates with
Table 1. Correlation coefficients $R$ and standard deviations (SD) of selected state variables of the ProDeMo model at observation stations in the southern Baltic in 1994–96 only

<table>
<thead>
<tr>
<th>Station</th>
<th>NO$_3$</th>
<th>NH$_4$</th>
<th>PO$_4$</th>
<th>Si</th>
<th>O$_2$</th>
<th>Number of observations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$R$</td>
<td>SD</td>
<td>$R$</td>
<td>SD</td>
<td>$R$</td>
<td>SD</td>
</tr>
<tr>
<td>P101</td>
<td>0.51</td>
<td>0.06</td>
<td>0.38</td>
<td>0.02</td>
<td>0.59</td>
<td>0.01</td>
</tr>
<tr>
<td>Gulf of</td>
<td>0.65</td>
<td>0.04</td>
<td>0.05</td>
<td>0.02</td>
<td>0.59</td>
<td>0.01</td>
</tr>
<tr>
<td>Gdańsk</td>
<td>0.83</td>
<td>0.03</td>
<td>0.18</td>
<td>0.01</td>
<td>0.80</td>
<td>0.02</td>
</tr>
<tr>
<td>ZN4</td>
<td>0.43</td>
<td>0.02</td>
<td>0.84</td>
<td>0.01</td>
<td>0.33</td>
<td>0.03</td>
</tr>
<tr>
<td>Gdynsk</td>
<td>0.35</td>
<td>0.07</td>
<td>0.65</td>
<td>0.02</td>
<td>0.37</td>
<td>0.02</td>
</tr>
<tr>
<td>K</td>
<td>0.84</td>
<td>0.08</td>
<td>0.61</td>
<td>0.02</td>
<td>0.77</td>
<td>0.01</td>
</tr>
<tr>
<td>P116</td>
<td>0.65</td>
<td>0.03</td>
<td>0.29</td>
<td>0.01</td>
<td>0.85</td>
<td>0.01</td>
</tr>
<tr>
<td>Bornholm Basin</td>
<td>0.60</td>
<td>0.04</td>
<td>0.42</td>
<td>0.02</td>
<td>0.67</td>
<td>0.03</td>
</tr>
</tbody>
</table>

* no statistical parameters owing to the small number of measurements.
Table 2. Correlation coefficients $R$ and standard deviations (SD) of selected state variables of the ProDeMo model at observation stations in the southern Baltic in 1994–96

<table>
<thead>
<tr>
<th>Z [m]</th>
<th>NO$_3$</th>
<th>NH$_4$</th>
<th>N$_{tot}$</th>
<th>PO$_4$</th>
<th>P$_{tot}$</th>
<th>Si</th>
<th>O$_2$</th>
<th>Number of observations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>SD</td>
<td>$R$</td>
<td>SD</td>
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<tr>
<td>0</td>
<td>0.88</td>
<td>0.13</td>
<td>0.72</td>
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<td>0.75</td>
<td>0.11</td>
<td>0.89</td>
<td>0.06</td>
</tr>
<tr>
<td>10</td>
<td>0.67</td>
<td>0.08</td>
<td>0.30</td>
<td>0.02</td>
<td>0.09</td>
<td>0.15</td>
<td>0.92</td>
<td>0.06</td>
</tr>
<tr>
<td>20</td>
<td>0.74</td>
<td>0.03</td>
<td>0.09</td>
<td>0.01</td>
<td>0.46</td>
<td>0.06</td>
<td>0.90</td>
<td>0.06</td>
</tr>
<tr>
<td>30</td>
<td>0.70</td>
<td>0.03</td>
<td>0.10</td>
<td>0.01</td>
<td>0.53</td>
<td>0.06</td>
<td>0.86</td>
<td>0.07</td>
</tr>
<tr>
<td>40</td>
<td>0.67</td>
<td>0.03</td>
<td>0.14</td>
<td>0.01</td>
<td>0.58</td>
<td>0.05</td>
<td>0.87</td>
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<tr>
<td>50</td>
<td>0.66</td>
<td>0.03</td>
<td>0.03</td>
<td>0.02</td>
<td>0.69</td>
<td>0.04</td>
<td>0.86</td>
<td>0.08</td>
</tr>
<tr>
<td>60</td>
<td>0.39</td>
<td>0.04</td>
<td>0.01</td>
<td>0.02</td>
<td>0.66</td>
<td>0.04</td>
<td>0.84</td>
<td>0.11</td>
</tr>
<tr>
<td>70</td>
<td>0.26</td>
<td>0.04</td>
<td>0.05</td>
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<td>0.78</td>
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</tr>
<tr>
<td>80</td>
<td>0.04</td>
<td>0.05</td>
<td>0.56</td>
<td>0.04</td>
<td>0.06</td>
<td>0.07</td>
<td>0.73</td>
<td>0.52</td>
</tr>
<tr>
<td>90</td>
<td>0.14</td>
<td>0.04</td>
<td>0.41</td>
<td>0.02</td>
<td>0.56</td>
<td>0.03</td>
<td>0.15</td>
<td>0.04</td>
</tr>
<tr>
<td>100</td>
<td>0.19</td>
<td>0.04</td>
<td>0.10</td>
<td>0.05</td>
<td>0.33</td>
<td>0.05</td>
<td>0.03</td>
<td>0.06</td>
</tr>
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<td>110</td>
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<td>0.05</td>
<td>0.05</td>
<td>0.06</td>
<td>0.48</td>
<td>0.06</td>
<td>0.08</td>
<td>0.05</td>
</tr>
</tbody>
</table>
measured concentrations at deep stations in the Gdańsk Basin and off Bornholm were satisfactory (0.58–0.85); for ammonia the range was from 0.29 to 0.52 (Table 1).

Comparison of the vertical modelled and observed distributions for the nutrient salts and oxygen dissolved in the Gulf of Gdańsk and the Gdańsk Basin showed the following regularities (Table 2):

- The correlation coefficients for nitrates, silicates, total phosphorus and oxygen decreased uniformly from the sea surface to the bottom.
- The correlation coefficients for phosphates, ammonia, total nitrogen decreased from the sea surface as far as the halocline, where they increased, and decreased abruptly in the near-bottom layer.
The depth-dependent decrease in correlation coefficients for dissolved oxygen was accompanied by a steady increase in the standard deviations (an expected regularity).

The features of correlation for total phosphorus at 80 m depth were the same as for dissolved oxygen.

The remaining variables with a model bias did not display such a correlation of the correlation coefficients or standard deviations.

Comparison of the available measurements of oxygen, silicon, phosphates and total phosphorus from three deep-water stations P1, P140 and P5 in 1998–2000 (not shown) with the modelled state variables yielded a high correlation (coefficients from 0.7 to 0.96). The correlation for the modelled nitrogen compounds was not so high: for nitrates the coefficients ranged from 0.52 to 0.7, for ammonia from 0.3 to 0.68, and for total nitrogen from only 0.12 to 0.16. Generally speaking, these results demonstrate the excellent quality of the modelled variables.

Except for the April vertical distribution, which was well correlated with observations, the modelled nitrate values were overestimated (Fig. 5). The vertical distributions of ammonium nitrogen concentrations to a depth of 80 m in spring should be taken as correct; in winter the simulations were overestimated, and in summer, below 30 m, they were underestimated. Phosphates were well mapped as far as the halocline (60 m); below this depth there were considerable discrepancies between modelled and measured values (Fig. 5). The vertical distributions of nitrate concentrations modelled for the 1999 season at stations P1, P140 and P5, respectively representing the Gulf of Gdańsk, Gdańsk Basin and Bornholm Basin, showed the closest similarity in spring (Fig. 6). The summer simulation showed no depletion down to 60 m depth, a situation endorsed by the measurements. For the remaining periods, modelled values were overestimated above the halocline and underestimated below it.

The seasonal vertical distribution of dissolved oxygen (Fig. 7) simulated at station P1 corresponded perfectly with the values measured on 8–9 February 1999 down to 70 m; at stations P140 and P5 the correlation held almost to the bottom. Moreover, the modelled and recorded values almost matched each other at these stations during other seasons. The vertical dissolved oxygen distributions were highly correlated with the measurements in each period and were the best modelled of all the parameters.

Generally speaking, the vertical distributions of nitrate nitrogen and phosphate phosphorus as far as the halocline were well mapped during summer periods. In 1994–96 modelled summer values of nitrate were
Fig. 5. Seasonal variability in 2000 of vertical distributions of nitrates, ammonia, phosphates observed (OBS) and modelled (MOD) in the Gdańsk Deep at station P1.

significantly overestimated, but in 1998–2000 they tallied more closely with measurements as far as the halocline at each station. In the entire period from 1994 to 2000, temporal variation was characterised by the exhaustion of nitrates in the spring and summer months in both the observed and modelled runs. In the same period the modelled distributions of phosphate...
Fig. 6. Seasonal variability in 1999 of vertical distributions of nitrates observed (OBS) and modelled (MOD) in the Gdańsk Basin (stations P1 and P140) and the Bornholm Basin (station P5).

Concentrations were satisfactory in relation to the measurements as far as the thermocline, but were significantly underestimated below it. State variables at the water surface, at the depth of the summer thermocline, the halocline and at the bottom were analysed at the standard depths for selected periods. Comparison of surface values at stations P1
Fig. 7. Seasonal variability in 1999 of vertical distributions of dissolved oxygen observed (OBS) and modelled (MOD) in the Gdańsk Basin (stations P1 and P140) and the Bornholm Basin (station P5)

and P5 in 1994–2000 demonstrated the recurrence of the annual cycles (Figs 8 and 9), indicating that the model functions well. A notable regularity at each of these stations was the summer depletion of nitrogen and phosphorus forms. However, the silicate concentration during this period was underestimated. Both measured and modelled DOC were higher
Fig. 8. The surface variability of the observed (OBS) and modelled (MOD) chemical and physical parameters: nitrates N-NO\(_3\), ammonia N-NH\(_4\), phosphates P-PO\(_4\), silicates Si-SiO\(_4\), dissolved oxygen O-O\(_2\), water temperature \(T\) in the Gdańsk Deep (station P1, depth – 0 m) in 1994–2000.

at lower temperatures. The correlation coefficients for silicate and DOC ranged from 0.79 to 0.97. Measured and modelled variability in phosphate phosphorus concentration at stations P140 and P5 and nitrate nitrogen at station P140 in the Gdańsk Basin were highly correlated. Modelled values of nitrate nitrogen in the Gdańsk Deep and the Bornholm Deep resembled
Fig. 9. The surface variability of observed (OBS) and modelled (MOD) chemical and physical parameters: nitrates N-NO$_3$, ammonia N-NH$_4$, phosphates P-PO$_4$, silicates Si-SiO$_4$, dissolved oxygen O-O$_2$, water temperature $T$ in the Gdańsk Deep (station P5, depth = 0 m) in 1994–2000.

The measured ones, the respective correlation coefficients being 0.67 and 0.69. The level of similarity was lower for the concentrations of silicate silicon, especially at station P5 in the Bornholm Basin. Despite a correlation coefficient of 0.33 for the Gdańsk Deep, the ammonium nitrogen simulations
were the least reliable (Fig. 8). The standard deviations of the differences between measurements and modelled values were similar at all stations. It should be pointed out that the modelled values for 1998–2000 did not differ much from the 1994–96 simulations.

Parameter variability was analysed at the following depths at station P1 in the Gdańsk Deep (not shown): the summer thermocline (30 m), the stable halocline (60 m) and at the bottom (100 m). The correlation coefficients decreased systematically from 0.69 at the surface, through 0.65 in the thermocline, 0.43 in the halocline, to 0.18 at the bottom, an indication that the model description of chemical processes was becoming less accurate towards the bottom. On the other hand the standard deviations for the differences between measurements and simulations were increasing. In relation to ammonia, the pattern for nitrate nitrogen was the same, despite the low correlation. The consistency with the measurements as regards modelled phosphate phosphorus concentrations was poor in the thermocline, but rather better in the halocline. Another significant feature was the underestimation of phosphate, especially in the deeper layers, evidence for which is provided by the vertical distributions (Figs 3–7). The variability in silicate concentration displayed similar correlations; nevertheless, the simulations were overestimated in the halocline, and underestimated at the bottom.

The vertical distributions of the correlation coefficient for each variable show that the modelled vertical distributions are satisfactorily consistent with the measured concentrations of dissolved oxygen, silicates, phosphates and total phosphorus. Correlation coefficients indicating a similarity between measured and modelled values tend to decrease towards the bottom. Records and modelled simulations of DOC variability as far as the halocline were highly correlated. Modelled DOCs were underestimated in the halocline but significantly overestimated at the bottom. While the measurements revealed an oxygen deficit, the simulations did not. This drawback is the result of the inadequate description of exchange processes at the water-sediment boundary. So far, the model has best described the sea water temperature, for which the high correlations from 0.97 at the surface to 0.90 in the thermocline fall to 0.59 in the halocline; at the bottom the model result was the reverse of the measured one (this was also demonstrated by the negative coefficient of the very low correlation). Validation turned out to be a positive test for the proper model functioning.

4. Statistical characteristics of the model quality

Measured and modelled values were correlated, regardless of whether the modelled ones were overestimated or underestimated in relation to the
measured ones. Nevertheless, the bias (Fig. 10) shows that a relation between modelled and measured values did exist. At the majority of the stations, modelled simulations overestimated nitrogen compounds and underestimated phosphates. Modelled concentrations of silicate silicon were significantly overestimated at station P140, but underestimated elsewhere. Simulations of DOC were slightly overestimated in the Gdansk Deep (station P1), and lower than the measured values in the Hoburg Channel (station 140). Modelled temperatures were closest to the observed values, but the salinity simulations were only slightly underestimated in relation to the measured ones. All measurements of nitrate and ammonia nitrogen concentrations were overestimated in relation to the simulations, the other variables were underestimated (Fig. 10).

![Graph showing bias of the model calculated for state variables in the ProDeMo model for 1994–2000](image)

**Fig. 10.** Bias of the model calculated for state variables in the ProDeMo model for 1994–2000

The correlation coefficient, together with the complementary criteria of conditional and unconditional bias, indicates the effectiveness of the simulation (Table 3, Fig. 11). The effectiveness of correlation, as expressed by the determination coefficient $r^2$, is usually an overestimated value, because it represents correlation when model bias is absent. The Nash-Sutcliffe coefficient $E$ makes allowance for such effectiveness-reducing bias and displays a correlation between the compared values. For a large bias, this effectiveness decreases to zero or less, which implies a lack of correlation (Fig. 11). In the spatial perspective, the differentiation in the effectiveness
Table 3. Correlations and bias for variables in the periods 1994–96 and 1998–2000 jointly

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$Q_m$</th>
<th>$C^2$</th>
<th>$B^2$</th>
<th>$E_{res}$</th>
<th>$E_{rec}$</th>
<th>$r$</th>
<th>$r^2$</th>
<th>$E$</th>
<th>$R_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PO$_4$</td>
<td>-0.012</td>
<td>0.170</td>
<td>0.067</td>
<td>0.0014</td>
<td>1.104</td>
<td>0.779</td>
<td>0.607</td>
<td>0.361</td>
<td>0.765</td>
</tr>
<tr>
<td>P$_{tot}$</td>
<td>-0.019</td>
<td>0.169</td>
<td>0.096</td>
<td>0.0017</td>
<td>0.883</td>
<td>0.731</td>
<td>0.534</td>
<td>0.268</td>
<td>0.842</td>
</tr>
<tr>
<td>SiO$_4$</td>
<td>-0.120</td>
<td>0.192</td>
<td>0.067</td>
<td>0.085</td>
<td>0.590</td>
<td>0.771</td>
<td>0.595</td>
<td>0.336</td>
<td>0.902</td>
</tr>
<tr>
<td>O$_2$</td>
<td>-0.010</td>
<td>0.013</td>
<td>0.0004</td>
<td>5.774</td>
<td>0.246</td>
<td>0.841</td>
<td>0.707</td>
<td>0.694</td>
<td>0.975</td>
</tr>
<tr>
<td>T</td>
<td>-0.130</td>
<td>0.0004</td>
<td>0.0004</td>
<td>2.816</td>
<td>0.256</td>
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<td>0.858</td>
<td>0.977</td>
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<td>S</td>
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<td>0.073</td>
<td>0.891</td>
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<td>0.928</td>
<td>0.861</td>
<td>0.687</td>
<td>0.994</td>
</tr>
<tr>
<td>NO$_3$</td>
<td>0.021</td>
<td>0.071</td>
<td>0.182</td>
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<td>0.604</td>
<td>0.365</td>
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</tr>
<tr>
<td>N$_{tot}$</td>
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<td>0.001</td>
<td>0.006</td>
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<td>0.337</td>
<td>0.138</td>
<td>0.048</td>
<td>0.920</td>
</tr>
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<td>0.0009</td>
<td>0.0007</td>
<td>1.479</td>
<td>0.242</td>
<td>0.058</td>
<td>-0.530</td>
<td>0.590</td>
</tr>
</tbody>
</table>

where: $Q_m$ – bias of model, $C^2$ – conditional bias of model, $B^2$ – unconditional bias of model, $E_{res}$ – mean square error, $E_{rec}$ – integral square error, $r$ – correlation coefficient, $r^2$ – coefficient of determination, $E$ – the Nash-Sutcliffe coefficient of efficiency $R_s$ – special correlation coefficient.

![Fig. 11. Coefficients of effectiveness for state variables at stations P1 (a), P140 (b), P5 (c) and all stations in 1994–2000 (d)](image)

of individual state variables was significant. At station P1 the effectiveness of the correlation between the measured and modelled concentrations of ammonia nitrogen was negative (–0.2). At station P140, it was significantly
lower for silicate silicon (even –1.56) and for nitrogen compounds (–0.4 to –0.62). In the Bornholm Basin, the effectiveness of modelled total nitrogen was also unsatisfactory (–0.08). Because of the higher correlation coefficient (0.09) at station P5, ammonia nitrogen was simulated more effectively there than in the Gdańsk Basin. If all the observation stations are taken into account, the best effectiveness was obtained for temperature, salinity and DOC (0.65–0.84), which testifies to the good quality of the hydrodynamic model. The correlation coefficient for measured and modelled phosphorus compounds was >0.7, but after allowing for bias, the simulation was only 40% effective, with a correlation coefficient of 0.4. For total nitrogen and nitrate nitrogen, the effectiveness decreased significantly, and for ammonia nitrogen it was even negative (Fig. 11d). Without allowing for bias, the correlation coefficients ranged from 0.24 to 0.93 (Table 3), thereby overestimating the quality of the model.

The Nash-Sutcliffe $E$ coefficient can be applied as an optimisation measure in further calibrations of the model. Its increasing values improve the correlation and reduce the bias of the modelled values.

The statistical analysis was carried out by comparing the simulations with the observations using a special correlation coefficient as a function of the total square error (Fig. 12). All the measurements from all the stations and dates for individual variables were used. Salinity and total nitrogen were correlated the best, ammonia the worst (Fig. 12). This means that the algorithm describing the circulation of ammonia compounds in this model is not yet sufficiently rigorous. The model simulations worked best for salinity, water temperature and oxygen, and quite well for phosphorus, total nitrogen and phosphate. The simulations of nitrate, ammonia and silicate were significantly different from the others. The parameters at near-bottom depths were rather lower than at the surface, which indicates that the simulated values were very different from the measured ones. In the spatial perspective, ammonia nitrogen and silicate silica were described the least accurately in each basin (Fig. 12).

The quality of the model for variables describing the character of the southern Baltic ecosystem is similar in the Gulf of Gdańsk, Gdańsk Basin and Bornholm Basin. The physical parameters (T, S, O$_2$) were simulated best in each basin, while the least convincing results were obtained for ammonia nitrogen and silicate silica in the Gdańsk Basin. The statistical measures describing the quality of the model based on the average square error (correlation coefficients and bias) and total square error (special correlation coefficient) indicated that the quality of the modelled simulations was very good with regard to the physical parameters, good as regards
Fig. 12. Special correlation coefficients as a function of integral square error: for state variables of all measurements (a) for stations P1, P140, P5 for the period 1994–2000 (b)

phosphate phosphorus, total phosphorus and silicate silica, and satisfactory for nitrate and ammonia nitrogen.

5. Discussion

The validation of the ProDeMo model as far as the relevance of the measured values to the modelled ones is concerned was carried out in a similar way to that of other ecosystem models (Baretta et al. 1995, Blackford & Radford 1995, Fennel & Neumann 1996, Marmefelt et al. 2000, Savchuk 2002). In this work the observation stations were chosen from
various basins, and measured values were compared with modelled values 
at ten standard depths. In the validation of other models, the sea was 
divided, for example, into depth layers – surface and near-bottom (Baretta 
et al. 1995) or basins – coastal, surface and near-bottom (Savchuk 2002).

Monitoring measurements are most often used for validating a model. 
The ERSEM model was validated by two series of monitored observed data 
on the North Sea – one from coastal basins, the other from distant 
basins (Lauenroth et al. 1983, Baretta et al. 1995). The model of the 
mesoscale variability of nutrient salts and phytoplankton in the western 
Baltic model (Fennel & Neumann 1996, Marmefelt et al. 2000) was validated 
by monitoring observations from three stations in the Arkona Basin. State 
variables at stations representing the Gulf of Gdańsk, Gdańsk Basin and 
Bornholm Basin in 1994–2000 were used for comparing ProDeMo-modelled 
values with monitoring measurements. A three-year period of observations 
(1988–90) was used for validating the ERSEM model (Blackford & Radford 
1995), and a primary production model of the German Bight was compared 
only with observations of an experiment during the spring bloom in 1991 
(Moll 1997).

The model simulations recreated the spring diatom blooms, the summer 
depletion of nutrients with limitation of nitrogen, and the intensified miner-
alsation of detritus in winter. Modelled fluctuations of water temperature 
showed a relation with the dissolved oxygen concentration. With every 
drop in water temperature there was a concomitant increase in oxygen 
concentration. During phytoplankton blooms, the oxygen saturation in the 
surface layers increased. Fluctuations in seasonal variability with respect 
to nutrients, oxygen and temperature, the relationship between light, heat 
and organic matter production, are indications of the internal logic of 
these processes, while the similarity between measured and modelled data 
demonstrate the reality of the results.

The ProDeMo simulations represented seasonal variability in the state 
variables, especially the nutrients. However, measured values of nitrate in 
the vertical distribution below the thermocline were lower than the modelled 
one, and the modelled seasonal variability cycle of ammonia was not highly 
correlated with the measurements. Similar effects were obtained as a result 
of the ERSEM model validation used in the research on the North Sea 
ecosystem. Overestimated in relation to measured concentrations, nitrate 
was modelled during summer and ammonia during the whole year (Baretta 
et al. 1995). The reason for this similarity in the results was the approximate 
approach in the formulation of the model algorithm.
6. Conclusion

Modelled and measured vertical distributions of nitrates, phosphates and DOC displayed decreasing correlation with depth from surface to bottom. A review of time runs revealed the regular summer depletion of the mineral forms of nitrogen and phosphorus. The seasonal variability in the modelled and measured oxygen concentrations and water temperatures was related: higher temperatures were accompanied by falling oxygen concentrations. The respective correlations between the modelled and measured values of these variables were 0.79 and 0.97.

The expected regularity regarding the increase in correlation coefficients and the decrease in standard deviations was obtained only for nitrate nitrogen and dissolved oxygen. The lack of such a relation for the other state variables was due to model bias. Absolute bias led to overestimation of the modelled concentration of nitrogen compounds and underestimation of phosphates, as well as local deviations in silicate concentrations. By including bias in the correlation relations between simulations and observations, the effectiveness of the model and the actual correlations were demonstrated. The effectiveness of 0.69–0.86 for the water temperature, salinity and oxygen of the hydrodynamic model, and from 0.4 for phosphates to ~0.5 for ammonia in the ProDeMo model testify to the good quality of both. The effectiveness coefficient enables the quality of the model in individual basins to be evaluated, and is a good optimisation measure for future calibrations of new variables.

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