

Documentation of the PROWQM model (version 3.2)

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1 Objectives and general description

PROWQM (PROVESS Water Column Model) is a one-dimensional integrated water column model, constructed and validated within the European PROVESS project. Its main objective is to provide a common framework and user-platform for the validation and testing of new or existing schemes for turbulence and of modules for biology and sediments prior to their implementation in three-dimensional numerical ocean models. Easily accessible interfaces are provided for (future) integration of new or alternative modules for biology and sediments without large computational and programming overheads. This allows to use PROWQM as a user-friendly platform for the testing and intercomparison of biological and sedimentological models and to assess their sensitivity on the formulation of vertical exchange processes (turbulence, resuspension).

The basic concept, structure and programming techniques are very similar to the ones used in the extensively documented COHERENS model (Luyten et al., 1999). A general structure map is given in Fig. 1. A number of novel features have been implemented such as:

- Several new turbulence closure schemes have been incorporated. Some of them have been developed during the MAST projects PROVESS and CARTUM.
- A link is provided with the recently developed one-dimensional GOTM model (Burchard et al., 1999).
- Incorporation of the PROVESS modules dealing with pelagic biology and benthic processes (Lee et al., ms).
- A new module for the deposition and resuspension of sediments which allows to simulate the damping of turbulence due to high sediment concentrations in the bottom layer via the equation of state of density.

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2 Model description

The program is written in FORTRAN 77 and has the following main components:

1. A physical “core” part containing the main physics and a general module for solving the time-evolution equation for momentum and scalar quantities (e.g. temperature, turbulent kinetic energy, biological concentrations, ...).
2. A series of modules allowing the user to select between an extensive series of turbulence schemes.
3. Two sediment models dealing with the resuspension and deposition of particulate matter.
4. Two microbiological models.

A series of switches (marked by a * below) allows the user to select whichever processes are required, for a particular simulation. The general characteristics of PROWQM are summarized as follows.

2.1 General

- The possibility is foreseen to run the program either as a 1-D or a 0-D model (*). In the latter case, the number of vertical grid points (NZ) must be set to 1. An example is the **batch** test case.
- The simulation of currents (*), temperature (*) and salinity (*) can be disabled/enabled. Either a slip or a no-slip condition can be applied at the sea bed (*).
- Compared to COHERENS, a more extended number of formulations for the surface fluxes are available (*).
- A module for wave-current interaction at the sea bed (*), similar to the one implemented in COHERENS is provided. The effect of surface waves on turbulence production in the surface layer can be included via the formulation of Craig and Banner (1994).
- Different schemes can be selected for the vertical advection of particulate matter (*). Vertical diffusion can be discretised implicitly (default), explicitly or semi-implicitly.
- Temperature and salinity are either calculated by the model or supplied externally using a simple data relaxation scheme (*).
- Various types of input can (optionally) be supplied by the user at selected intervals: meteorological data, wave parameters, attenuation coefficient, surface slopes and elevation.

- Harmonic analysis can optionally (*) be performed on user-defined variables.
- The type of model output can either be specified by the user in one of the pre-defined formats (file format, output times, variables; time series, harmonic or time-averaged) or given in a completely user-defined format.
- Error traps are implemented which stop execution of the program after improper initialisation and in some other cases, and which provide an explanatory message.
- Default values are assigned for all model parameters and switches, which can be changed by the user.
- The integration of new models for biology and/or sediments by the user is facilitated via a series of built-in subroutine calls.

2.2 Turbulence

The form of the turbulence scheme is selected using a total of 19 switches. The schemes can be classified into three main groups selected by the switch IOPTK:

- algebraic formulations as in COHERENS (switch ITCFORM);
- “second-moment” closures (see below);
- schemes implemented in the GOTM model.

The basic concept of the second-moment closures is the down-gradient parameterization of the vertical fluxes of momentum, temperature and all scalar quantities. This gives:

$$-\overline{u'w'} = \nu_t \frac{\partial \overline{U}}{\partial z}, \quad -\overline{v'w'} = \nu_t \frac{\partial \overline{V}}{\partial z}, \quad -\overline{w'\phi'} = \lambda_t \frac{\partial \overline{\phi}}{\partial z} \quad (1)$$

where an overbar denotes an ensemble average, a prime a fluctuating quantity, (U, V) are the horizontal current components, ϕ is a scalar quantity and λ_t, ν_t are the coefficients of eddy viscosity and diffusivity. The following options are available:

- ν_t and λ_t are either parameterized (switch ITCPAR) using the $K - \varepsilon$ approach

$$\nu_t = S_u K^2 / \varepsilon, \quad \lambda_t = S_b K^2 / \varepsilon \quad (2)$$

or using the $K - l$ formulation

$$\nu_t = S_m K^{1/2} l, \quad \lambda_t = S_b K^{1/2} l \quad (3)$$

where K is the turbulent kinetic energy, ε the dissipation rate, l the (“master”) mixing length and (S_u, S_b) or (S_m, S_h) the so-called stability functions.

- A general generic form for the stability functions is derived from the parameterized second-moment equations. The following options are included:

- type of formulation (switch **ITCMOD**): Mellor and Yamada (1982), Kantha and Clayson (1994), Burchard and Baumert (1995), default **COHERENS** version after Hossain and Rodi (1982), Canuto et al. (2001), as derived from LES data (Andr n and Moeng, 1993), from a renewed calibration of model parameters with neutral flow data;
- method of solution (switch **ILEV**): quasi-equilibrium after Galperin et al. (1988) or non-equilibrium method (Mellor and Yamada, 1982);
- a more complex parameterization including Coriolis effects (switch **ITCROT**). In that case equations (1) are replaced by the more complex forms:

$$\begin{aligned}
-\overline{u'w'} &= \nu_{uu} \frac{\partial \overline{U}}{\partial z} + \nu_{uv} \frac{\partial \overline{V}}{\partial z} + \nu_{ub} \frac{K}{\varepsilon} N^2 \\
-\overline{v'w'} &= \nu_{vu} \frac{\partial \overline{U}}{\partial z} + \nu_{vv} \frac{\partial \overline{V}}{\partial z} + \nu_{vb} \frac{K}{\varepsilon} N^2 \\
-\overline{w'\phi'} &= \lambda_t \frac{\partial \overline{\phi}}{\partial z}
\end{aligned} \tag{4}$$

where N^2 is the (squared) buoyancy frequency. For more details see e.g. Kantha et al. (1989), Hassid and Galperin (1994).

- The number of evolution equations for turbulence parameters is selected by the switch **NTRANS** (with separate options for selecting Dirichlet or Neumann type of boundary conditions):
 - 0-equation: Mellor-Yamada “level 2” model using an algebraically prescribed mixing length (switch **ILENG**);
 - 1-equation: K -equation with L prescribed algebraically (switch **ILENG**);
 - 2-equations: K -equation plus either an equation for KL (or “ q^2l ”) as in the Mellor-Yamada theory or for ε as in the standard $K - \varepsilon$ model (Rodi, 1984). The choice between the two versions is made with the switch **ITCPAR**.
 - 3-equation: the same as the 2-equation model now including an additional equation for scalar variance as in the Mellor-Yamada “level 3” method.
- Different parameterizations can be selected for the vertical diffusion term in the evolution equations for turbulence quantities (switch **ITCDIF**). For details see Luyten et al., ms.
- Background mixing can be added in the following ways:
 - uniform values (switch **IOPTK**);

- using a limiting theory for turbulent length scales (Luyten et al., ms) (switch ILIM);
- using the Large et al. (1994) and Kantha-Clayson (1994) internal wave mixing scheme (switch ITCIW).

2.3 Biology

Two different microplankton modules (*) can currently be selected. The first is the module, already implemented in **COHERENS**. The second is a benthic-pelagic module, developed within the MAST-PROVESS project (Lee et al., ms). A documentation of the latter model is presented in an associated document (Tett et al., 2001).

2.4 Sediment

Two different models (*), dealing with the deposition and resuspension of particulate matter, are implemented. The first is taken from **COHERENS**, the second from the **GOTM** model. Different sediment fractions with different particle sizes and fall velocities can be defined by the user.

3 Installation, test cases and applications

The instructions for installing the present version 3.2 of the **PROWQM** code and preparing/simulating a test case or a realistic application are almost the same as described in the **COHERENS** documentation (Chapter I-2 of Luyten et al., 1999). The main difference is that occurrences of **COHERENS** and **release_8.4** are replaced by **PROWQM** and **prowqm_3.2**. Note that a postprocessor for converting model output into netCDF format has not yet been provided. A new feature is the directory **prowqm_3.2/data** which contains a series of subdirectories holding the data needed for the initialization, the forcing and the validation of certain applications.

The code of **PROWQM** is supplied with ten pre-defined applications. To prepare and run an application under a **UNIX** or **LINUX** environment, use the **Prepare** and **Run** scripts as described in Section 2.2 of Chapter I-2 of the **COHERENS** documentation. The scripts are executed with an auxiliary argument, given by a capital letter (e.g. **A**), which indicates the type of experiment conducted with the simulation. The meaning of each experiment is shortly explained by commented lines in the **Prepare** file. The following test cases and realistic applications have been defined:

pycno : evolution of a wind-driven boundary layer without rotation as in the Kato-Phillips experiment;

csnsp : seasonal evolution of temperature at station CS in the North Sea;

- tides** : simulation of a tidal cycle of deposition and resuspension under homogeneous conditions using either of the two sediment models;
- batch** : idealised “batch” culture experiment where populations of microplankton are grown in mesocosm under controlled conditions;
- nsbi1** : simulation of the seasonal biological cycle and SPM dynamics in the North Sea using simplified forcing conditions and with the **COHERENS** microplankton module;
- nsbi2** : as **nsbi1** now using the **PROVESS** microplankton and benthic modules;
- papa** : simulation of a seasonal temperature cycle at Ocean Weather Station Papa (Martin, 1985);
- november** : simulation of a seasonal temperature cycle at Ocean Weather Station November (Martin, 1985);
- flex** : simulation of the temperature field at station FLEX in the North Sea from April 4 to June 7 1976 (see e.g. Burchard et al., 1999);
- lagmag** : simulation of convective cooling at Lake Maggiore in December 1995;
- irism1** : simulation of turbulence dissipation rates at the mixed station M₁ within the Irish Sea in March 1993 (Simpson et al., 1996);
- iriss1** : simulation of turbulence dissipation rates at the mixed station S₁ within the Irish Sea in July 1993 (Simpson et al., 1996);
- pronns** : simulation of temperature and turbulence parameters at the **PROVESS** northern North Sea site. Two types of simulations can be conducted: (a) a full year run, (b) a simulation for the **PROVESS** measurement period forced by observational data (see Luyten et al., ms). To run one of the two cases, use **Preparea**, **Runa** instead of **Prepare**, **Run** for case (a) and **Prepareb**, **Runb** for case (b).
- probio** : simulation of the biological cycle at the **PROVESS** northern site. Two types of simulations can be performed: (a) a two-year run with climatological mean forcing; (b) a one-year run for 1998 using real-time surface forcing.

Test cases **pycno**, **csnsp**, **batch** and **nsbi1** are the same as implemented in **COHERENS**, although with a different setup of the experiments (except for **batch**). The results of **papa**, **november**, **flex**, **lagmag**, **irism1**, **iriss1** and **pronns** can be compared with data supplied on the **CARTUM** CD-ROM. More extended data for the **PROVESS** sites are found on the **PROVESS** CD-ROM.

A user-application is installed by creating a number of **FORTRAN** source files. For details see Chapters I-2 and I-3 of the **COHERENS** documentation. Generic example files for model setup are found in the **/tests/examples** subdirectory.

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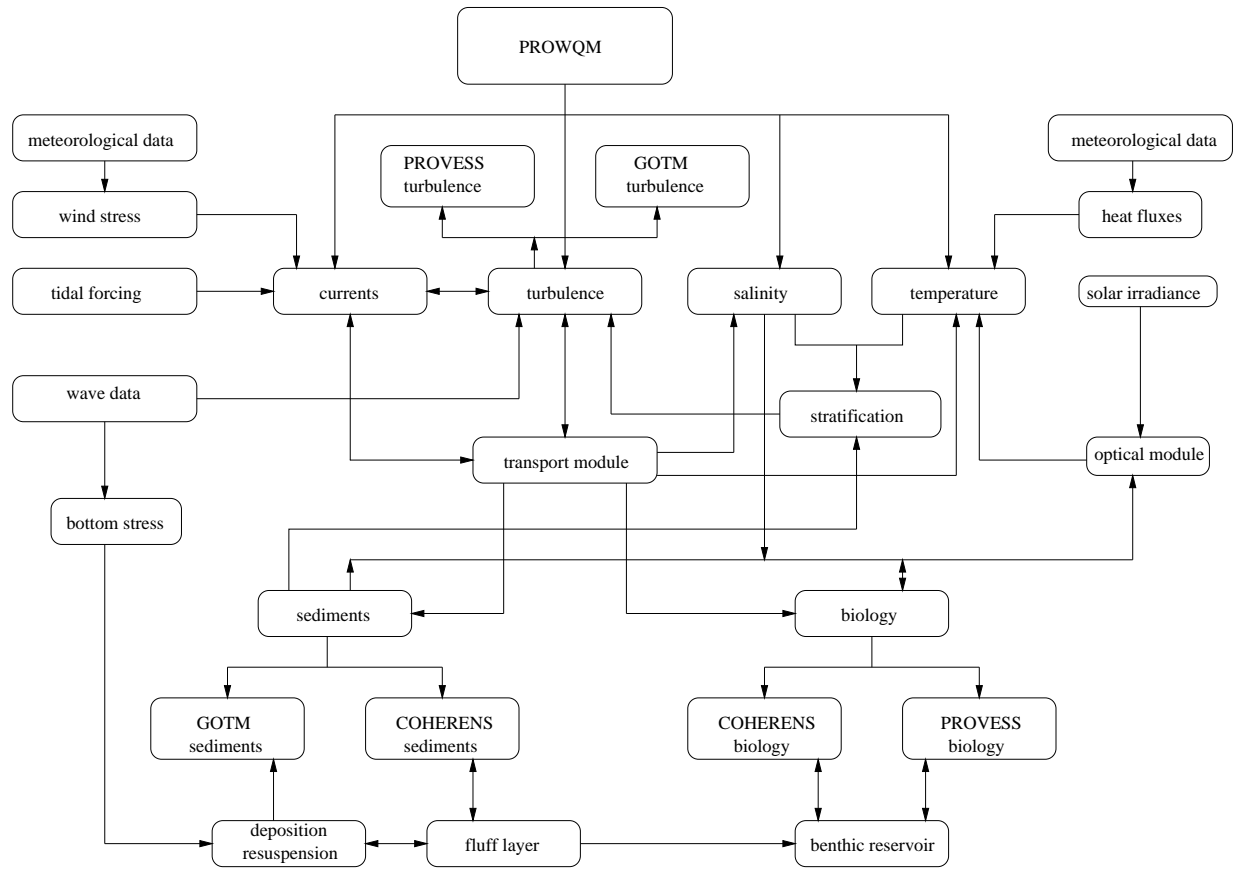


Figure 1: Structure map of the PROWQM model.