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Contributions of IT and SE in Water Sciences Modelling

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Advent of computers and computational techniques as well as rapid advancements in the development of fast computing systems had significant contributions on enormous successes in investigations in the fields of aquatic ecology, environmental and/or water science/engineering. Most of the computational outputs in the fields of water science are complex and not easily comprehensible by common people. As such different visual animation techniques have been used in the past for demonstrating complex computational outputs to common people. Through advancement of software technology, development of utility tools to create visualization of several ecological/environmental/hydraulic processes has become comparatively easy. Through charismatic colour schemes, these visualizations often produce significant impressions to the end-users and audience. People tend to forget the accuracies of these visualization clips/videos, often not demonstrated along with sufficiently acceptable scientific supporting accuracy protocol/measurements.

In regards to nature of investigations 'water science' can be broadly categorised in to three categories: 1) physical water science, 2) chemical water science and 3) biological water science. All of these categories usually have close interactions, however in early days computational tasks predominantly dealt with the physical water science mainly due to following reasons: many of the chemical and biological processes were unknown, most of the chemical and biological processes are complex and concerns on water quality was not that prominent. However, with the ever increasing urbanisation and increase in population, water quality (WQ) issues becoming more and more critical. For the investigations of most of the water quality issues chemical and biological water sciences are inter-related. Physical water science problems can be dealt independently, however chemical and biological water science problems require solutions on physical science matters as well, unless the concerned system is closed and non-dynamic/stagnant.

In early days the physical water science problems were investigated with the help of simple 'water balance modelling' concept, basic principle of which is that for a water/liquid system difference of volumes of inflow and outflow equals to the change of storage in the system. However, this simple concept is not accurate enough for many water science problems, especially for unsteady, non-uniform, dynamic and multi-dimensional flows. To gain higher accuracy, for many water systems a three-dimensional analysis is recommended. As for example, a large lake, a large river, a large aquifer and the ocean systems warrant a three-dimensional analysis. Consideration of three-dimensionality becomes more crucial when chemical and biological parameters are to be analysed for those systems. Three-dimensional flow equations for those systems are complex, difficult to solve and require suitable numerical representations. With the advancements of numerical techniques and fast computing solutions of those problems became easy.

In regards to surface and ground water hydrology/hydraulics, computational methods and processes are fairly simple and well-established. Integration of water quality components also simple and do not warrant the need for super-computing and further development of IT/SE. However, it is possible to reduce the computational time for some long-period simulations.

For the large water systems, in addition to considering three-dimensionality, stratification or multi-layered flows add further complexity. Phenomena of mixing among adjacent layers are more complex. With the application of advanced numerical techniques it is possible to solve these problems with sufficient accuracy. However, the greatest challenge of these computations remains the 'numerical instability', which often produces unrealistic results and causes an immature termination of the computations. Applied mathematics needs to be developed more to overcome this issue or to be able to solve complex PDEs without the use of numerical representations. Development of IT had significant effects on reducing computational time related to those investigations.

With the rapid urbanisation and population growth, the emerging need is to deal with critical WQ issues. In the past WQ investigations were mainly limited to expensive field monitoring and laboratory testing. With the developed modelling techniques it is possible to incorporate WQ parameters in all the above-mentioned modelling tasks. Accurate calculations of some WQ parameters such as carbonate/bi-carbonate and pH still requires lots of improvements and in some cases yet to be established through physical laws. Calculations of micro-organisms and nutrients are generally performed through simple equations using conceptual models. For a dynamic system, variations of WQ parameters are largely influenced by physical parameters (flow, volume, velocity etc.), which is defined as convection. As such for the calculations of WQ parameters, accurate calculation of physical parameters is also important. It is a common practice that variations of WQ parameters due to physical and chemical/biological actions are calculated separately, then these two/three variations are averaged within a short time-step to achieve the final variations. This averaging simplification is acceptable only for very short time-step, which requires fast computing to get solutions within reasonable time.

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