

---

2010

## Numerical Modelling of Contaminant Transport Hydrodynamics

Follow this and additional works at: <https://scholarsarchive.byu.edu/josh>

---

### BYU ScholarsArchive Citation

(2010) "Numerical Modelling of Contaminant Transport Hydrodynamics," *Journal of Spatial Hydrology*.  
Vol. 10 : No. 2 , Article 2.

Available at: <https://scholarsarchive.byu.edu/josh/vol10/iss2/2>

This Article is brought to you for free and open access by the Journals at BYU ScholarsArchive. It has been accepted for inclusion in Journal of Spatial Hydrology by an authorized editor of BYU ScholarsArchive. For more information, please contact [scholarsarchive@byu.edu](mailto:scholarsarchive@byu.edu), [ellen\\_amatangelo@byu.edu](mailto:ellen_amatangelo@byu.edu).



## Numerical Modelling of Contaminant Transport Hydrodynamics

*Yasser Hamdi*

### Abstract

Modelling of contaminant transport on watersheds is a problem of concern with regard to the protection of water ecosystems. This paper presents a numerical model, using the finite element method, to simulate contaminant transport hydrodynamics. Spatial and temporal progression of a spilled toxic substance was compiled for the Macks-Creek basin located in United States. It is shown that the developed tool, based on coupled terrain and surface runoff models, provided adequate results in terms of runoff velocities and height. Results from this compute served as an input of a computer based system that we developed to simulate the real-time contaminant behaviour and spreading since its spillage.

The developed model can be used in both simulating and forecasting modes. Obtained predictions are of practical relevance to hydrologists and water resources managers for applications in environmental management strategies during infrastructure and urban planning phases as well.

**Key words:** runoff, contamination, environment, numerical modelling, real-time, simulation, forecasting, hydrodynamic, management.

### 1. Introduction

Growing population and economic activities near rivers increase the risk of water ecosystems pollution and the need for environmental management (Van de Meent et al., 2000; UNEP, 2001). Surface water transforms landscapes by moving large amounts of contaminant soils which are eroded by runoff, transported by river systems, and eventually deposited in surface water reservoirs. The ecological risk assessment of chemicals in surface waters was studied by many scientists over the world (Metcalf et al., 2003; Whitall et al., 2001; Solomon et al., 1996)

The intensive use of chemicals in many economic sectors makes our ecosystem more vulnerable to contamination (UNEP, 2001). The most common practice in the agricultural sector is to use chemicals to improve the quality and quantity of products. Pionke et al. (1999) showed the importance of modelling nutrient concentrations and loading patterns in stream flow draining agricultural Hill-Land watershed. This can be helpful in the economic activities but it has serious consequences on the water quality and it can cause serious deterioration of surface and underground water reservoirs used not only for water supply and irrigation but also as aquatic systems. Radtke et al. (1980) showed the effects of agriculture on stream water quality by combining a physically based groundwater and overland flow models with a transport one. Many other existing models are not always applicable to natural systems having irregular boundaries, and where physical and hydrological characteristics vary substantially in space and time. For example, the Rhone watershed represents 20% of France surface, 50 of the existing 72 species of fishes live in the Rhone River. It was shown in many reports, published by the environmental ministries over the world and particularly in France, that many species of fishes assuring the diversity of water ecosystems and biologic

heritages, are seriously menaced by pollution. In our days, toxic substances in aquatic systems have the potential to reach levels that could impair fish reproduction (Keith et al., 2001; Kannan et al., 2001a). Sekhar (2001) presented some approaches for modelling dissolved solids in a river. In recent years, restrictions on the use of chemicals have been introduced in many countries. This reflects a need for developing not only efficient non-chemical methods but also models to deal with a contaminant spill when it occurs.

Pollution of underground water reservoirs takes place slowly, over days, weeks and months (Javadi et al., 2006, 2007) but contamination of rivers and surface water reservoirs occurs much faster. In some cases, runoff flows and flooding events can transport contaminants to rivers in fewer minutes. Runoff is the major component of the water cycle that causes erosion and contributes to the replenishment and contamination of rivers and water surface reservoirs. There are no models in the literature that allow a real-time visualisation of a contaminant movement on a natural watershed and compute its duration and 2D velocities.

In another context, contamination can also happen through extreme hydrological events that generally cause severe material damage and toxic substances spills on watersheds. The question to which managers have to answer immediately when accidental or voluntary chemical spills occur on a watershed is how to stop the contaminant spreading before it reaches a given point? This point can be the principal river or its outlet. Direct runoff and water contamination prediction have been studied extensively as separate subjects and systems (Hanks and Bowers 1962; Kibler 1968; Rubbin 1966; Whisler and Klute 1965; Woolhiser and Liggett 1967).

A considerable number of mathematical descriptions of runoff can be found in the literature. Taylor (1976), Baxter et al. (1990), Blandford and Meadows (1990) used conservation of both mass and momentum which are the basis for the Navier-Stokes and continuity equations that describe runoff. Li et al. (1999) presented a finite element method for contaminant transport in unsaturated soils. A numerical runoff model using the finite element method (FEM) is presented in this paper. Remote sensing and aerial photography analysis produce digital terrain models that can be used as input for runoff models (Hamdi, 2001). Those surface elevation models are structured as a grid of irregular triangles, which is similar to the finite element philosophy. Taking advantage of this similarity, a 2D finite element hydrodynamic model that calculates the spatial and temporal distribution of a direct runoff hydrograph is developed. An approximate solution to the governing flow equation can be obtained by the FEM. This method is based on an integral formulation of the governing equation, where the approximation is done on sub-domains. The flexibility of the FEM to represent complex geometries is well-suited for free surface problems, where there is a need to represent natural channels having irregular boundaries. A robust numerical scheme that allows for the correct simulation and the Newton-Raphson linearization method are used, with variable time step sizes. This model incorporates the runoff flow and accounts for infiltration as a time and space dependent phenomenon. In this paper we use the Green and Ampt formula to describe the cumulative infiltration process as a non-linear function of time based on Darcy's Law (Craig et al., 2010).

In the present paper, a new contaminant transport technique is proposed. It is based on temporal progression and spatial distribution of imaginary particles that represent the contaminant on a natural basin. We simply developed a technique that allowed us to attach a particle to a vector in movement and we coupled this technique to the runoff model that gave the velocities vectors. The idea was very simple but results were impressive. With the developed tool, one can visualise a real-time

contaminant movement on the watershed. This will help managers to intervene efficiently when a chemical spill occurs for example.

## 2. Hydrodynamic model

Conservation of both mass and momentum are the basis for the Navier-Stokes and continuity equations that describe surface water flows.

$$\left\{ \begin{array}{l} \frac{\partial H}{\partial t} + \frac{\partial UH}{\partial x} + \frac{\partial VH}{\partial y} - (r - i) = 0 \\ H \frac{\partial U}{\partial t} + UH \frac{\partial U}{\partial x} + VH \frac{\partial U}{\partial y} + gH \frac{\partial \eta}{\partial x} + \frac{f}{8} \frac{U \sqrt{U^2 + V^2}}{\cos(\alpha_x)} - (\hat{r} - \hat{i})U = 0 \\ H \frac{\partial V}{\partial t} + UH \frac{\partial V}{\partial x} + VH \frac{\partial V}{\partial y} + gH \frac{\partial \eta}{\partial y} + \frac{f}{8} \frac{V \sqrt{U^2 + V^2}}{\cos(\alpha_y)} - (\hat{r} - \hat{i})V = 0 \end{array} \right. \quad (1)$$

where  $H$  is the depth of flow, with respect to the soil surface (Fig 1),  $U$  and  $V$  are the mean velocities in the  $x$  and  $y$  directions, respectively.  $\alpha_x$  and  $\alpha_y$  are the slopes of the ground surface in the  $x$  and  $y$  directions, respectively. Hydrological components such as rainfall rate in space and time  $\hat{r} = r(x, y, t)$ , infiltration rate in space and time  $\hat{i} = i(x, y, t)$  per unit area are included in the mass conservation equation.

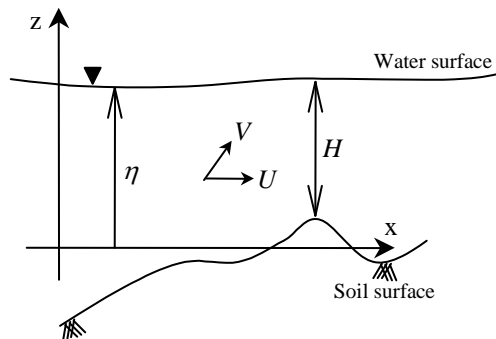


Figure 1. Schematic representation of the mathematical model

A sloping surface is considered here to account for cases where the slopes are large enough such that they cannot be neglected.  $g$  is the gravitational acceleration and  $f$  is the friction coefficient. Friction stresses based on Colebrook and White theory are used.

## 3. Infiltration model

This section presents a method of describing the cumulative infiltration process as a non-linear function of time based on Darcy's Law. A modified Green and Ampt equation (2) is used to compute cumulative infiltration. The Newton-Raphson linearization method is used to resolve the equation. The equation was tested by comparison with Richards numerical solution. In order to see how the infiltration rate behaves in response to variations in all of the input data, a sensitivity study was also carried out. The concluded results of the equation indicate that a theoretically based model can be used to describe infiltration when appropriate physical parameters can be obtained.

The infiltration equation used in this paper is also based on the recognition of two separate infiltration phases, with and without surface ponding. This allows us to take into account the fact that at the beginning of the rainfall event, the infiltration rate is equal to the precipitation one and infiltration decreases exponentially only after a time  $t_p$  called ponding time.

As opposed to common practice, we added the runoff depth in the mathematical development of the infiltration equation. Let  $w$  be the rainfall rate and  $k_h$  is the saturated hydraulic conductivity. During a precipitation event, temporal variation of infiltration rate  $f(t)$  can be expressed as:

$$\left\{ \begin{array}{l} f(t) = \xi \cdot w + (1 - \xi) \cdot \left[ K_h + \frac{I}{\frac{t-t_p}{\phi_e(y_f(t))} + \frac{I}{w-K_h} - \frac{I}{K_h} \text{Log} \left[ \frac{w}{w-K_h} \frac{(f(t)-K_h)}{f(t)} \right]} \right] \\ \xi = 1 \text{ for } t \leq t_p \\ \xi = 0 \text{ for } t > t_p \end{array} \right. \quad (2)$$

Where  $\phi_e$  is the effective porosity of the soil;  $y_f(t)$  is the total height of runoff and the mean pressure head at the infiltration front. The infiltration rate was computed in every node of the used mesh in a production function.

#### 4. Finite element formulation

The two-dimensional finite element model, briefly described here, provides numerical solutions to equation 1 from the Galerkin weighted residual method. We use linear interpolation functions and divide into sub-domains to obtain a set of algebraic equations to solve. The solution represents an approximation at the nodal points.

$$\left\{ \begin{array}{l} W_u = \int_D \delta U \left[ H \frac{\partial U}{\partial t} + UH \frac{\partial U}{\partial x} + VH \frac{\partial U}{\partial y} + gH \frac{\partial \eta}{\partial x} + \frac{f}{8} \frac{U \sqrt{U^2 + V^2}}{\cos(\theta_x)} - (r - i - e)U \right] dD = 0 \\ W_v = \int_D \delta V \left[ H \frac{\partial V}{\partial t} + UH \frac{\partial V}{\partial x} + VH \frac{\partial V}{\partial y} + gH \frac{\partial \eta}{\partial y} + \frac{f}{8} \frac{v \sqrt{U^2 + V^2}}{\cos(\theta_y)} - (r - i - e)V \right] dD = 0 \\ W_h = \int_D \delta H \left[ \frac{\partial H}{\partial t} + \frac{\partial UH}{\partial x} + \frac{\partial VH}{\partial y} - (r - i - e) \right] dD = 0 \end{array} \right. \quad (3)$$

A nodal approximation functions are introduced in the integral formulation to obtain, for each element, an algebraic equation. An assembly is then performed over all elements:

$$[M] \{\dot{q}\}_t + [K(q)] \{q\}_t = \{F\}_t \quad \text{where } \{q\}_t = \begin{Bmatrix} u \\ v \\ \eta \end{Bmatrix}_t \quad (4)$$

A finite difference representation of the first-order temporal variation,  $\dot{q}$ , is assumed in the model. To avoid numerical instabilities, an implicit Euler temporal scheme is used. Equation 4 is non linear and the Newton-Raphson linearization technique is used in the model for its solution.

## **5. Case study**

The finite element model is applied to the Macks Creek watershed area. The Macks Creek experimental watershed is a 31.64 km<sup>2</sup> sub-basin of the Reynolds Creek watershed located in mountainous south-western Idaho in United States. The watershed contains two principal rivers: the Macks-Creek and the Cottle-Creek (Fig 4-b). This watershed area is monitored by American Agricultural Research Service. The catchment is quite steep, with an elevation drop of 750 m in 8 km. Surface slopes approach 30% in portions of the basin. Two main channels with slopes averaging 5% and lengths near 10 km collect surface runoff. This watershed area is characterised by its diverse spatial and temporal variability of the rainfall, soil type, slope, and roughness. During July, August, and September, most of the basin is subject to convective storms. These storms have resulted in severe flooding events. However, major floods of record were caused by winter storms with rain and snow melt.

In order to apply the model, the Macks Creek drainage basin area is subdivided into systems of subwatershed areas. The subdivision is performed depending on the topography. The highest points on each subwatershed area are considered as a closed boundary line with zero depth boundary value. Infiltration parameters given by the American Soil Conservation Soil are used. The developed model requires good topographical data and a well adapted finite element mesh.

### **5.1 Automatic adaptive finite element mesh**

An Automatic Adaptive Mesh (AAM) method was used to take into account the considerable spatial variability of the physiographic parameters. To apply the method, one needs to start with an initial mesh (Fig 2-a). Another good reason to use such a technique is the radical change in flow characteristics between runoff and river flow. The AAM is a reliable and efficient approach in spatial hydrology modelling. In some cases, however, big challenges are faced when constructing the adaptive meshes that have a good quality. In this paper, a local refinement technique using Delaunay triangulation method is developed for these purposes (Fig 2-b). Specific treatments were used to deal with dry elements and basin boundary. The application and evaluation of the method show that a satisfactory result has been obtained for the Macks-Creek watershed.

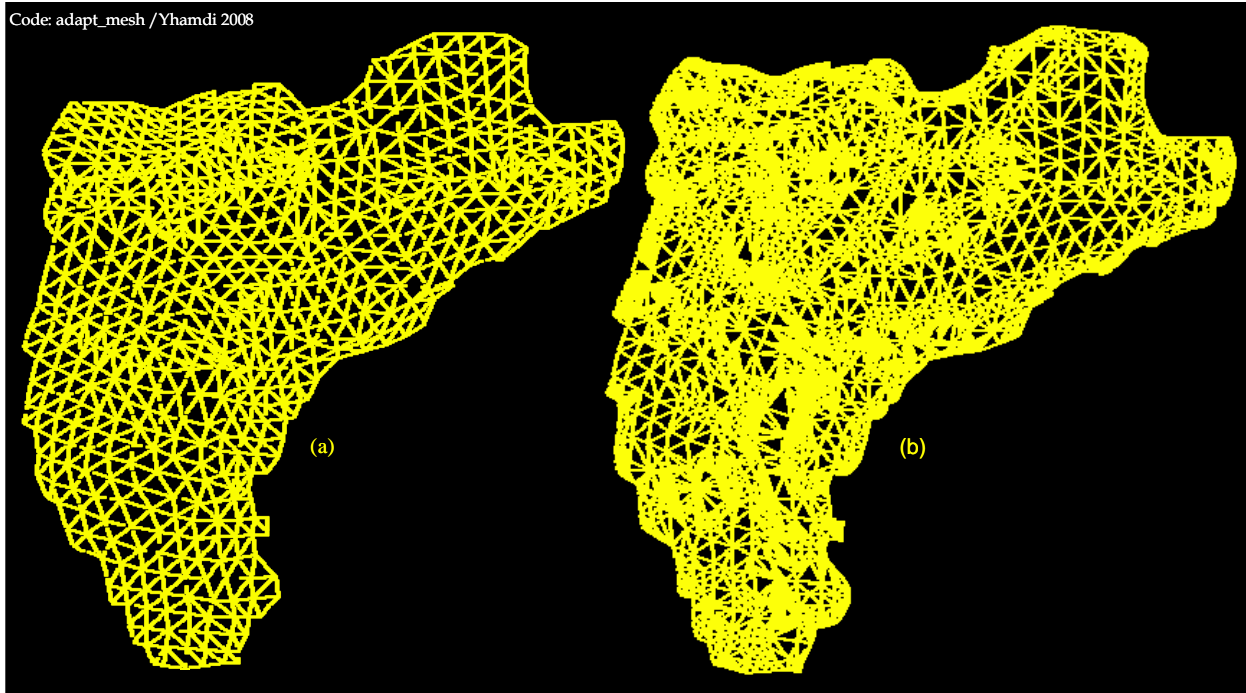


Figure 2. Basin discretisation (Macks Creek watershed). (a) Initial mesh; (b) Adaptive mesh.

## 5.2 Illustrative example: the spillage

To apply the model in an environmental context, we supposed an accidental spill that caused the contamination of a considerable zone (1000 m<sup>2</sup>) in the northern-east portion of the Macks Creek basin. It is important for the reader to know that the properties and characteristics of the spillage do not matter in the calculation as it can move in water runoff. We can simply assume that a toxic chemical was accidentally spilled somewhere on the watershed. Two successive meteorological events were used for the simulation. To test the performance and endurance of the developed model, we supposed that the spillage took place on more than a sub-watershed at the same time. We also tested the model when many spills occur in different locations on a watershed. In table 1, some parameters used for the Macks Creek basin are summarized. In the present study, the soil porosity, the initial water content and the saturated hydraulic conductivity are the most important parameters (according to the sensitivity analysis). The reader is referred to Hamdi (2001) for a review of such model parameters values.

Table 1: Les paramètres de Green et Ampt utilisés pour le bassin Macks Creek

Soil	$\phi$ (%)	$\theta_0$ (%)	$K_{hsat}$ (cm/hr)
Sandy Loam	0.412	32	1.09
Loam	0.434	33	0.34
Clay Loam	0.309	25	0.10
Silt Loam	0.486	34	0.65
Sandy Clay Loam	0.330	25	0.15
Rock	0.000	0	0.00

The evaluation of the findings of the developed model put forth that the most critical part in terms of pollution progression is the difference between runoff on the watershed and fluvial flow in rivers. This

result was expected because of the radical increase of velocities when water reaches a river. To put things right, we simply used an adapted mesh by using small elements around rivers. When the spill simulation is conducted for the Macks Creek basin with the existing natural conditions of the accident, it is observed that the spilled substance has been spread in accordance with runoff. This finding was expected and results are shown in figure 3. The inspection of the figure indicates the efficiency of the model in reproducing runoff heights and water depths (represented by iso-colours) in the hydrographical network. These results, flow patterns in term of velocities, not presented in this paper, can be displayed by the model. What is important in the figure, with regard to the focus of the present paper, is the progression of the white particles (that represent the contaminant) in time and space. We can see how the toxic substance move on the watershed one week after the accident when the first rainfall event occurs and caused a runoff sufficient to move the contaminant near the principal river (Fig 3-a). In a next step and 2 weeks after, another meteorological event was able to relocate the substance to the river and then to the outlet (Fig 3-b). As illustrated by figure 3, the model provides a good description of the hydrodynamic behaviour of the spilled contaminant and as we can see from the same figure, the movement and spreading of the particles are predicted correctly.

In order to determine the effect of each parameter in the model and to estimate the model uncertainties and error, we conducted a sensitivity analysis study. The study showed how the variation (uncertainty) in the output of the developed model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input of the model. The reader is referred to Hamdi (2001) for a review of these analyses. As a result of the sensitivity analysis, the initial water content and the saturated hydraulic conductivity of the soil can have serious effects on the model results. Care must be taken when using these parameters in the proposed model.



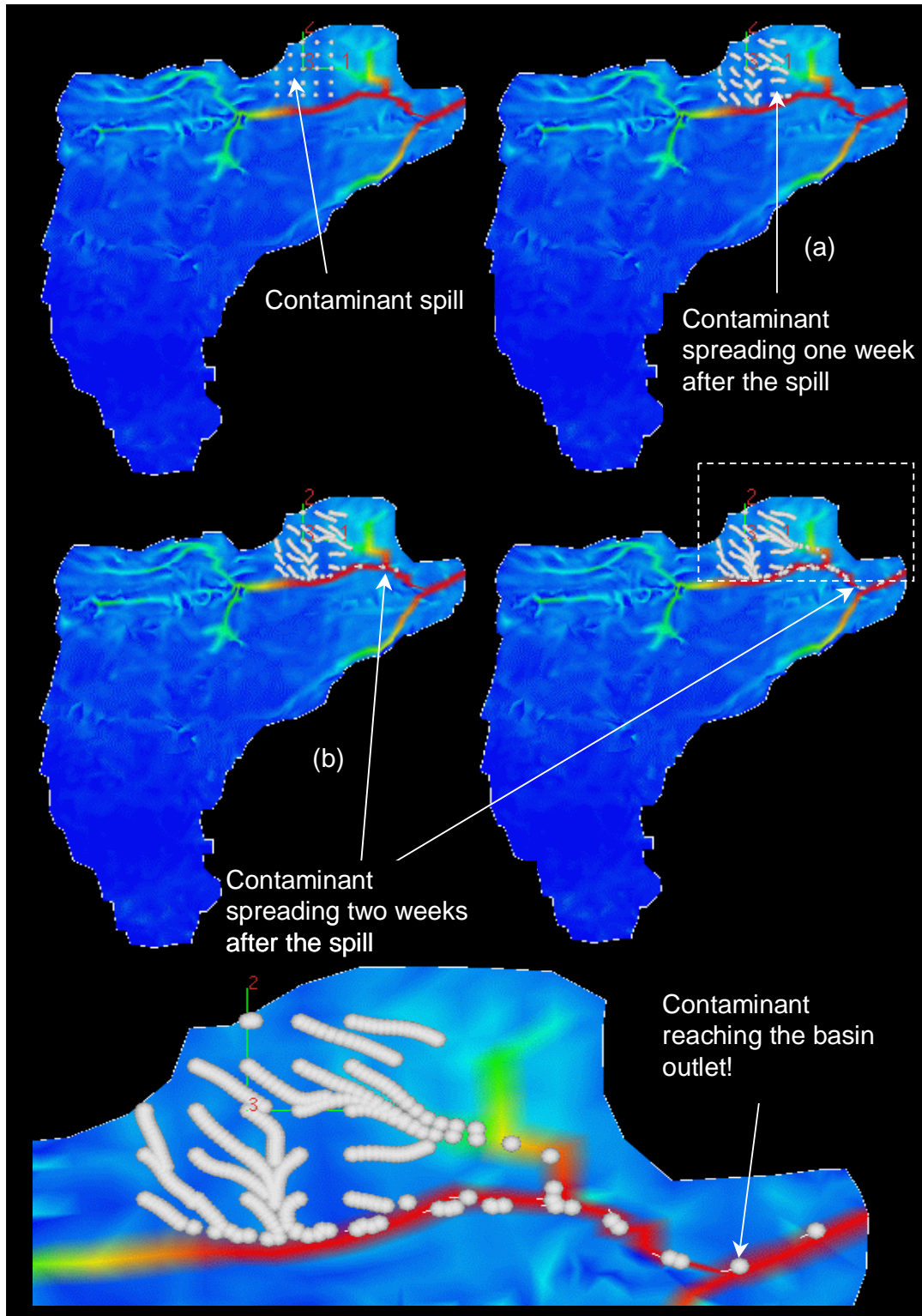


Figure 3. Contaminant distribution on the Macks Creek watershed. (a) After the first hydro-meteorological event one week after spill. (b) After the second hydro-meteorological event two weeks after spill.

### 5.3 Other results

One of the benefits of the developed model is its ability to predict runoff and river flow patterns (runoff depth & 2D velocities). Such information may be used by water resources managers to identify flooding zones and to assist the erosion management assessment and plan for example. It is also useful in soil and water conservation works. The compiled water depth and velocity at 40 minutes after the storm event is displayed in Figure 4 and Figure 5. It clearly demonstrated the usefulness of the modelling as high floods areas could be identified graphically.

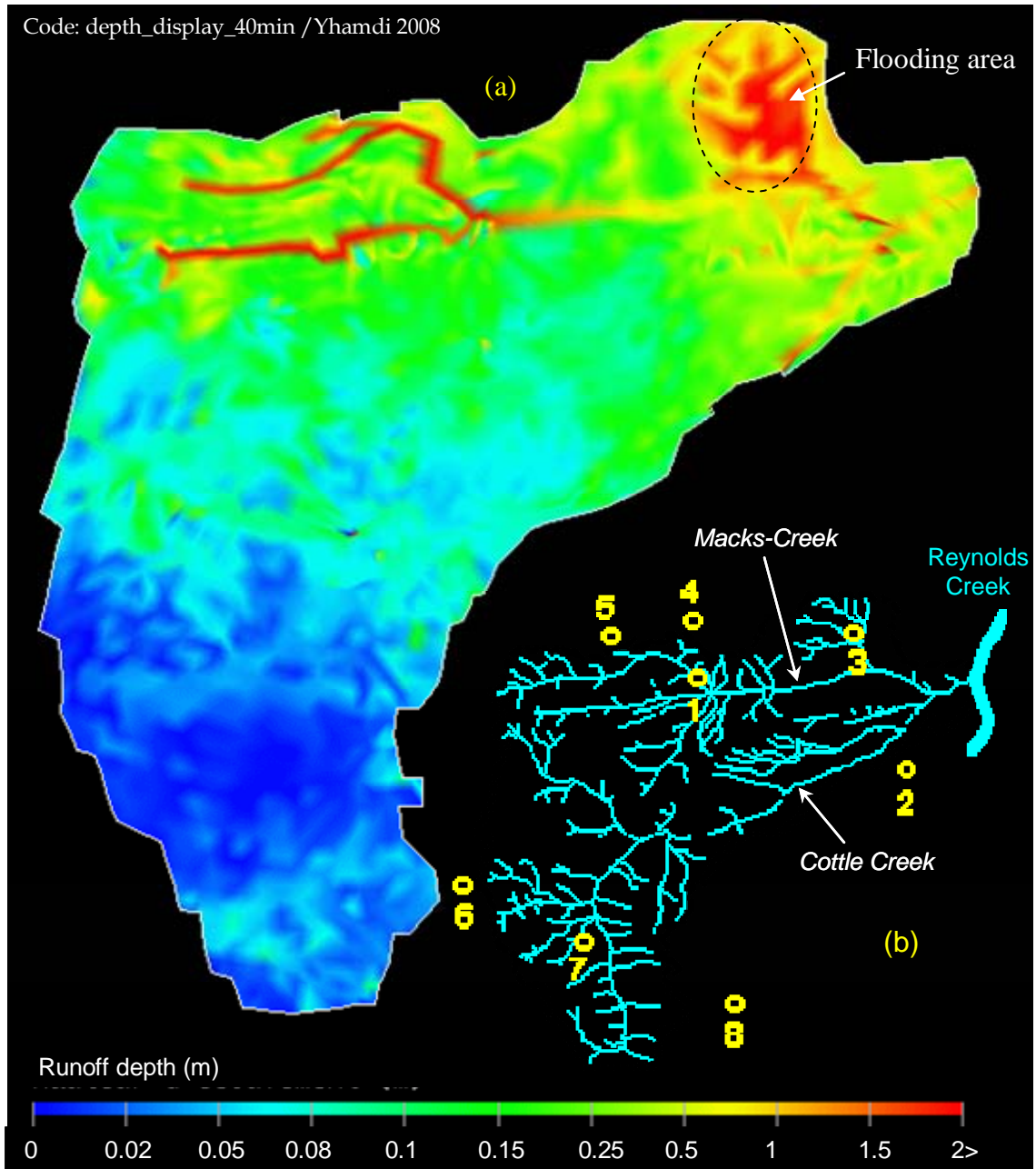


Figure 4. Spatial variability of runoff depth (Macks Creek watershed). (a) Iso-colours of runoff depth 40 minutes after rainfall starting. (b) Hydrographical and Meteorological networks.

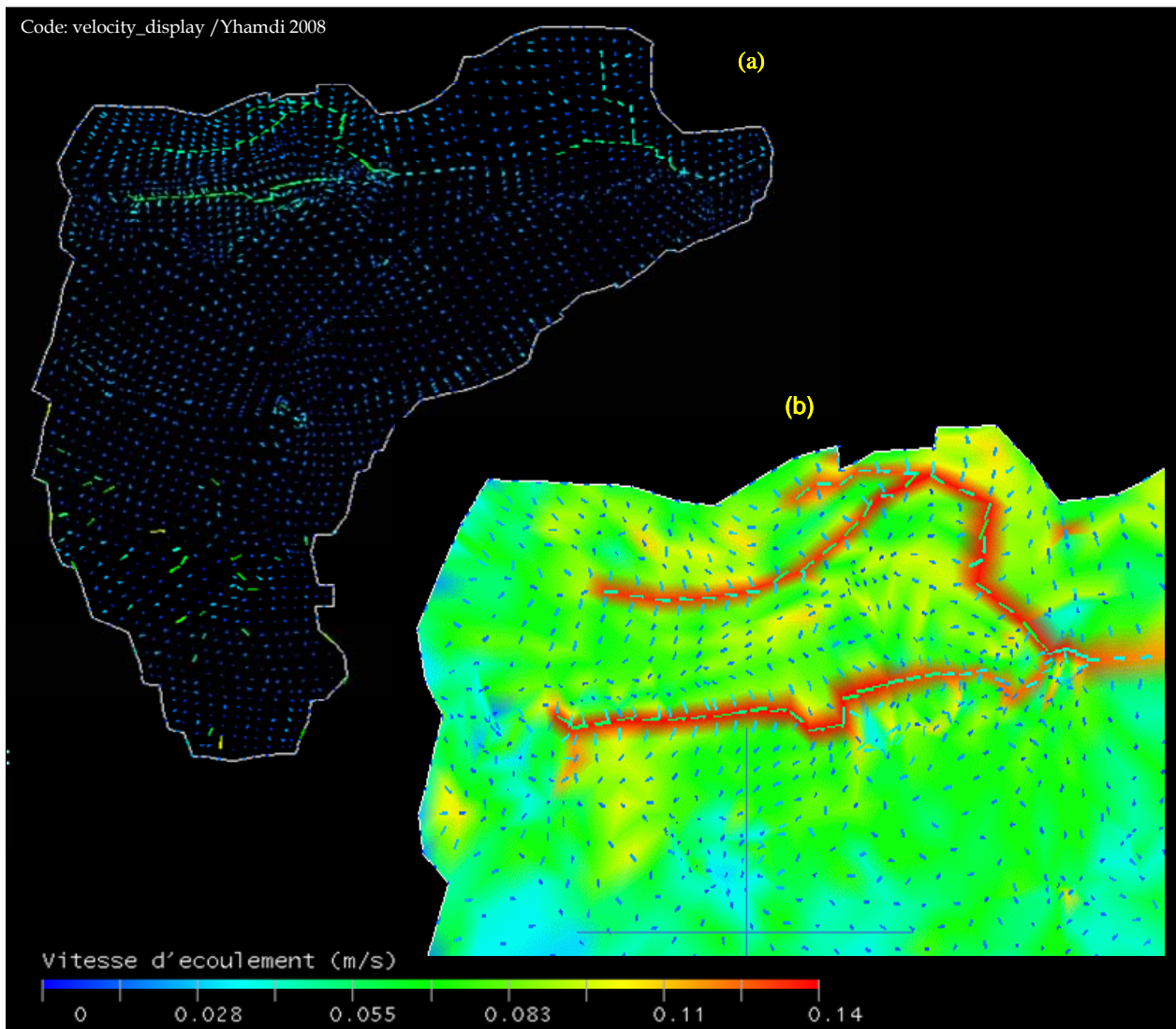


Figure 5. Spatial variability of runoff velocity (Macks Creek watershed). (a) Iso-colours of runoff velocities. (b) Runoff depth & velocity (Zoom).

## 6. Conclusion and Summary

The present study is an example of modelling efforts to help to predict the movement and spreading of toxic substances on watersheds immediately after voluntary or accidental spills. This is very useful for determining a strategy of intervention and detailed surveillance.

The main objective of this paper consisted in presenting a hydrodynamic finite element model, vertically integrated, to simulate the hydrodynamic contaminant transport, including runoff. The model incorporates the effects of sloping topography, spatial and temporal variation in the input parameters, and time and space dependence of the infiltration rate.

A contaminant spill simulation is conducted for the Macks Creek basin using an imaginary scenario for the spill conditions and the meteorological events. It is observed that the impact of two successive rainfall events on the spill spreading was considerable. The contaminant reached critical points on the watershed such as the principal river and its outlet. The developed model allowed the localisation of the contaminant in space and time. It was also shown that the model can take advantage of the database generated by terrain models, which are a series of triangular faces constructed from aerial or satellite photographs.

As a recommendation, the use of such a computer modelling in toxic spills predictions can be integrated into a *National Contaminant Spill Contingency Plan*. In conjunction with the integrated computer simulation, a contingency plan should include components such as an early warning system combined with a rapid response mechanism to control the spreading of the contaminant in case of accidental spills. It will be also important to combine the developed model with a 2D groundwater flow one.

## REFERENCES

- Van de Meent, D., McKone, T.E., Parkerton, T., Matthies, M., Scheringer, M., Wania, F., Perudy, R. and Bennett, D.H. (2000) Persistence and transport potential of chemicals in a multimedia environment. In: Klečka, G. et al. (Eds). Evaluation of Persistence and Long Range Transport of Organic Chemicals in the Environment: SETAC Special Publ. Series, SETAC Books, Pensacola FL, pp. 169-204.
- Metcalfe, C.D., Miao, X.-S., Koenig, B.G. and J. Struger. (2003) Distribution of acidic and neutral drugs in surface waters near sewage treatment plants in the lower Great Lakes, Canada. *Environ Toxicol Chem* 22:2881–2889.
- Whitall, D.R. and Paerl, H.W. (2001) Spatio-temporal variability of wet atmospheric nitrogen deposition to the Neuse River Estuary, North Carolina. *J Environ Qual* 30: 1508-1515.
- Solomon, K.R., Baker, D.B., Richards, R.P., Dixon, K.R., Klaine, S.J., La Point, T.W., Kendall, R.J., Weisskopf, C.P., Giddings, J.M., Giesy, J.P., Hall, L.W. and Williams, W.M. (1996) Ecological risk assessment of atrazine in north american surface waters. *Environ Toxicol Chem* 15: 31–76.
- UNEP: United Nations Environment Program (2001). Final Act of the Conference of Plenipotentiaries on The Stockholm Convention On Persistent Organic Pollutants. UNEP, Geneva, Switzerland. 44 pp.
- Pionke, H.B., et al. (1999) Seasonal Flow, Nutrient Concentrations and loading Patterns in Stream Flow Draining Agricultural Hill-Land Watershed. *Journal of Hydrology*, 220, 62-73.
- Radtke, D.B. and McConnell, J.B. and Carey, W.P. (1980) A Preliminary Appraisal of the effects of Agriculture on Stream Water Quality in South-West Georgia, U.S. Geological Survey, Open File Report, 80-771.
- Keith, T.L., Snyder, S.A., Naylor, C.G., Staples, C.A., Summer, C., Kannan K., and Geisy, J.P. (2001) Identification and quantification of nonylphenol ethoxylates and nonylphenol in fish tissues from Michigan. *Environ Sci Technol* 36: 10 13.
- Kannan, K., Franson, J.C., Bowerman, W.W., Hansen, K.J., Jones, P.D. and Giesy, J.P. (2001a) Perfluorooctane sulfonate in fish-eating birds including bald eagles and albatrosses. *Environ Sci Technol* 35: 3065-3070.
- Sekhar, M.C. (2001) Immission Approach for Modelling Dissolved Solids in a River and Separation of Point and Nonpoint Loads. Ph. D. Thesis, Regional Engineering College, Warangal, India.

- Javadi, A., AL-Najjar, M., Elkassas, A.S.I. (2006) Numerical modelling of contaminant transport in unsaturated soil. In: 5th Int Cong Env Geotechnics. Cardiff University, U.K. 1177–1184
- Javadi, A., AL-Najjar, M., Evans, B. (2007) Flow and Contaminant Transport Model for Unsaturated Soil. Springer Proceedings in Physics, Volume 113, Part II, 135-141.
- Hanks, R.J. and Bowers S.A., (1962) Numerical solution of the moisture flow equation for infiltration into layered soils. *Soil Sci. Soc. Amer. Proc.*, 26(6), 530-534.
- Kibler, D.F. (1968) A kinematic overland flow model and its optimisation. PhD dissertation, Colorado State University, Fort Collins, USA.
- Rubbin, J. (1966) Theory of rainfall uptake by soils initially drier than their field capacity and its application. *Water Resour. Res.*, 2(4), 739-749.
- Whisler, F.D., Klute, A. (1965) The numerical analysis of infiltration, considering hysteresis into a vertical soil column at equilibrium under gravity. *Soil Sci. Soc. Amer.*, 29(5), 489-494.
- Woolhiser, D.A., and Liggett, J.A. (1967) Unsteady, one-dimensional flow over a plane: The rising hydrograph. *Water Resources Research*, 3, 753-771.
- Taylor, C. (1976) A Computer Simulation of Direct Runoff. *Finite Element in Water Resour.* Gray, W.G. Pinder, G.F., Pentech Press, London, U.K., 4,149-163.
- Baxter, E.V et al. (1990) Finite element watershed modelling: One-dimensional elements. *Journal of water resources planning and management*, 116(6), 803-819.
- Blandford, G.E. and Meadows, M.E. (1990) Finite element simulation of non-linear kinematic surface runoff. *J. Hydrol.*, 119, 335-356.
- Li, X., Cescotto, S., Thomas, H.R. (1999) Finite element method for contaminant transport in unsaturated soils, *J Hydrologic Engineering* 4:265–274
- Hamdi, Y. (2001) Contribution à la modélisation numérique du cycle de l'eau. PhD, Université Laval, Québec, Canada.
- Craig, J.R., Liu, G., Soulis, E.D. (2010) Runoff-infiltration partitioning using an upscaled Green-Ampt solution. *Hydrological Processes*, Vol. 24, No. 16. pp. 2328-2334.