DEVS-Scheme simulation of stream water quality

Piotr L. Jankowski
University of Idaho
and
Jerzy W. Rozenblit
University of Arizona

Abstract

This article describes an approach to simulation modelling of natural system by employing Multifaceted Modelling Methodology. Basic tenets of the modelling framework and its implementation are explained. The application is focused on modelling stream water quality. An example of multi-segment stream water quality model is developed using Discrete Event System Specification. Preliminary simulation results are presented and compared with conventional single-constituent models.

1. Multifaceted Simulation Modelling

Multifaceted methodology denotes a modeling approach which recognizes the existence of multiplicities of objectives and models in any simulation project. It provides formal representation schemes that support the modeler in organizing the model construction process, aggregating of partial models, and in specifying simulation experiments (Zeigler, 1984). Modeling objectives drive three fundamental processes in the methodology; they facilitate the construction, retrieval, and manipulation of entity structures (Rozenblit and Zeigler, 1986, 1988), selection of model structures, and specification of experimental conditions under which models are evaluated by a simulation study.

The entity structure is a knowledge representation based on a tree-like graph that encompasses the boundaries, decompositions and taxonomic relationships that have been perceived for the system which has been identified as a component in one or more decompositions. Each such decompositions is called an aspect. Thus entities and aspects are thought of as components and decompositions, respectively. In addition to decompositions, there are relations termed specializations. A specialization relation facilitates representation of variants for an entity. Called specialized entities, such variants inherit properties of an entity to which they are related by the specialization relation.

Aspects can have coupling constraints attached to them. Coupling constraints restrict the way in which components (represented by entities) identified in decompositions (represented by aspects) can be joined together.

In addition to coupling constraints, there are selection constraints in the system entity structure. Selection constraints are associated with specializations of an entity. They restrict the way in which its subentities may replace it in model construction process. Synthesis constraints restrict ways in which entities selected from specializations may be configured to represent the structure of the system being designed (Rozenblit and Huang, 1987). The process that employs the production rule formalism to support automatic selection of entities and synthesis of model structure is called rule-based driven model structure generation.

Models can be expressed in special formalisms depending on the problem at hand. Typical specifications include differential equations, finite state machine, or discrete event. Each formal model description specifies a system and selects a class of subsystems by placing constraints on the possible static and dynamic structures it encompasses. A characterization of such constraints is given in (Zeigler, 1984). The model construction process involves the specification of the static and dynamic structure. In our methodology, models are developed using Discrete Event System Specification (DEVS) formalism. This formalism underlines the construction of models in the simulation environment - DEVS-Scheme.

2. Stream Representation in a Water Quality Model.

In modeling of water quality in streams with relatively stable flow conditions a *steady-state* assumption is commonly used. This assumption implies that one can distinguish a section of stream, called in the literature a *reach* (Loucks et al. 1981, Orlob et al. 1983) or a *segment* (Dorfman et al. 1972, Hanssmann 1976), in which mass inflow and outflow are constant in time. Hence, under steady-state conditions, a stream treated as a one-dimensional, contiguous body of water can be represented as a cascading sequence of segments (non-branching network). Such a network of connected segments (reaches) has been the dominant conceptual scheme of representing a stream in water quality models (Grimsrud et al. 1976, Loucks et al. 1981, Orlob et al. 1983, Whitehead 1983). An important issue in such a conceptual representation is the creation of segments along the course of a modeled stream. The criteria for the stream segmentation can be stream topological properties (e.g. a point of tributary inflow) as well as the indicators of changes in hydrological and biological conditions.

3. System-Analytical Specification of Stream in a Water Quality Model.

In systems analysis terms the system under study - a stream or a section of a stream can be viewed as a collection of components - stream segments (Wilson 1981). Such a collection can be abstracted as a set S and its components as $\{s_1,s_2,s_3,\ldots,s_k\}$, where $s_i \neq s_j$ and $i, j \in (1,2,3,\ldots,k)$. A structure of the system can be represented by the set S and a coupling of its components (Zeigler, 1984). A coupling of the system components can be defined as a structure:

$$N = < S, I_l, M_l >$$

where in the case of a non-branching, single stream:

I_l is a set of stream segments preceding segment s_i , $i \epsilon (1,2,3,...,k)$, $l \epsilon (1,2,3,...,k)$,

M_l is a mapping function that connects a s_{i-1}-th segment with a s_i-th segment.

In a more general case of a branching stream channel (see Figure 1), M_l is a mapping function that connects multiple s_j segments, where $j < i$, with s_i segments.

A non-branching network is an appropriate model for the coupling scheme of stream segments. The concepts of coupling as the scheme of linking the stream segments can serve as the conceptual basis of hierarchical, modular system specification. Such a specification provides a modeling paradigm for prediction of stream water quality that is an alternative to the traditional and widely used nonhierarchical one-model specification. In the hierarchical, modular system specification the modeled system is always viewed as an entity comprising of some finite number of entities distinguished at each level of hierarchical decomposition. The structure and behavior of each entity is described by its model. The models describing terminal entities are called atomic models. The models describing higher level entities are called coupled models. In the stream water quality modeling context, an atomic model can represent a single-constituent water quality model of one segment and a coupled model can represent the water quality model of a stream consisting of multiple single-constituent (not necessarily the same ones) segment models. At the higher level of hierarchical specification one can have a coupled multiconstituent model of a stream.

4. System Entity Structure Framework for Hierarchical and Modular Specification for Stream Water Quality Models.

System Entity Structure (SES) (Zeigler 1984, 1987a) is a declarative knowledge representation scheme that can be used to express hierarchical and modular specification of stream water quality models. The entity structure for a single-constituent water quality model represents a model space from which alternative configurations of a single-constituent stream water quality model can be derived. A prototype of the entity structure tree for a stream water quality model is presented in Figure 2 (Jankowski, 1989).

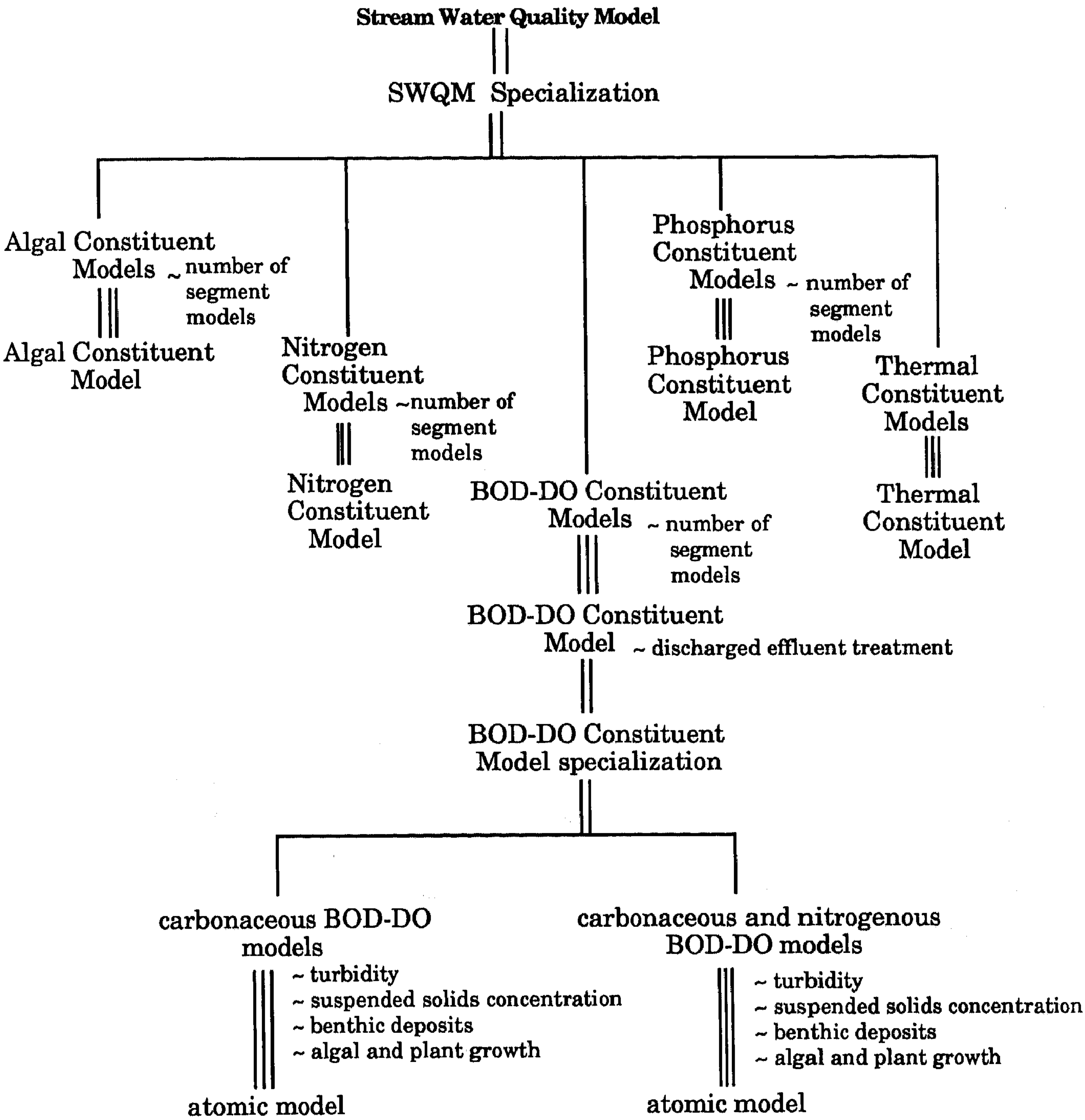

Figure 1. An entity structure tree for single-constituent stream water quality models.

The root entity - named "Stream Water Quality Model" - denotes a single-constituent model of a river basin or a section of it. It is specialized into five entities: "Algal Constituent Model", "BOD-DO Constituent Model", "Nitrogen Constituent Model", "Phosphorus Constituent Model", and

"Thermal Constituent Model". Each specialized entity has the attached variable "number of segment models" which, together with the multiple specialization, represent the number of segments partitioning upon the segmentation criteria (topological, hydrological, geomorphic, and biological) a given stream, and the number of single-segment, single-constituent models.

Each of the five entities can be specialized into subentities denoting a constituent-specific type of atomic segment-model. In the design of the system prototype, presented in this research, only the subentities resulting from the specialization of the "BOD-DO Constituent Model" entity are further specialized. This is sufficient to demonstrate the validity of the proposed entity structure for the entire modeling domain. The entity "BOD-DO Constituent Model" representing a BOD-DO model type is specialized into two entities: "carbonaceous BOD-DO models" denoting those BOD-DO models which take into account only the carbonaceous oxidation of the organic matter contained in the discharged sewage, and "carbonaceous and nitrogenous BOD-DO models" representing those BOD-DO models which account for the carbonaceous and nitrogenous oxidation of organic waste components. A variable "discharged effluent treatment" attached to the "BOD-DO Constituent Model" entity can receive the values: none, mechanical, biological. These values play the role of pointers to two specialized entities "carbonaceous BOD-DO models" and "carbonaceous and nitrogenous BOD-DO models". The "carbonaceous BOD-DO models" entity is further specialized (multiple specialization) into a segment-specific atomic model. Similarly, the "carbonaceous and nitrogenous BOD-DO models" entity is specialized into a segment-specific atomic model representing carbonaceous-nitrogenous BOD-DO atomic segment-model.

5. DEVS-Scheme Implementation of Hierarchical and Modular Specification for Stream Water Quality Models.

The DEVS-Scheme software environment is based on the Discrete Event System Specification (DEVS) formalism for representation of discrete event simulation models (Zeigler, 1976, 1984). In this formalism a model is defined by the structure:

$$M = \langle X, S, Y, \delta int, \delta ext, \lambda, ta \rangle$$

where:

- -X is the external input event set,
- -S is the sequential state set,
- -Y is the set of external output events,
- -δint is the internal transition function dictating state transitions due to internal events,
- -δext is the external transition function dictating state transitions due to external events,
- -λ is the output function,
- -ta is the time advance function.

An important property of this formalism is that a DEVS model is closed under coupling (Zeigler, 1984), which means that any composite model obtained by coupling of DEVS models is itself a DEVS model.

The DEVS model definition is compatible with the network specification of the model of a river or its section. Hence, an atomic segment-model employed to calculate values of water quality indicators for the given segment can be implemented as a discrete event model in which:

-X is the set of constituent values and parameters characterizing the sewage effluent and the upstream quality of water entering the given segment (as well as values of bio-chemical reaction rates pertinent for the segment),

-Y is the set of constituent values calculated for the end of the segment. These values are transferred by the output function λ from a k-l segment as its output to a k-l+1 segment as its input,

-S is the set consisting of two states: active - when the model is engaged in calculations upon receiving an external input x, and passive - after the results have been transferred to the next contiguous atomic segment-model and the next external input has not yet arrived,

-δint changes the active state to the passive state after an output event has occurred,

-δext calculates constituent values for the set of spatially oriented (along the longitudinal dimension of the water flow) points inside of the segment, upon receiving the initial constituent values,

-ta advances the time for which a model is allowed to stay in the active state without the occurrence of the external input event.

As a result of the closure under coupling property the coupled model of a river or its section consisting of the DEVS-implemented atomic segment-models is also a DEVS model.

The DEVS-Scheme implementation of the entity structure for point-source, single-constituent stream water quality models is depicted in Figure 3 (Jankowski, 1989).

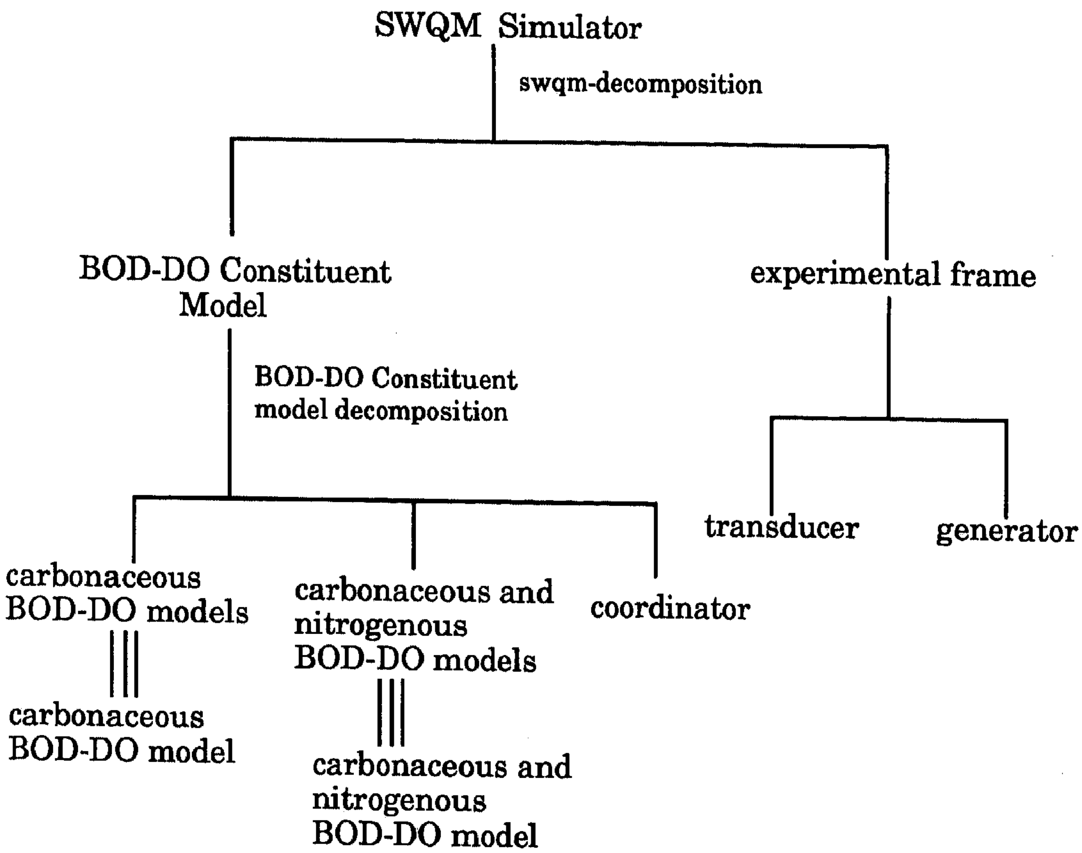

Figure 2. A composition tree underlying the structure of the DEVS-Scheme simulator for a stream water quality model (SWQM).

Figure 2 presents the DEVS-Scheme implementation of the system entity structure depicted in Figure 1. Comparing Figure 2 with Figure 1 one can notice some differences between the design (Fig.1) and its implementation (Fig. 2). In the DEVS-Scheme implementation the root entity "SWQM Simulator" is decomposed into "BOD-DO constituent-model" and "experimental frame" entities. The "BOD-DO constituent model" entity is is further decomposed into two entities representing atomic segment-models: carbonaceous BOD-DO models, carbonaceous and nitrogenous BOD-DO models, and a model coordinator labeled as "coordinator". The multiple decomposition of the entities carbonaceous BOD-DO models and carbonaceous and nitrogenous BOD-DO models represents the multiple instances of both models.

The entity "coordinator" in the Figure 2 represents an atomic model whose function is to coordinate a sequence of inputs and outputs of the atomic segment-models during the simulation. The function of the model coordinator is depicted in Figure 3. The coordinator receives input values from the generator. The input values represent various conditions of of water quality, upstream from the first segment of the given river basin or its section,

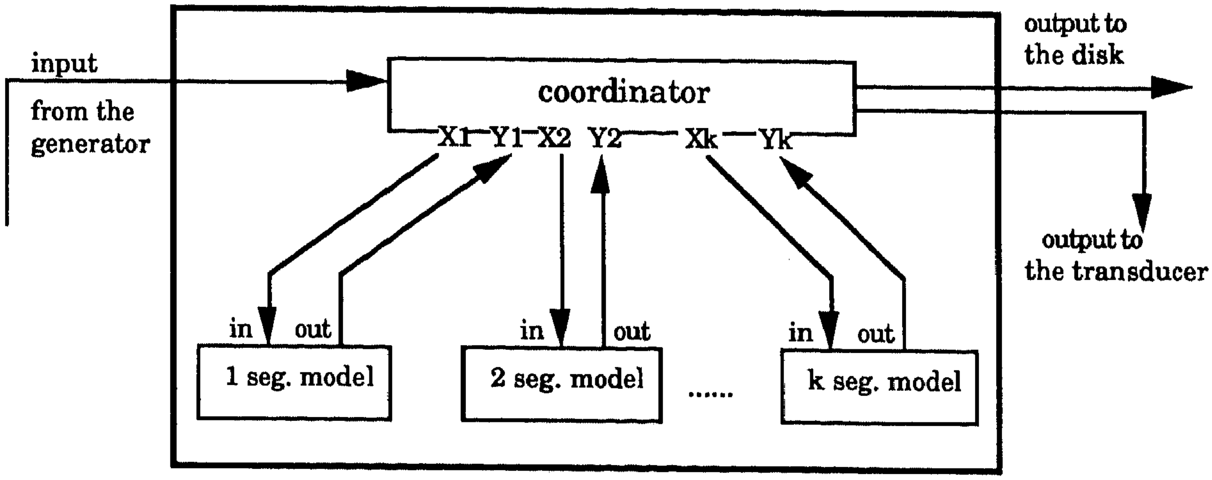

Figure 3. Functional specification of the model coordinator.

expressed by dissolved oxygen deficit (DOD) and biochemical oxygen demand (BOD). The input value pairs (DOD, BOD) are transmitted from the coordinator through the output port X1 to the first segment-model's input port "in". Values of DOD and BOD, for the endpoint of the first segment, are then calculated by an atomic segment-model selected for the "1 seg. model". Subsequently, the calculated (DOD,BOD) pair is sent out of the "1 seg. model" through the port "out" and received by the coordinator on the input port "Y1". The coordinator transmits the pair of values (DOD,BOD) to the next segment-model, "2 seg. model", through the output port "X2" and simultaneously sends it to a log-file on the disk. The process continues until the last pair (DOD,BOD) is calculated for the endpoint of the last k-th segment. The last value pair (DOD,BOD) is sent to a file and also to the transducer - a component of the simulation frame.

6. Evaluation of Simulation Results.

Preliminary simulation tests were run to assess the performance of the DEVS-Scheme implemented hierarchical and modular specification for stream water quality models. A 222 km long section of the Warta River, the main tributary of Odra River and the third largest river in Poland, was used for the test. The simulation was run for the initial value pair: BOD = 17 [g/m^3] and DOD = 8 [g/m^3], reflecting average water quality conditions for the summer period, upstream from the first segment of the section. The initial BOD and DOD values reflect the high level of water pollution in the river. The results of the simulation runs were than compared with the observed values of water quality indicators and values obtained by simulating a nonchierarchically specified single-constituent model. The average error of water quality prediction obtained from the DEVS-Scheme specified model was 4% versus the average error of

12% for a traditionally (nonchierarchically) specified single-constituent model. These results, however very preliminary, suggest that a DEVS-Scheme based hierarchical and modular model specification can be robust in modeling and simulation of stream water quality.

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