Peer Review of the Regional Simulation Model

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Introduction

The South Florida Water Management District held an expert workshop to review recent enhancements to the Regional Simulation Model (RSM) numerical solutions on April 23, 2019. This resulted in reports from two experts (Dr. Murugesu Sivapalan and Dr. Gabor Tóth) on the appropriateness of numerical formulations used in RSM. These reports can be found in Appendices B and C.

The South Florida Water Management District then commissioned a panel to perform a peer review of the Regional Simulation Model and its elements, the Hydrologic Simulation Engine (HSE) and the Management Simulation Engine (MSE). The members of the Panel were Dr. Rafael L. Bras (Chair), Dr. Victor M. Ponce, and Dr. Daniel Sheer. The Panel reviewed material and prepared for a workshop that was held July 24 and 25, 2019 at the offices of the SFWMD in West Palm Beach, Fl. This report is based on the outcome of that workshop and the review of material before and after the meeting.

The Scope of Work listed the following goals for the Peer Review:

1. "Determining if object-oriented design and computational sequencing used in HSE/MSE of RSM is suitable for simulating the hydraulics, hydrology, and the operations control needs of the south Florida hydrologic system;"
2. "Evaluating if the "multiple editions" approach to numerical solutions is appropriate for use in regional hydrologic modeling in south Florida, and if this perpetual evolution is leveraging the proper disciplines and approaches and translating them correctly; "
3. "Determining if the RSM is generally applicable for hydrologic modeling in south Florida."

In the process of seeking answers to the above questions, the Panel raised several issues that we will discuss in some detail in the body of the report. Our responses to the questions can be summarized in the following way:

1. The object-oriented modular design of RSM is valuable. The idea that elements can be added almost at will and solved within the same numerical framework is attractive. The platform can effectively integrate the expertise of many. The downside is that the framework is computationally complicated and its mastery challenging.
2. The Panel found the "multiple editions" confusing at times, although the appropriateness of solutions and techniques is not in question. As will be pointed out, the Panel advocates for a true integration of models.
3. The Panel feels that the RSM formulation is appropriate to the hydrology of south Florida. See also Appendices B and C for additional expert comments on the numerical

formulations within RSM.

Before going further, the Panel wishes to express its appreciation to the staff of the District for its preparation and cooperation. Furthermore, the Panel states that the District has a good product and dedicated employees who work well under resource-limited conditions.

The following sections address issues that arose during the workshop, all related to the three questions above.

What is the mission? What is the right level of complexity?

It is important that model development be guided by the problem at hand. Once the problem is identified and understood, then the question is what is the proper modeling approach to solve that problem. It is easy to be absorbed by the modeling and the tool development and lose sight of why we are doing it and what is the problem to be solved. Complexity does not necessarily "make best."

MSE development

1) The existing MSE is quite coarse, with a limited number of rule forms available to a user.
2) Creating objects that implement new rule forms requires programming in C++, and is and will be beyond the capability of other than model developers or those rare individuals with both programming and water resource management experience.
3) A simple language that allows a non-programmer user to create new operating strategies for both individual objects, basins, and system wide would be highly desirable. A parser could translate that language to XML.
4) The use of assessors to describe implement complex, multi-structure, multi-objective operating policies presents many challenges. It requires complex custom coding in C++, often including custom and complex iteration schemes. In non-dendritic systems, the use of optimization schemes may be required. An LPSOLVE based scheme for implementing management strategies has been formulated and implemented for the RSM as an alternative to the use of assessors. A more capable formulation with a simple language to aid users in formulating new rules is recommended, along the lines of OASIS (which uses OCL) or CALSIM (which uses the WRESL and WRESL+ languages). These languages allow complete user control of the optimization formulation based on the system state at the current (or previous) time step, including meteorological and other forecasts. In addition, capabilities for continuous balancing of weighted deviation from targets, iteration to convergence, and others that require the iteration of the solver itself are highly desirable. The OCL MINIMAX and SOLVE commands provide examples of this capability.

5) The SFWMD may wish to consider if model utility is the overarching goal of RSM development. If so, tradeoffs between utility, cost, time to completion, open source and other coding requirements should be carefully weighed.
6) To be truly useful to those without access to the model developers, the MSE needs a fully functional GUI. There are many water management simulation software packages with GUIs that can serve as design guides. Features such as metadata inclusion, automatic documentation of model modifications, and ability to include information on the rationale for changes will be extremely important if the model is to be used for operations support. Ability to easily input operations changes will be extremely important. Input of physical data that is less likely to change between alternatives might be handled separately. The New York City Operations Support Tool, CALSIM, RESIM, WEAP, RIVERWARE, MIKE BASIN, and other commercial GUI's all have features that will be desirable in a GUI for the RSM.

Models integration

It is difficult to follow the different "model editions". The Panel was confused with and surprised by the fact that the basin model and the mesh model (above and below the "red line") were not integrated. The lack of integration limits utility and make full utilization of RSM by other than agency staff very difficult. The lack of integration should be made very clear in any presentation or discussion.

The approach of setting gate openings and running a much shorter time step holds promise for computational efficiency, temporal resolution and linkage with MSE. In particular, a Basins-structured LP-based MSE could determine flows at structures. These flows could be converted to gate openings, and the grid-based model run. Actual flows at gates set by MSE would be different coming out of the grid solve. These could be set as constraints in the MSE which would then be resolved to provide a consistent solution for both models. This approach might resolve the problem of integrating the Basins and grid solutions and should be pursued.

Another example of lack of integration is the "hydrologic process modules" output serving as input to the mesh model. Logically, it should be integrated into a common model. This can lead to reconciliation, compatibility problems, particularly in natural systems. It was argued that subsurface storm runoff was a dominant process in the region. The Panel doubts this is the case, which was also questioned by Dr. Sivapalan in his review (Appendix B). The discussion seemed to imply that the issue is one of nomenclature and the solution is valid for the various alternative runoff mechanisms (i.e., Horton, saturation from below). This should be clarified and if the argument for subsurface storm runoff is to be made then some evidence of its dominance must be provided.

SFWMD has long recognized the need for higher spatial and temporal resolution models for particular issues in both planning and regulation. The Miami-Dade RSM implementation (MDRSM) is an example of such a model. This integration presents a challenge. A standard protocol for obtaining and validating boundary conditions for smaller scale models from the larger scale RSM must be developed. Such a scheme might set tolerances for agreement on boundary flows where heads are used as boundary conditions (or vice versa).

The RSM code contains a large number of features that can be combined in a variety of ways to address problems of varying complexity. The developers have combined various sets of features into “editions” to assist modelers in using features that have been tested to work together appropriately. There is source code control and versioning, and every modeling project report specifies the code version number that was used for a specific edition or model application. This can be confusing and there is a need to provide clarity on the concept of RSM editions to avoid confusion for model implementers.

Model management/Modeling documentation

As stated previously, the RSM is complicated to run, maintain and use. At the same time, it is a key and accepted tool (as was well articulated in the meeting by state and federal agencies and non-profits working on the Everglades and south Florida). The Panel recommends:

1. Users manuals and complete documentation are urgently needed. The Panel understands that resources are barely sufficient to keep the system going. The Panel urges the SFWMD to invest in documentation; this should be a priority.
2. Ease of use and access must be a goal. The model needs a Graphical User Interface.
3. Users should have access to documented tools for the display of model output. This includes graphical displays. A suite of such tools should be made generally available. Output formats should remain stable for long periods to facilitate user development of new display and interpretation tools.
4. The District may wish to consider hosting RSM for outside use on a server. This may greatly simplify maintenance issues. It would also facilitate agency review of model runs by outside parties. Nevertheless, the inevitable outcome of opening access will be increasing demand for help and advice.
5. Provision should be made for external access to SFWMD data bases so that external users can set up their own models
6. External model developers may create enhancements to the SFWMD. When providing the RSM to outside users the SFWMD should, to the extent possible, encourage or require that such enhancements be available to the SFWMD for internal use, or better, for general use. This includes external development of performance metrics.
7. Thought may be given to the formation of a users’ group, possibly involving licensing, sharing of development and of model use experiences.
8. It is inevitable that others will challenge the results of RSM using competing models. Thought should be given and guidelines developed on methods to compare the results of differing models.
9. The District needs to develop standard procedures for the review and verification of both internal and external runs.

10. The Panel is concerned about continuity of staffing and expertise. At the moment there is a cadre of senior experts that are irreplaceable. Younger people need to be brought in and/or expertise has to be developed throughout a broader community.
11. Desktop computer CPUs with up to 64 cores/128 threads are now or will soon be available for ~$5K or less. The bottom line is that computational facilities continue to get faster and cheaper. Further, distributed computational cycles are readily available at very affordable prices from providers "in the cloud". The potential for using such options should be investigated since they could greatly reduce run times for the mesh portions of the model.

Model and input error

1) There was no comprehensive analysis of the nature of overall model errors, the difference between observed and simulated results. It is important to note that there are errors in model simulation of physical parameters, e.g. flows and stages, and there are errors in the model simulation of performance metrics. While these are related, they are NOT the same, and both need to be analyzed.
2) A close examination of time series comparisons of model errors and scatterplots is likely to reveal the existence of systemic errors, and a more thorough statistical examination of the relationship between errors and model input, output and perhaps most importantly performance metrics values may reveal the existence of systemic errors. It is desirable to have the relationships between errors and input, output, and performance metrics values be normally distributed and homoscedastic. If they are not, empirical corrections may be added to model output to correct systemic errors. There are many techniques for making such adjustments and they are likely to improve the relationship between presented values and realistic expectations of the impact of alternatives being evaluated. This should improve estimates of variance of results and otherwise greatly improving the utility of model results. Some references to techniques for model error analysis are attached.
3) The time series of model errors from calibration and verification can be useful as direct corrections to model runs. They can be added to model results as either innovations (percentages) or absolute values depending on the underlying processes, when the same historical drivers are used in simulation runs. In other cases, or where longer simulations are needed, time series of synthetic errors can be developed using the statistics of the calibration/verification errors, and these time series added to the model results. Care must be taken to preserve both serial and spatial correlation of errors in the synthetic error time series.
4) Model inputs, and particularly meteorological inputs are subject to substantive deviations from actual values and contribute to model error. It is useful to understand the nature of these errors and to identify systemic errors in order to understand and correct for remaining sources of model error. Modifications made to model physical

parameters are sometimes made to reduce model errors that are largely due to errors in estimation of model drivers. There is substantial literature on methods to account for systemic errors in meteorological data. Use of these methods may considerably improve model calibration. The methods used by the NWS to correct such errors may be aimed squarely at the middle of the distribution of values, where the SFWMD's interest may concern correcting the value of the inputs at the extremes.

5) Once adjustments have been made for systemic errors and the implications of errors in model inputs (drivers) are understood, the effect of the approximations used in model formulation can also be better understood, and a priority scheme for implementing changes in model formulation can be developed.

Use of the full unsteady flow equations for flow in a horizontal channel

In the typical case, the forces acting on a 1-D formulation of unsteady open-channel flow are: (1) gravity, (2) friction, (3) pressure gradient, and (4) inertia. Significantly, in a horizontal channel the gravitational force vanishes, while the three other forces remain. This renders the Manning equation inappropriate, since the driving force in this equation is the gravitational force. Thus, for modeling unsteady flows in horizontal channels (the case of south Florida) there appears to be no other choice than to use the full Saint-Venant equations. A diffusion wave formulation may not suffice, because it neglects inertia. The latter is bound to play an increasing role in the momentum balance as the gravitational force vanishes.

The need to include lateral contributions (seepage in and out of the control volume) in the analysis of wave propagation in south Florida applications remains to be fully clarified. Great strides along these lines have already been made by SFWMD scientists. The additional terms in the mass and momentum balance equations need to be carefully identified. Their relative importance may be determined following the work of Ponce (1982). (see Appendix A for references)

Dynamic hydraulic diffusivity in convection-diffusion modeling of surface runoff

An established approach to modeling flood flows used in RSM is that of Hayami (1951), who combined the governing equations of continuity and motion (the Saint Venant equations) into a second-order partial differential equation with discharge *Q* as the dependent variable. This equation, effectively a convection-diffusion model of surface runoff, has been widely used in practice. It consists of: (1) a rate-of-rise term, (2) a convective term, of first order, and (3) a diffusive term, of second order. In Hayami's formulation, the coefficient of the convective term is the kinematic wave celerity (Seddon celerity); the coefficient of the diffusive term is the hydraulic diffusivity (Hayami diffusivity).

The hydraulic diffusivity used in RSM follows the original Hayami formulation of a diffusion wave, wherein the inertia terms (in the equation of motion) are neglected. This approximation works well for low Froude number flows. However, for high Froude number flows, the neglect of inertia proves to be increasingly unjustified. As shown in Ponce (1991), the true hydraulic diffusivity of the convection-diffusion model of flood flows is the *dynamic* hydraulic diffusivity, which is a function of the Vedernikov number (Powell, 1948). In fact, for Vedernikov ***V*** = 1, all wave diffusion vanishes and the flow is poised to develop physical surface instabilities, *i.e.*, the so-called *roll waves*. This fits admirably with physical reality, confirming the theoretical basis of the Vedernikov-dependent diffusivity, *i.e.*, the *dynamic* hydraulic diffusivity.

We recommend that a dynamic hydraulic diffusivity be incorporated into all instances where surface-water convection-diffusion is being modeled in RSM. This extension provides *a lot of bang for the buck*, since the structure of the computation remains basically the same. Ponce's formulation clarifies the work of Dooge and his associates, as recounted recently by Nuccitelli and Ponce (2014).

Numerical Methods, Accuracy and Errors

Computational efficiency

1) Run times for the models are currently undesirably, but perhaps not unavoidably, long
2) There was discussion of neural net and other AI based emulators for the model. This subject was outside the scope of work but is something to be further investigated.
3) All comments on error analysis made above apply to any model emulators as well. Errors should be assessed against data as well as against RSM results.
4) If a linear programing solver is used for the MSE it may well be possible to solve both the MSE and HSE in a single pass. This would largely eliminate the need for custom iteration schemes, except when linear approximation tolerances are exceeded. This should be pursued
5) Solvers other than LPsolve (the GNU solver tested) should be tested. Commercial solvers may be substantially more computationally efficient.

The appropriateness of the TVDLF

In its newest implementation, the RSM model uses the Total Variation Diminishing Lax-Friedrichs method (TVDLF), which is shown to be accurate and stable for both kinematic and diffusion flows such as those prevalent in Southern Florida (Lal and Toth, 2013). The method uses a linearized conservative implicit formulation of the simplified St. Venant equations, thereby avoiding the iterative formulations that would normally be necessary when solving a nonlinear scheme. SFWMD scientists have extensively tested the method, with favorable results in terms of numerical accuracy and runtime.

The success of the method in simulating a wide array of problems, including dry channel bed and steep bottom slopes, must be attributed to its use of weighting factors to incorporate numerical diffusion as needed to control the instabilities that would normally appear in connection with sharp (*i.e.*, nonlinear) changes in model variables. The panel welcomes the use of the TVDLF method and supports its continued use; the downside, however, is the increased level of complexity, compared to more conventional methods.

Stability and Convergence

The laws of mass and momentum conservation, which underpin all physical-process modeling of unsteady flows, may be combined, through appropriate linearization, into a single second-order, convection-diffusion equation (Hayami, 1951). In one extreme, when the diffusion term vanishes, the equation becomes hyperbolic; in the other extreme, when the convection term vanishes, the equation becomes parabolic.

Numerical models of hyperbolic systems are subject to the Courant law, which expresses the ratio of physical celerity (c) to numerical celerity ($\Delta x/\Delta t$), also referred to as the *grid ratio.* On the other hand, numerical models of parabolic systems are subject to what has sometimes been referred to (for lack of a better name) as the cell Reynolds number law, which expresses the ratio of physical diffusivity (ν) to numerical, or grid, diffusivity $[(\Delta x)^2/\Delta t]$. Both Courant and cell Reynolds numbers control the properties of numerical models of unsteady flow; their values should be calculated *a priori* (Ponce *et al.*, 2001).

The properties of numerical schemes may be analyzed using various tools of advanced mathematics. A time-tested approach uses Fourier analysis to develop amplitude and phase portraits following the pioneering work of Leendeertse (1967). Significant strides along these lines have already been accomplished by SFWMD scientists. Further clarification of various concepts appears to be in order at this juncture.

In hyperbolic systems, an assessment of numerical accuracy (*i.e.*, convergence) focuses on the spatial resolution $L/\Delta x$, where L is the predominant wavelength of the perturbation and Δx is the chosen space step. Generally, numerical models of hyperbolic systems are shown to be more accurate when the grid size follows the characteristic lines, *i.e.*, for a Courant number $C = 1$, wherein the physical celerity c matches the grid ratio $\Delta x/\Delta t$. In theory, selecting a sufficiently high spatial resolution, say, $L/\Delta x \geq 100$ and a Courant number $C = 1$ should suffice. In practice, however, a certain scheme may lack enough numerical diffusion to confront the high-frequency perturbations that are likely to appear in well-balanced schemes; thus, additional filtering (numerical diffusion) is normally required to render the system workable.

For instance, there is a wealth of accumulated experience on the numerical properties of the well-known Preissmann scheme, wherein stability and convergence are determined by the spatial resolution $L/\Delta x$, the Courant number C, and the weighting factor ϑ (Ponce *et. al.*, 1978). The latter is required to control nonlinear instabilities which tend to plague the computation as the scheme approaches second order. Values of the weighting factor in the range $0.55 \leq \vartheta \leq 1$ are recommended, with values near the lower limit approaching convergence (to second order) at the expense of stability, and values near the upper limit approaching stability at the expense of convergence.

Choice of spatial resolution for good modeling practice

The determination of the proper spatial resolution lies at the crux of good modeling practice, as the experience with RSM clearly shows. No amount of time spent on this effort is wasted. Our recommendation is to start with a target spatial resolution $\Delta x / L \geq 100$. [The number 10 is definitely too low, and 1000 may be impractical]. Calculating spatial resolution entails an estimation of: (a) the mean flow velocity, (b) the wave celerity corresponding to the prevailing type of friction and cross-sectional shape, and (c) the wavelength of the predominant perturbation. Values of wave celerity for a comprehensive set of frictional formulations and cross-sectional shapes have been presented by Ponce (2014).

We recommend that the selected wave sizes remain within the diffusion wave range, since the dynamic wave range is very likely to be too diffusive to be of any practical interest (Lighthill and Whitham, 1955). The dimensionless wave propagation chart of Ponce and Simons (1977) may be used as a suitable indicator of the appropriate wave scale required to nail down the proper spatial resolution (see appendix).

So*lution Methods*

While implicit schemes are unconditionally stable, a similar statement may not follow for explicit schemes. This is certainly the case for both surface and groundwater flows. On this basis, implicit schemes are generally preferred over explicit schemes.

It may be true that implicit schemes are not subject to *an upper limit* on the time step in order to remain stable. However, the use of time steps greatly exceeding this limit renders the model inaccurate (nonconvergent). Thus, the use of implicit schemes with Courant numbers greatly exceeding 1 ($C >> 1$) must be viewed with extreme caution, begging for a Fourier analysis for proof of convergence. Furthermore, certain explicit schemes are not subject to a stability condition, as demonstrated by Ponce *et al.* (1979) in connection with convection modeling.

The tradeoffs between explicit and implicit schemes are, therefore, clear: While implicit schemes are more stable, they require matrix inversion and the actual time step is effectively limited in size by accuracy considerations. Explicit schemes, on the other hand, are simpler to develop and execute, requiring no matrix inversion and no downstream boundary (Ponce *et al.*, 1979; Ponce *et al.*, 2001). Viewed in this light, explicit schemes are poised to remain along implicit schemes in the tool bag of the numerical modeler of unsteady flows.

Summary

South Florida is one of the most intensely managed environments in the world. The control of its water resources dates back hundreds of years and is essential to the social, economic and ecological well-being of the region. During our visit several constituents including federal and state agencies, as well as not for profit institutions stated the need of a reliable, stable and credible representation of the region; a model that allows them to explore management alternatives, do planning, or study the impact of future climatic conditions. The Panel concludes that RSM serves that purpose and is suitable for simulating the hydraulics, hydrology, and the operations control needs of the south Florida hydrologic system. It builds on a legacy of models customized to represent the unique physical and water management demands of south Florida. The Panel does have several observations and recommendations discussed in the body of this report. Some of the key conclusions are:

1. There is concern about continuity of expertise. This is a complicated model, very much dependent on a few very knowledgeable individuals.
2. There is a need of investment on appropriate user interfaces (like GUIs), manuals and ways to facilitate access by outside users.
3. Model integration is important and encouraged, to allow the inclusion of basin and mesh footprints within one implementation. Hydrologic Process Modules should also be part of the model integration and not seen as super imposed models that provide boundary conditions at the soil surface.
4. Dominant runoff production mechanisms should be identified.
5. Model and input errors must be quantified and used to improve model results.
6. A diffusion wave formulation may not suffice in all parts of south Florida, because it neglects inertia. The TVDLF method is a good generic approach to the various formulations.
7. A dynamic hydraulic diffusivity should be incorporated into all instances where surface-water convection-diffusion is being modeled in RSM.
8. Criteria for determining time and space discretization must be founded on solid theoretical foundations.
9. Model complexity should be in tune with the problem at hand.

Appendix A

By Victor M. Ponce

This Draft Report contains Panelist Victor M. Ponce's contributions and recommendations after attending the South Florida Water Management District (SFWMD) Peer Review of the Regional Simulation Model's (RSM), held in West Palm Beach, Florida, on July 24-25, 2019. The specific focus of the peer review is on identifying strengths, weaknesses, and possible applications of the RSM model, with regards to its suitability for simulating the hydraulics, hydrology, and operations control needs of the south Florida hydrologic system. This report is a contribution to the Draft Report to be prepared by the Panel based on input of its three members and discussion thereof.

This review has concluded that the methodologies included in RSM are adequate for its use in south Florida. To improve and complement current efforts, the author recommends that District scientists spend additional time on the issues of numerical accuracy, particularly on the determination of the applicable Courant and cell Reynolds numbers for specific model runs. The author's experience in this area is offered to serve as a suitable framework for the analysis.

1. On strategies for model control to manage instabilities

All numerical models, and RSM is no exception, have a way of becoming unstable under a certain set of circumstances. Thus, it seems appropriate, at the start, to provide a general discussion on strategies for model control to manage instabilities. A good physically based mathematical model is based on generally accepted partial differential equations describing the relevant physical processes. RSM uses 1-D and 2-D formulations of watershed, channel, reservoir, and groundwater flow, coupling them as appropriate to better represent the physical reality at the chosen level of abstraction.

All numerical models suffer from problems of stability and convergence. Stability is related to roundoff errors; convergence to discretization errors (O'Brien *et al.*, 1950). A model run on a computer of infinite word length would theoretically be free from roundoff errors; therefore, stable. However, such a computer does not exist. The computers in use today typically have a 32-

bit word length, that is, each rational number is represented by a collection of 32 zeros (0) and ones (1), with an accuracy of approximately seven (7) significant digits. In practice, however, this accuracy is not enough; in the longer runs, roundoff errors propagate beyond the stated accuracy, eventually rendering the solution unstable.

Convergence, which is akin to accuracy (in the sense of *convergence to* the analytical solution), is determined by the size of the discretization, *i.e.*, the values of the discrete space and time steps, which are chosen by the person performing the modeling. In theory, the steps should be small enough to reduce the (n+1)th-order errors of an n-th order scheme to insignificant amounts. This is normally obtained by a careful choice of the discrete steps in order to achieve good spatial and temporal resolutions. The temptation may be to choose very small discrete steps; however, generally this is not the answer. Decreasing the discrete steps *increases* the number of computations required to reach a solution, thereby *increasing* the chance for round-off errors to propagate, not to mention the increased computer time required to get a solution.

In practice, the control of numerical instability is seen to be a careful balancing act: How to build a scheme that has enough numerical diffusion to handle the high-frequency perturbations that are responsible for the instability, while at the same time making sure that the solution itself is not being substantially affected by the artificially introduced numerical diffusion. This dilemma is at the crux of all numerical modeling.

The laws of mass and momentum conservation, which underpin all physical-process modeling of unsteady flows, may be combined, through appropriate linearization, into a single second-order, convection-diffusion equation (Hayami, 1951). In one extreme, when the diffusion term vanishes, the equation becomes hyperbolic; in the other extreme, when the convection term vanishes, the equation becomes parabolic.

Numerical models of hyperbolic systems are subject to the Courant law, which expresses the ratio of physical celerity (c) to numerical celerity ($\Delta x/\Delta t$), also referred to as the *grid ratio.* On the other hand, numerical models of parabolic systems are subject to what has sometimes been referred to (for lack of a better name) as the cell Reynolds number law, which expresses the ratio of physical diffusivity (ν) to numerical, or grid, diffusivity [$(\Delta x)^2/\Delta t$]. Both Courant and cell Reynolds numbers control the properties of numerical models of unsteady flow; their values should be calculated *a priori* (Ponce *et al.*, 2001).

The properties of numerical schemes may be analyzed using various tools of advanced mathematics. A time-tested approach uses Fourier analysis to develop amplitude and phase portraits following the pioneering work of Leendeertse (1967). Significant strides along these lines have already been accomplished by SFWMD scientists. Further clarification of various concepts appears to be in order at this juncture.

In hyperbolic systems, an assessment of numerical accuracy (*i.e.*, convergence) focuses on the spatial resolution $L/\Delta x$, where L is the predominant wavelength of the perturbation and Δx is the chosen space step. Generally, numerical models of hyperbolic systems are shown to be more accurate when the grid size follows the characteristic lines, *i.e.*, for a Courant number C = 1, wherein the physical celerity c matches the grid ratio $\Delta x/\Delta t$. In theory, selecting a sufficiently high spatial resolution, say, $L/\Delta x \geq 100$ and a Courant number C = 1 should suffice. In practice, however, a certain scheme may lack enough numerical diffusion to confront the high-frequency perturbations that are likely to appear in well-balanced schemes; thus, additional filtering (numerical diffusion) is normally required to render the system workable.

For instance, there is a wealth of accumulated experience on the numerical properties of the well-known Preissmann scheme, wherein stability and convergence are determined by the spatial resolution $L/\Delta x$, the Courant number C, and the weighting factor ϑ (Ponce *et. al.*, 1978). The latter is required to control nonlinear instabilities which tend to plague the computation as the scheme approaches second order. Values of the weighting factor in the range $0.55 \leq \vartheta \leq 1$ are recommended, with values near the lower limit approaching convergence (to second order) at the expense of stability, and values near the upper limit approaching stability at the expense of convergence.

An excellent example of the use of Fourier analysis in numerical modeling of flood flows is that of the Muskingum-Cunge model, a diffusion wave model that is based on the matching of physical and numerical diffusivities (Cunge, 1969). A review of the amplitude and phase portraits of the Muskingum-Cunge model, including an online calculator, has recently been accomplished by Vuppalapati and Ponce (2016).

2. On the appropriateness of the TVDLF model implemented in RSM

In its newest implementation, the RSM model uses the Total Variation Diminishing Lax-Friedrichs method (TVDLF), which is shown to be accurate and stable for both kinematic and diffusion flows such as those prevalent in Southern Florida (Lal and Toth, 2013). The method uses a linearized conservative implicit formulation of the simplified St. Venant equations, thereby avoiding the iterative formulations that would normally be necessary when solving a nonlinear scheme. SFWMD scientists have extensively tested the method, with favorable results in terms of numerical accuracy and runtime.

The success of the method in simulating a wide array of problems, including dry channel bed and steep bottom slopes, must be attributed to its use of weighting factors to incorporate numerical diffusion as needed to control the instabilities that would normally appear in connection with sharp (*i.e.*, nonlinear) changes in model variables. The author welcomes the use of the TVDLF method and supports its continued use; the downside, however, is the increased level of complexity, compared to more conventional methods.

3. On the use of a dynamic hydraulic diffusivity in convection-diffusion modeling of surface runoff

An established approach to modeling flood flows used in RSM is that of Hayami (1951), who combined the governing equations of continuity and motion (the Saint Venant equations) into a second-order partial differential equation with discharge Q as the dependent variable. This equation, effectively a convection-diffusion model of surface runoff, has been widely used in practice. It consists of; (1) a rate-of-rise term, (2) a convective term, of first order, and (3) a diffusive term, of second order. In Hayami's formulation, the coefficient of the convective term is the kinematic wave celerity (Seddon celerity); the coefficient of the diffusive term is the hydraulic diffusivity (Hayami diffusivity).

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4. On the choice of spatial resolution for good modeling practice

The determination of the proper spatial resolution lies at the crux of good modeling practice, as the experience with RSM clearly shows. No amount of time spent on this effort is wasted. Our recommendation is to start with a target spatial resolution $\Delta x / L \geq 100$. [The number 10 is definitely too low, and 1000 may be impractical]. Calculating spatial resolution entails an estimation of: (a) the mean flow velocity, (b) the wave celerity corresponding to the prevailing type of friction and cross-sectional shape, and (c) the wavelength of the predominant perturbation. Values of wave celerity for a comprehensive set of frictional formulations and cross-sectional shapes have been presented by Ponce (2014).

We recommend that the selected wave sizes remain within the diffusion wave range, since the dynamic wave range is very likely to be too diffusive to be of any practical interest (Lighthill and Whitham, 1955). The dimensionless wave propagation chart of Ponce and Simons (1977) (Fig. 1) may be used as a suitable indicator of the appropriate wave scale required to nail down the proper spatial resolution. Figure 1 is global and based on theory; therefore, it is preferable to alternative approaches containing empirical components.

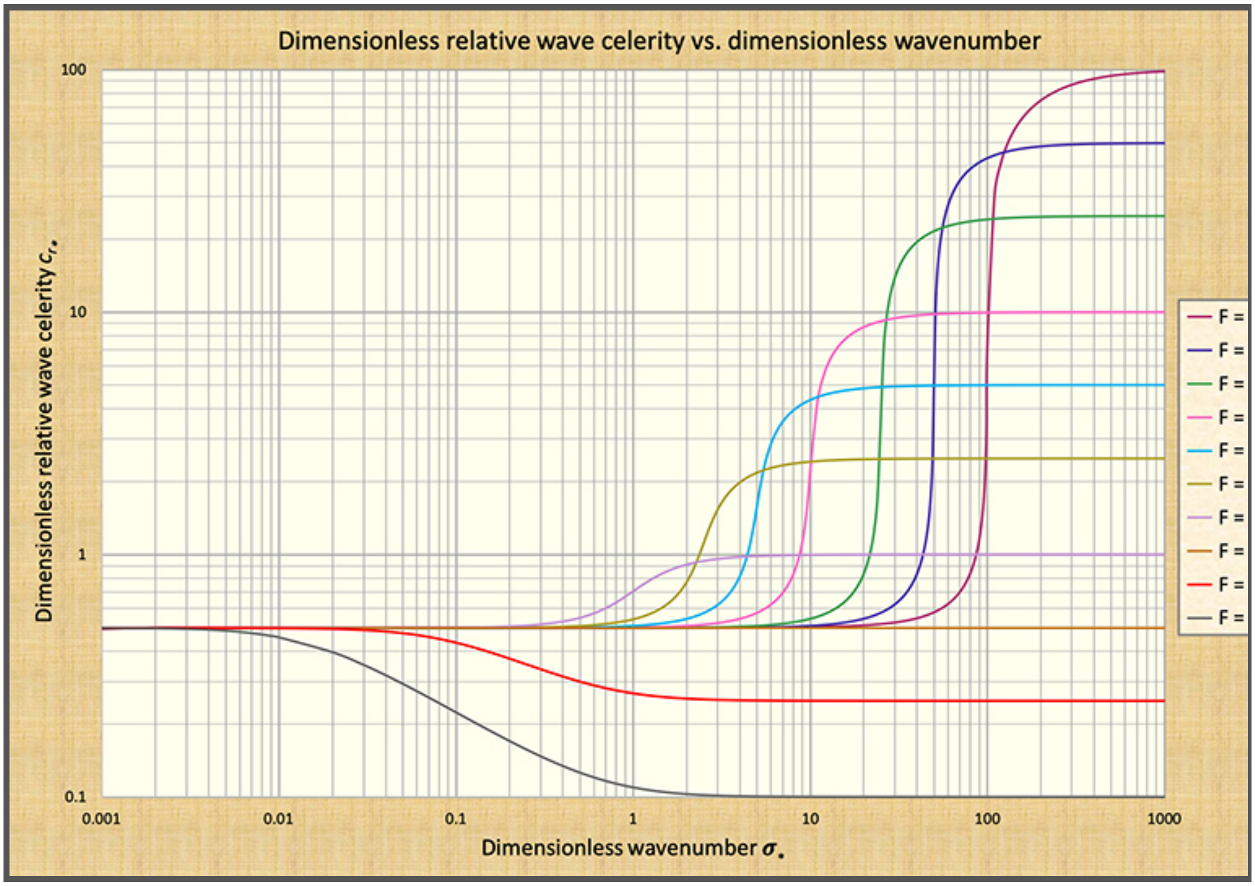

Fig. 1 Dimensionless relative wave celerity vs dimensionless wavenumber in open-channel flow.

5. On the comparative advantages of implicit vs explicit schemes

The choice between explicit and implicit schemes continues to haunt numerical modelers. While implicit schemes are unconditionally stable, a similar statement may not follow for explicit schemes. This is certainly the case for both surface and groundwater flows. On this basis, implicit schemes are generally preferred over explicit schemes, but the complete story remains to be told.

It may be true that implicit schemes are not subject to *an upper limit* on the time step in order to remain stable. However, the use of time steps greatly exceeding this limit renders the model inaccurate (nonconvergent). Thus, the use of implicit schemes with Courant numbers greatly exceeding 1 (C >> 1) must be viewed with extreme caution, begging for a Fourier analysis for proof of convergence. Furthermore, certain explicit schemes are not subject to a stability condition, as demonstrated by Ponce *et al.* (1979) in connection with convection modeling.

The tradeoffs between explicit and implicit schemes are, therefore, clear: While implicit schemes are more stable, they require matrix inversion and the actual time step is effectively limited in size by accuracy considerations. Explicit schemes, on the other hand, are simpler to develop and execute, requiring no matrix inversion and no downstream boundary (Ponce *et al.*, 1979; Ponce *et al.*, 2001). Viewed in this light, explicit schemes are poised to remain alongside implicit schemes in the tool bag of the numerical modeler of unsteady flows.

6. On the need to use the full unsteady flow equations for flow in a horizontal channel

In the typical case, the forces acting on a 1-D formulation of unsteady open-channel flow are: (1) gravity, (2) friction, (3) pressure gradient, and (4) inertia. Significantly, in a horizontal channel the gravitational force vanishes, while the three other forces remain. This renders the Manning equation inapproriate, since the driving force in this equation is the gravitational force. Thus, for modeling unsteady flows in horizontal channels (the case of south Florida) there appears to be no other choice than to use the full Saint-Venant equations. A diffusion wave formulation will not suffice, because it neglects inertia. The latter is bound to play an increasing role in the momentum balance as the gravitational force vanishes.

The need to include lateral contributions (seepage in and out of the control volume) in the analysis of wave propagation in south Florida applications remains to be fully clarified. Great strides along these lines have already been made by SFWMD scientists. The additional terms in the mass and momentum balance equations need to be carefully identified. Their relative importance may be determined following the work of Ponce (1982).

7. On the need for RSM model version numbers

The term "RSM model" is being currently used to describe any and all activities under the RSM modeling framework. This explains the District's (SFWMD) reluctance to engage in explicit model version numbers to describe what amounts to activities of varied scope and in many areas. The review failed to shed additional light on this important issue. We do not have a clear answer to solve this problem, namely, the inability of RSM to connect the various modeling activities and individual projects in time and space. We encourage SFWMD scientists to continue to focus on resolving this issue. [Chair note: see last paragraph of the Model Integration Section for clarification of the meaning of this comment]

8. On the need for consistency in model documentation

We recommend that SFWMD consider a thorough and full documentation of the RSM model via a technically edited User Manual, accompanied by a Reference Manual, as a way to ensure that potential users of the model will be able to use it in the future. Background material would consist of relevant published papers listed in the bibliography and included therein with hot links to online pdf files.

As an alternative, one certainly requiring fewer resources, the District could sponsor a publications series to be entitled, for example, *RSM Tecnical Monographs.* For consistency, each monograph would follow the same (or similar) format and describe in detail a specific portion of the model, using graphics and color as appropriate. This approach has the advantage that progress is not defined in terms of project completion.

9. Other miscellaneous recommendations

We offer the following miscellaneous recommendations:

a. The 2-D momentum equations originate in the 3-D Navier-Stokes equations, and, as such, are technically *not closed* (Flokstra, 1976; 1977). Some sort of surrogate for the missing effective stresses appears in order (Kuipers and Vreugdenhil, 1973). This is an obscure subject, perhaps deserving of more attention than that given so far.
b. Caution is recommended when using a 2-D formulation of a diffusion wave, wherein the inertia terms are neglected. Neglecting inertia is bound to eliminate physical circulation (Ponce and Yabusaki, 1981). However, it may be a reasonable assumption in the largely convective 2-D flows that prevail in south Florida.
c. The Muskingum-Cunge model of 1-D flood flows, effectively a diffusion wave model, has been analytically verified by Ponce *et al.* (1996). We suggest that the District consider including this verification test in their set of cases for model verification.

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Appendix B

Report of Peer review of Hydrological Model Used to Simulate South Florida Hydrology

Part 2: Hydrology and Hydraulics

Reviewer: Murugesu Sivapalan, Professor of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign , June 27, 2019

The "Regional Simulation Model" RSM is the hydraulic/hydrologic model currently used for simulating floods, flows through wetlands, etc. in south Florida by the SFWMD and the US Army Corps of Engineers. The model is designed to assist with water management in general and, in particular, assist with flood control, water supply, and address other environmental issues that are unique to South Florida.

This report is the outcome of a peer review of the latest version of the model and was focused on two aspects of the model: (1) Computational Methods – to make sure that the computational methods used to simulate the physical processes are accurate; (2) Physical Hydrology – to make sure that the physical processes in the hydrologic system are correctly represented in the computer model RSM.

The peer review was meant to determine if the methods, standards and procedures followed are acceptable under current hydrologic and hydraulic modeling practices, find out flaws that increase project risk, make corrections if needed, find improvements, and create a basis for documentation in the future. In particular, the reviewers were asked to comment on the following issues:

1. Determining if object oriented design and computational sequencing used in HSE/MSE of RSM is suitable for simulating the hydraulics, hydrology, and operational needs of the south Florida system;
2. Evaluating if the physical process identifications, conceptualizations, and numerical methods used in the model are appropriate for use in regional modeling in south Florida;
3. Confirming that the use of the governing equations and the theoretical foundation used in RSM is appropriate for south Florida conditions and the SFWMD mission;
4. Confirming the use of RSM as a framework for regional model implementation at SFWMD;
5. Confirming the presence of an open environment to incorporate new and evolving modeling concepts for changing conditions;
6. Recommending that the peer-reviewed model is a stronger candidate for certification by the US Army Corps of Engineers for use in CERP projects.

This part of the review (Part 2) focuses on the second aspect of the RSM model, i.e., physical hydrology (hydrology and hydraulics), especially in the upper parts of the upper basin, especially the appropriateness and fidelity of process descriptions. However, in some places I will comment on or raise questions about the numerical aspects of the model. The review, and the recommendations that arise from it, are based on various presentations made during a one-day workshop held at the Headquarters of the SFWMD at West Palm Beach, copies of which were made available to the review panel. The panel was provided with other supporting documentation (including papers), which guided me in my review. I also made copious notes during the presentations, which helped me to put together this report.

This review should be read in conjunction with the responses to my comments and recommendations from the modeling team. Some of the questions I have posed in this report may be beyond the scope of the review. I understand that they may be addressed in future extensions of the model and in future documentations of the model.

1. Overall Modeling Framework of RSM

Some of the unique features of South Florida hydrology that influenced the particular design of the Regional Simulation Model (RSM) include: (i) highly managed canal network, (ii) complex landscape, with slow reacting wetlands and highly reacting urban and agricultural areas, and (iii) interactive surface water and ground water and a system of unlined canals. The overall framework adopted in the RSM is geared uniquely towards capturing these features.

The following design choices have been made from the start of the development of RSM, and represent its main strength and uniqueness:

- Finite Volume Method
- Object Oriented Methodology (C++)
- Implicit solution using a sparse matrix solver
- Encapsulate the effects of local hydrology into Hydrologic Process Models (HPM)
- Separate Hydrology and Management
- Complexity derived through assembly of simple components.

The "Volume" in the Finite Volume formulation can include: canal segment, basin, lake, impoundment and WCD (water control district). These are the building blocks, or cells, of the model, which can represent different types of functions in the landscape and within the model:

- Water bodies that *retain* specific water masses
- Water movers that *move* specific water masses between waterbodies
- SV and VS converters for storage mapping
- Hydrologic Process Modules (HPMs) for simulating local hydrology

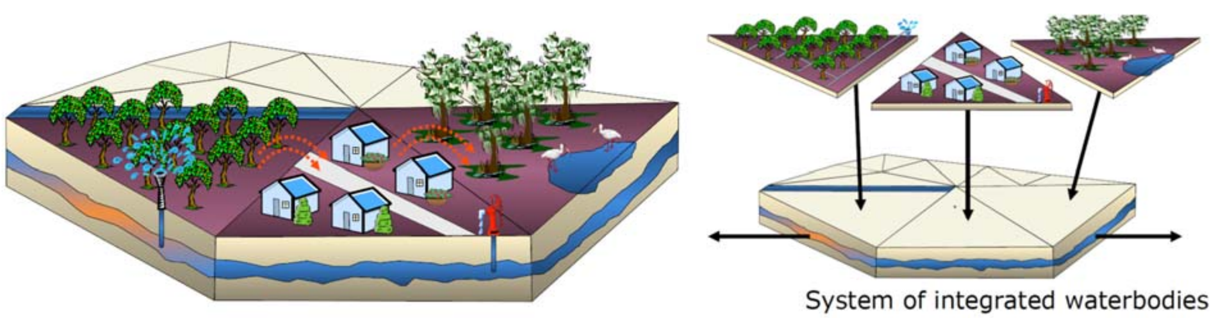

Figure 1: Partitioning of the landscape into different functional units or cells, as reflected in RSM

Development of the Finite Volume model involves application of the Reynolds Transport theorem to discrete elements (water bodies, water movers etc.), some of which include 2D surface and groundwater flow and some include 1D canal flow, and their interaction across mutual interfaces.

Development of the model also involved conversion from volume (storage) to water level, which is achieved through appropriate constitutive relationships (stage-volume relationships). The model also requires closure relations to represent exchange fluxes between different components (e.g., cell to cell surface and groundwater mesh flow, segment to segment canal flow, canal segment to mesh cell streambank flow, water body to water body flows via structures and pumps). These relationships are critical to achieving closure of the balance equations.

Hydrological Process Modules (HPM) include: rainfall-runoff models, evapotranspiration-infiltration processes, and surface, water management. Hydrological processes included in these HPMs include unsaturated-zone hydrology, surface hydrology, land water management practices, stormwater retention, water supply (consumptive use). Essentially these are aimed at fully resolving the complexity and heterogeneity of sub-grid processes, either explicitly through distributed models, or implicitly through parameterized, lumped representations. Inputs to the models are based on soils and land use derived from GIS geodatabases. The link-node configuration presented in Figure 2 illustrates well the overall framework adopted in RSM for a realistic application.

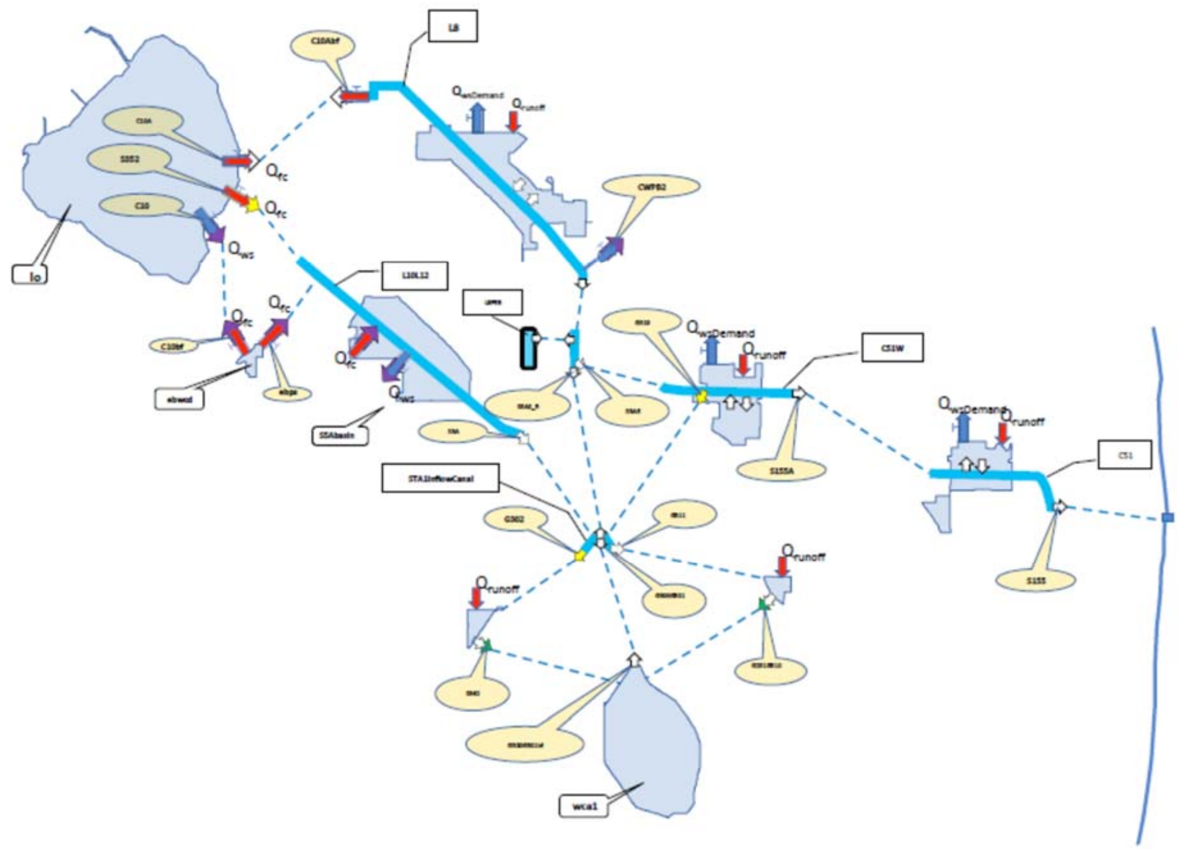

Figure 2: Link-node configuration of model implementation in a realistic setting.

There have been a wide range of applications of the model, which not only illustrate the adaptability of the model, but have also helped to bring out the enormous complexity and heterogeneity of water distribution across South Florida, and the challenges of water management. Two applications included in the documentation, one in Florida (Lal, van Zee and Belnap, 2005; see Figure 3) and the other in Colombo, Sri Lanka, are illustrative of the potential of the model.

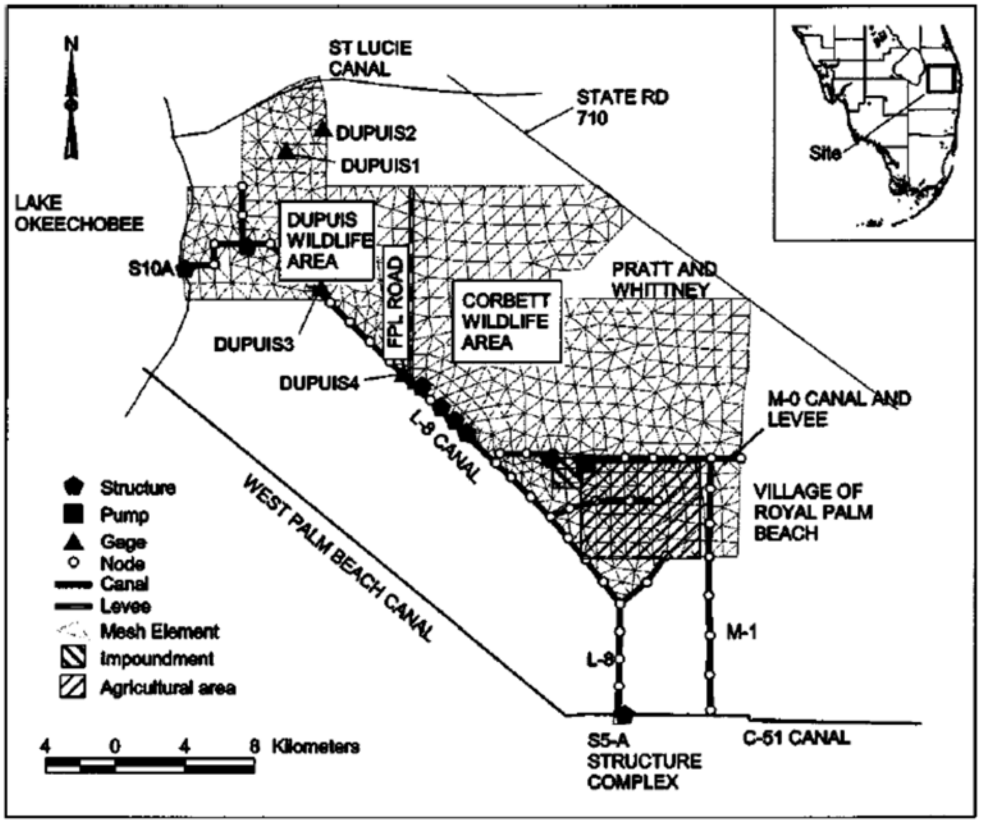

Figure 3: Example application of RSM in South Florida: L-8 Basin

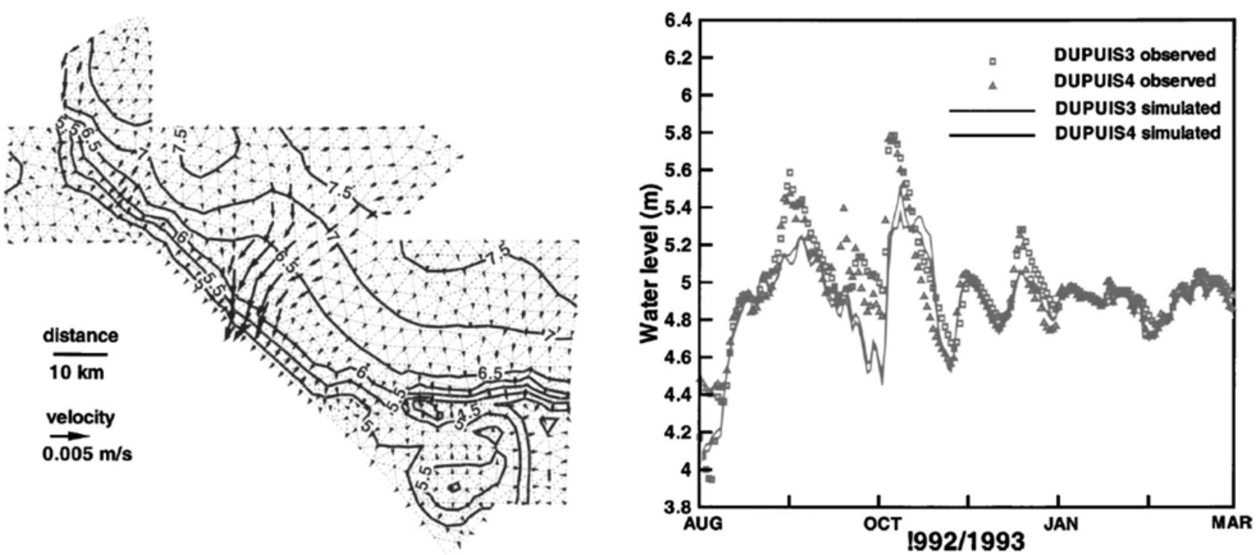

Figure 4: Typical results of application of RSM to the L-8 Basin: (Left) water levels and flow velocities; (b) comparison of observed and simulated water levels at an outlet.

2. Recent Model Improvements

The model documentation provided to the review team goes into considerable detail about recent efforts to capture more accurately localized flow features (e.g., within cells). These include improved parameterization of flow resistance to overland in wetlands, representation of runoff generation and routing in hillslope elements in steeper, headwater basins, and explicit accounting of the effects of micro-scale features in the exchange of fluxes between cells.

Mapping Functions between Abstract and State Variables: These, otherwise known as constitutive relationships, are needed to make the governing equations determinate. They appear in all physically based hydrological models (e.g., Richards equation for flow in the unsaturated zone requires a soil moisture characteristic curve that relates pressure to saturation in the vadose zone). They also play an important role in Finite Volume method adopted here, because it treats each cell as a lumped system.

Resistance to flow in vegetated landscapes: A lot of focus on small-scale (local) hydrodynamics, including more physically based parameterizations of flow resistance (as opposed to traditional, cruder methods based on Manning's formula). This could be crucial in flatter wetlands, where vegetation plays a key role in slowing down water movement.

Upslope Hydrologic Representation: There has also been considerable effort to capture improved representation of rainfall-runoff processes (including runoff generation and runoff routing) in the steeper parts of the region, for example, subsurface stormflow, in addition to infiltration excess (Horton) and saturation excess (Dunne) mechanisms of overland flow generation.

Hydraulic Structures and other Water Movers: There has also been a lot of effort in recent times on improved parameterizations (i.e., closure relations) of fluxes across human-made hydraulic structures and other water movers, which are at a scale smaller than that of the cells that form the RSM.

3. Review Comments on Hydrology and Hydraulics Process Representations

I will start my review by commenting on the overall framework adopted by RSM. I am referring to the Objected Oriented Methodology built around the Finite Volume Method, which partitions the landscape or hydrologic system into water bodies, water movers, and the links that connect them, i.e., that govern exchange of water fluxes between them. The RSM framework is the best and the wisest approach that I have seen adopted anywhere, and in my opinion, perfectly fitting to the hydrology and hydraulics of South Florida. I applaud its choice.

As part of the review, I was asked to comment on some of the recent extensions to the model, aimed at more detailed descriptions of sub-grid scale processes. I will say that, taken individually, these improved process descriptions are compatible with the current state of the art, both in terms of process understanding and in terms of modeling.

I have no major concerns about these, either of the two aspects: the broader framework, and the improved descriptions of sub-grid process complexity. My comments below will focus on some of the applicability of the improved process descriptions to Florida conditions, and in particular, on the appropriateness and success of their integration into the broader RSM framework.

These comments are not at all meant to be criticisms of the wisdom that is behind the RSM framework and the continued, excellent efforts you have made to implement it and make improvements to various aspects of the model.

(1) A lot of focus was given during the presentations, and in the documentation provided, to improved process representation at small scales, especially within HPMs. This is a laudable exercise, especially for understanding and predicting processes at local or small scales in this environment.

However, first and foremost, it is not clear how these small-scale (micro-scale) representations are embedded into the larger (regional) scale model structure? My understanding of the Finite Volume Method is that, the effects of sub-grid variability will need to be incorporated within the macro-scale model in some kind of parameterized form, i.e., as constitutive relationships and closure relations. Do they go into RSM in resolved form (within each cell), or in parameterized form? This was not made clear in the presentations or documentation provided.

(2) Secondly, I need to be convinced that these small-scale process heterogeneity and complexity has any effect beyond the cells within which they occur.

An example of this is the issue of micro-topography. I can see that micro-topography influences runoff generation, runoff movement and evapotranspiration at local scales, but how is this parameterized at the scale of the water bodies or water movers? What impact does it have on the exchange fluxes across cells? I would like this issue clarified, and the emphasis on its detailed treatment better justified.

(3) Thirdly, if the numerical scheme adopted is able to explicitly resolve the micro-scale process heterogeneity and complexity, as well as the larger, macro-scale framework of RSM, how is this done

(4) The dominant time scales and space scales of the processes involved and their parameterizations are vastly different. Combining them into one framework is challenging, to say the least. ? How is such a model to be optimized? These are partly questions of numerics, and beyond the scope of my part of the review, partly hydrologic/hydraulic questions. By letting treatment of small scale processes and numerics dominate there is a danger that some macro-scale hydrologic/hydraulic processes and numerical issues may be ignored, to the detriment of RSM's ability to reproduce both local scale and regional scale phenomena.

(5) It is true that when it comes to water management problems everything is local: we want to be able to predict water levels, fluxes and possible water-related hazards in places where people live. However, in the highly inter-connected system that you have in South Florida, these water problems may have origins not only locally but also regionally, and local natural or management changes can have impacts both locally but also regionally.

Therefore, there are two kinds of questions or challenges one faces in such a modeling environment: (a) how do local scale (within water bodies) impact regional scale phenomena, and (b) how regional scale phenomena or dynamics impact local scale phenomena or dynamics.

(6) In most hydrological systems, including in South Florida, processes happen at all scales, not just at the scales that we are familiar with, as in hydrodynamics. Inundation of parts of Florida when the connectivity of water movers (e.g., canals) exceed their capacity, is also a (large scale) process, a regional scale phenomenon resulting from process interactions at smaller scales! An example of this may be the breaching of a levee, which might lead to extensive flooding over a large area, irrespective of local scale processes. These may be exacerbated, let's say, as a result of a larger scale weather system, or larger scale human intervention that leads to interruption of system connectivity. What efforts have been made to address emergent phenomena caused by breakdown of connectivity?

(7) This big picture view is missing in the presentations and the documentation provided. Climate change, sea level rise, combined flooding and storm surges, are examples of regional scale phenomena. How do they propagate to the smaller, local scales? Land use change, local water management may have impacts on large-scale water movement and water availability. What efforts have been made to study these at the regional scale and discover hidden vulnerabilities in the model structure, rather than merely focusing on the small-scale details, which may or may not have significant impact on regional processes?

(8) Now, I come to some of the improved process descriptions at small scales, especially in the steeper parts of South Florida, e.g., headwaters of the Kissimmee River Basin. What are the dominant runoff generation mechanisms in South Florida? Has there been any detailed (observational) study of runoff generation mechanisms in South Florida? I ask this question because I would have thought infiltration excess (especially during the hurricane season due to heavy rainfall intensities) and saturation excess because of shallow groundwater tables will be the dominant mechanisms in Florida.

I need to be convinced that subsurface stormflow is a viable mechanism in this region. I accept that the upper Kissimmee River Basin is steeper, but only in a relative sense compared to the rest of South Florida. I am tempted to think that it is still much flatter compared to regions of the world that I am familiar with, where subsurface stormflow is a dominant mechanism. What field evidence is there to justify the effort to include subsurface stormflow? Also, how is subsurface stormflow captured in the model? Many schemes are mentioned in the presentations (e.g., kinematic storage, Boussinesq etc.), but I could not find anything conclusive. Please clarify.

(9) In fact, one of the streamflow hydrographs presented in one of the powerpoint presentations caught my attention. It indicated to me the occurrence of saturation excess overland flow, combined with slow groundwater flow (seepage) that appeared to remain constant through the season, and independent of storm events. I am tempted to think that, in this flat and humid environment (and based on the hydrograph evidence), that there might be more pervasive (large, slow), shallow regional groundwater flow system that contributes to lakes and wetlands, as well as delivering slowly responding baseflow to streams. Surface runoff, and perhaps some shallow subsurface flow (if at all it exists), is probably superimposed on the regional groundwater system. How is this regional groundwater system accounted for within RSM. This was not made clear in the documentation provided. What is the model used? I may be wrong, but I would like some discussion and justification of this.

(10) Even (so-called) physically-based, distributed models have a parameter estimation problem. How does one estimate or specify the parameter values for this model, not only at the sub-grid level

(which you might claim that you use DEMs and soil databases for these), but also at the cell level, where model parameterizations are lumped? How does one validate such a distributed model to demonstrate that it captures the small-scale effects, as well as macro-scale effects?

(11) The questions I have raised above then lead to my final comment. This is about communication. There needs to be some kind of documentation of the model that addresses the issues I raised above in a clear way to a reader, and especially to a potential model user. The presentations and documentation provided to me did not give me a clear perspective on how the various components fit together into a coherent whole. It is insufficient to depend on scores of publications and reports that focus on particular detailed aspect of the model (e.g., complexity of sub-grid processes) to get an accurate description of the model and to see how various model components fit together. This is especially important considering loss of institutional memory when current developers of the model move on, and new model developers and users come on board who may not have the perspective of the earlier model developers.

Appendix C

Report to South Florida Water Management District Following Site Visit on April 23, 2019

Gabor Toth, PhD
5/30/2019

1. General Assessment

Unified approach. The RSM design strategy has been using a general object oriented approach to a complex system, which involves natural and artificial water systems and structures. This is a great concept and it allows the RSM to provide accurate and reliable answers to problems involving the whole system. The recent changes further improve the generality and robustness of the model by using better numerical schemes, more complete system of equations and better parameterizations of subgrid scale processes. These efforts combined will not only make the RSM a better model for the SFWMD, but it may become a powerful tool that can used for other regions with steeper topography. As I have emphasized at the review, a well-designed general model often finds unexpected applications and provides more benefits than originally anticipated.

Switching to the implicit TVDLF scheme. The main advantage of the implicit TVDLF scheme is that it works robustly for a wide range of conditions. This means that the same solver can be used for slow and fast flows, and in fact some of the complexities related to previous solvers can be removed. For example the model can find basins by itself, potentially eliminating the need to predefine basins, which may even become incorrect under flood conditions.

The use of mapping functions is a very good approach. It allows flexibility and software reuse. The implementation of the mapping functions were not discussed in detail. I assume that some tabulated values are used (lookup tables). Often it is necessary to map in both directions, and it is often important to make the inverse function exact, i.e. if the original function is approximated with f and it's inverse is approximated with, we want g(f(x)) = f(g(x)) = x. This is relatively easy to ensure with linear interpolation, but the efficiency depends on the algorithm.

Verification and validation effort. The correctness of the implementation has to be carefully *verified* proving that the *model solves the equations right*. The presented verification tests showed convincingly that this is indeed the case. *Validation* aims at showing that *the model solves the right equations*, which contain the important physics and provide accurate solution for the physical system under the expected range of conditions. Again, the presentations showed that the SWFMD conducted a comprehensive set of validation tests and overall the results showed that the model performs well. It should be noted that complete verification (proving that the implementation is perfect) may not be practical, and complete validation (proving that the model provides reasonable solution under all possible circumstances) is impossible. In my judgement the verification and validation effort done is adequate and the results are satisfactory.

Summary. Overall the new RSM is a well-designed and well tested model that outperforms the previous models in terms of generality, flexibility, robustness and accuracy. Based on the presented results I would recommend its adaptation for use by the SFWMD and other users. Several comments and suggestions for further development are provided below, but none of these preclude using the current implementation of the code.

2. Comments on Numerical Algorithms

Triangle shapes. The advantage of triangular grids are flexibility in matching boundary conditions and adjustable grid resolution according to the requirements of the problem. Disadvantages include the complexity of the discretization compared to Cartesian grids and the difficulty of achieving accuracy and robustness (positivity) at the same time. In general, the quality of the solution depends on the triangulation. Highly skewed triangles tend to increase numerical errors. Triangle shapes need to be controlled by the grid generation software. The numerical schemes should also be chosen to be appropriate for the triangles produced by the grid generation. For example, using the circumcenter as the center of the cell or an interpolation scheme with weights proportional to the triangle areas (eq. 24 in presentation 13. "Two dimensional TVDLF method"), may be acceptable for relatively regular triangular grids, but may be exceedingly inaccurate for highly irregular triangular grids. For the latter case the circumcenter should be replaced with the center of mass (centroid) and a least square fitting to the centroids of the triangles should be used, which is an accurate and reliable algorithm for arbitrary triangles. In general, the weights of the closest points should be largest, which means that the weighting should not be proportional to areas of the triangles, as the center of larger triangles are further away.

Time step control. While the fully implicit TVDLF scheme provides stable and positive solutions under a wide range of conditions, the accuracy of the solution still depends on the time step. The current approach is to experiment with different time steps, establish some recommendations, and then expect the user to set fixed time steps that hopefully adhere to these recommendations. A more reliable and user friendly approach is to implement some form of time step control into the code. The simplest approach is to check if the conditions of accuracy are satisfied or not and produce warnings or stop the execution if the conditions are violated. A more sophisticated approach is to set the time step to satisfy the accuracy conditions. This can be done either based on some theoretical formula, such as the CFL number (the time step divided by the time the fastest wave takes to cross the grid cell), or based on the changes in the solution, for example requiring that the water head does not change more than some fraction anywhere. Both approaches have been used successfully in the magnetohydrodynamics models developed at the University of Michigan, including adaptive time step control for fully implicit solvers [Toth et al. 2006, section 2.2.4] similar to the one used by RSM.

3. Software engineering aspects

Object oriented approach. The 2005 version of RSM uses an object oriented approach, which is highly recommended for any complex software. This has benefited the RSM in many ways, and it is one of the main strength of the software. It also allowed improving the numerical methods without a need for major changes in the rest of the model.

Version control. The RSM is under the SVN version control system, which is appropriate. Switching to newer systems, like Git, should be relatively straightforward (there are tools that can do the conversion without losing the development history) but not really important, unless SVN becomes unavailable or unsupported on some platforms that the RSM should be used on. Peer pressure can also play a role. Our group at Michigan has recently switched from CVS to Git to keep up with current practices.

Regular and comprehensive testing. Frequent and comprehensive testing is a crucial requirement for any complex software that is under development and/or used by a wide range of users on various platforms. Response given to my question suggested that there are some tests that are performed after code changes. This is a good software engineering practice. Ideally the tests should cover all typical usage of the code on multiple platforms.

Portability is important for multiple reasons. An increasing user base will try to run the code on different platforms. In addition, compilers keep evolving, which requires updates. Having frequent testing with different compilers allows discovering issues early and makes finding and fixing issues relatively straightforward.

Documentation. I am not sure about the state of documentation. It is an absolute must if the RSM to be used by other users. Good documentation saves time for the users and the developers too. Functionality tests provide the best basis for documentation, as they provide working examples that are continuously maintained.

4. Responses to questions

Q: Is it acceptable to limit the numerical flux to avoid unphysical backward flow due to a numerical flux that has opposite direction and larger amplitude than the physical flux?

A: Limiting the numerical flux is acceptable in an implicit scheme, see for example Toth et al. [2011]. The implicit scheme provides stability. Reducing the numerical flux locally may make the scheme non-TVD, but given the diffusive nature of the equations, spurious oscillations are unlikely to develop.

Q: Is it OK to limit water levels at a structure flow that fills up the canal faster than the time step?

A: Limiting the result to physically meaningful values is acceptable and it is often done in hydrodynamic models to preserve positivity of density and pressure, for example. An alternative approach is subcycling, i.e. taking multiple small time steps locally where needed.

Q: Does the transverse derivative of the water head (which contributes to the slope) need to be considered in the implicit solver and/or the numerical flux of the 2D TVDLF scheme?

A: If the dependency on the transverse gradient is very stiff, it is probably important to handle it implicitly. If the dependency is not stiff, using an explicit evaluation for this term may work as long as the normal gradient is evaluated implicitly. The matrix-free method allows a fully implicit evaluation with no extra cost. Multiplying an arbitrary vector (in the Krylov solver) with the matrix can be evaluated as

$$(I - \Delta t \frac{\partial R}{\partial h})\Delta h = \Delta h - \frac{R(h^n + \epsilon \Delta h) - R(h^n)|}{\epsilon}$$

where h is the vector of water levels, Δh is the change from time level n to $n+1$, R is the right hand side vector of the PDE including the source terms and the physical and numerical fluxes, and ε is a small scalar parameter.

The Lax-Friedrich numerical flux at face i+1/2,j is

$$\frac{1}{2} c^n_{i+\frac{1}{2},j} (h^{n+1}_{i+1,j} - h^{n+1}_{i,j})$$

should be simply based on the amplitude of the fastest wave speed c (which involves the transverse derivative but it is evaluated at time level n) and the jump in the normal direction, which does not involve the transverse gradient.

5. Suggestions

Adjustable grid resolution and time step. I have already pointed out the usefulness of adjustable, or preferably, adaptive time step. A similarly important feature is adjustable grid resolution not only for testing, but also for the practical use. Using a single fixed grid resolution makes it very difficult to assess the contribution of numerical truncation errors. Truncation errors are proportional to some power of the grid resolution Δx and the time step Δt:

$E \propto \Delta x^k \ \Delta t^m$

where E is the difference between the exact solution and the numerical solution at some fixed time after the initial conditions, and k and m are the spatial and temporal order of accuracy of the scheme, respectively (typically 1 or 2 for the schemes used in the RSM). By comparing the solutions at different grid resolutions and time steps, one can estimate the truncation error and see if it is negligible or significant for the quantities of interest.

I was told during the visit that one issue of changing the RSM grid is that the structures, canals, etc. are connected to particular grid cells identified with a grid index, which would change if the grid was modified. The coupling between the grid cells and the structures should be based on the location, size and shape of the grid cells, and not on the index. This would allow modifying the grid more easily.

Parallel execution. Executing the RSM for many time steps on the current grid may be feasible on a single core, but increased grid resolution and/or smaller time steps may make the run times unacceptably slow. The best way out of this is the use of parallelization. Some compilers can do auto-parallelization of simple loops and speed up the code. A more reliable approach is to use OpenMP parallelization, that provides explicit control over the multi-threaded execution. With the ever increasing number of cores per processor, OpenMP parallelization can easily speed up the code by a factor of 10 to 20. An even more powerful approach is to use MPI parallelization, which distributes the data as well as the work. This requires introducing communication among the processors, typically with the use of ghost cells. Once the explicit solver is MPI parallel, extending the parallelization to the implicit solver is quite straightforward. Essentially all global dot products in the Krylov solver need to be followed by an MPI_allreduce operation to perform the summation over the processors, and of course the matrix-vector multiplication, which is based on the explicit scheme, needs to be parallel. Using MPI parallelization can speed up the code by several orders of magnitude, mostly depending on the size of the computer and the problem size. For 1 million grid cells, for example, a speed up by a factor of several hundreds should be possible. For larger grids, the achievable speed up factor will be larger too, of course assuming that the SFWMD has access to (super) computers with that many cores. Recently we have shown weak scaling (fixed problem size per core) of an implicit magnetohydrodynamic model up to 250,000 cores using a combination of MPI and OpenMP parallelization.

Numerical fluxes for system of equations. Solving the St. Venant equations in 1 or 2 dimensions requires the solution of a system of partial differential equations. There are several choices for the flux function which depends on the left and right states. Roe's scheme has the least diffusion (minimum numerical flux) but it can sometimes give problems for non-linear system of equations, especially in 2D. It also requires the eigen vectors of the Jacobian matrix, which may not always be possible to obtain analytically for complicated system of equations. There are several alternatives, such as the HLLE and Lax-Friedrich fluxes. The LF flux uses the magnitude of the largest eigenvalue, and it is the most diffusive option. The HLLE scheme uses the left and right going wave speeds [see Einfeldt, 1991] and it has some nice properties, such as preserving positivity. Unlike the Roe scheme, it does not need the eigenvectors. This method was also used by Valiani et al. [1999].

6. References

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