C-128

# A NUMERICAL SIMULATION ON THE FLOW OF WATERSHED FILTRATION REACTORS USING LIGNOCELLULOSIC MATERIALS

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## ABSTRACT

Pinyon juniper, a small-diameter and underutilized (SDU) lignocellulosic material, was harvested in New Mexico, identified as Juniperus monosperma at the USDA Forest Products Laboratory, chipped, fiberized and chemically modified to remove pollutants from wastewater. This juniper species was selected as a raw material through screening test for removal of pollutants and proved to be one of a best lignocellulosic material. Resultant fiber was made into a Rando mat using 10% HC-105 binder, with mat density of 0.109 to 0.131 g/cm$^3$, thickness of about 1.3cm. The hydraulic conductivity was 6.4 x 10$^{-4}$ cm/s. Mats were cut into 61 cm x 61 cm pieces, fitted into stainless steel frames, and installed into a model filtration reactor. The aim of this study is to simulate the flow by computational fluid dynamics (CFD) and provide information on flows inside the system to aid the design of an ideal reactor. The major influential parameters of the flow inside the reactor can be designated such as porosity, height, width, number of filters, and distances between the baffles. Due to the flow resistances between the filters, the water level is continuously decreasing with waves propagating on it. Different flow characteristics can be obtained by changing the shape of the reactor and porosity of the filter.

Keywords: Lignocellulosic material, hydraulic conductivity, filtration reactor, CFD, free surface

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## 1. INTRODUCTION

The water supply system of New York City consists of two reservoir systems, the Catskill/Delaware system and the Croton system. The 375-mi' Croton watershed, located east of the Hudson River, contains 10 reservoirs and 3 controlled lakes. The area of the Catskill/Delaware system is 1,594 $m^2$; this watershed includes 6 reservoirs west of the Hudson River and 3 reservoirs in Westchester County.

In the Catskill/Delaware watershed, approximately 350 dairy and livestock farms and 90 other agricultural enterprises are in operation. Various pollutants, such as Cryptosporidium, nutrients, pesticides, and sediment, originate from the activity of those farms and enterprises, which deteriorate the quality of water in the reservoirs. One potential problem in the New York Watershed is eutrophication of the reservoirs due to the excess supply of nutrients including phosphorus (NYCDEP, 1999a; NYCDEP, 1999b).

The New York City Department of Environmental Protection (NYCDEP) operates several wastewater treatment plants to reduce phosphorus loadings into the watershed. The size of plants varies from 4,200 to 5.6 million L/day, and the phosphorus removal process is based on precipitation techniques. The approach proposed by the Forest Products Laboratory is to decrease phosphorus loading by installing small filtration systems at the outlet of wastewater at dairy farms. In the fixed-bed filtration system, the selection of an adsorbent is important. Red mud, which is a waste material in alumina production and whose main components are ferric and aluminum oxide, activated alumina, and polymeric ligand exchangers have been studied as a sorbent for phosphate removal (Akay et al., 1998; Ayob et al., 2001; Zhao and Sengupta, 1998).

Lignocellulosic fibers are low cost unconventional sorbents and have been examined for potential use as heavy metal removal sorbents (Friedman and Waiss, 1972). Some scientists have modified lignocellulosic fibers with several chemicals to improve their filter performance (Morita et al., 1987; Saliba et al., 2000). Among lignocellulosic fibers, juniper (Juniperus monosperma) was chosen as an appropriate sorbent since it is inexpensive and has relatively high heavy metal sorption capacity (Han, 1999).

Recently, juniper fibers were processed into a mat-type filter medium and used to restore the watershed affected by acid mine drainage (AMD) in the Wayne National Forest in Ohio. The AMD water contains iron, sulfates, aluminum, manganese, and other dissolved and suspended solids because of its strongly acidic condition (Drever, 1997). The juniper filter media were installed into a filtration system to remove the dissolved metal ions and suspended solids from the water.

In the present study, the modified lignocellulosic filter media were installed into system and their performance as filter media were examined (Han et al, 2003). The flow inside the filtration reactor having porous filters and baffles was analyzed numerically by commercial CFD program STAR-CD. STAR-CD was developed by Gosman's group of the Imperial College in England and can simulate complicated geometries (Computational Dynamics, STAR-CD Manuals).

The flow inside the reactor is very complicated due to the free surface movement. Porous filters and baffles further complicate the flow. The aim is to simulate the flow numerically and provide information on flows inside the system to aid the design of the filtration reactor. The influence parameters to affect the flow inside the reactor such as porosity and height and number of filters and baffle distances need to be investigated.

## 2. SIMULATION

### 2.1. MATERIALS

The raw filter material was juniper (Juniperus monosperma), a small-diameter and underutilized (SDU) lignocellulosic material that is distributed in the southern region of the United States. Juniper trees were shredded into small chips, refined (fiberized or pulped), and chemically modified. Resultant fibers or pulp was made into a Rando mat using 10% HC−105 binder. Mat density was 0.109 to 0.131 g/cm$^3$ and thickness was about 1.3 cm. Mats were cut into 61-cm by 61-cm pieces. The filter mats were initially used at the Wayne National Forest to reduce metal contents from the water affected by AMD. After being used for 3 days, the filter mats were dried and shipped to the Forest Products Laboratory in Madison, Wisconsin. The filter mats were washed with clean water to remove components soluble to water and dried again. All the filter mats except for the part that was used for the laboratory-scale test were shipped to the field site in New York State to be reused for the removal of phosphorus from water.

### 2.2. NUMERICAL MODELING

The filtration reactor was designed at the Forest Products Laboratory and made of fiberglass by Empire Fibreglass Products, Inc. (Little Falls, New York). The filter frames were fitted into 13 slots in the reactor. Twelve lignocellulosic filter mats were placed in the reactor. Figure 1 shows the filtration reactor and filter frames.

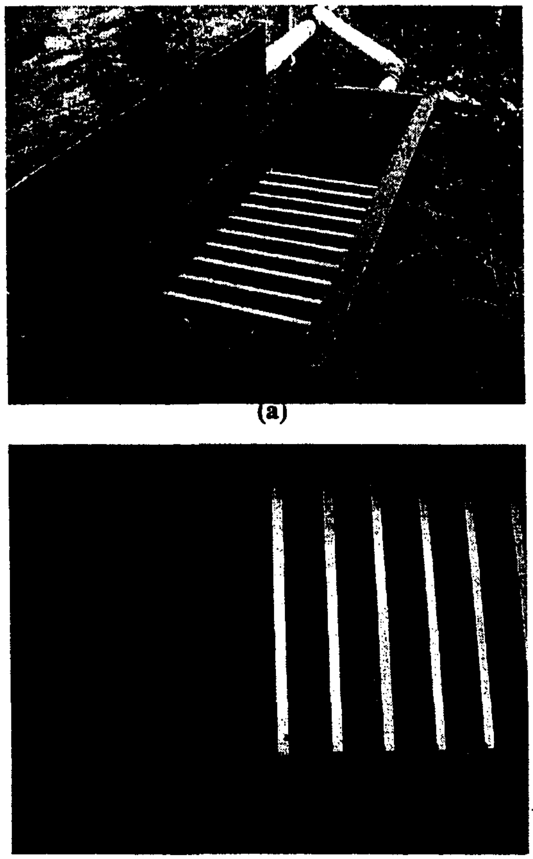
The numerical model is based on solving the Reynolds-Averaged Navier-Stokes Equation (RANSE) taking into account the free surface via the Volume of Fluid (VOF) method. A commercial CFD program, STAR-CD where such methods are implemented is used in the study. Brief information on the software is given in the Appendix along with example depicting the capability of solving transient free surface problem. For the simulation of turbulent flow a standard two equation k-ε model is used in the study. Equations (1) and (2) are called Reynolds-averaged Navier-Stokes equations.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho \mu_i) = 0 \qquad (1)$$

$$\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}(-\rho\overline{u_i' u_j'}) \qquad (2)$$

They have the same general form as the instantaneous Navier- Stokes equations, with the velocities and other solution variables representing ensemble-averaged values. Reynolds stresses, $-\rho\overline{u_i' u_j'}$ must be modeled in order to represent the effects of turbulence. Reynolds stress is

$$-\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\left(\rho k + \mu_t \frac{\partial u_i}{\partial x_i}\right)\delta_{ij} \qquad (3)$$



(a)

(b)

**Fig. 1 Filtration reactor (a) and filter frames (b) inside filtration reactor**

The advantage of this approach is the relatively low computational cost associated with the computation of the turbulent viscosity, $\mu_t$. Two additional transport equations (for the turbulent kinetic energy, k, and the turbulence dissipation rate, E) are solved to get turbulent viscosity

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

The models of turbulence, which are simple and complete at the same time, are two-equation models in which the solution of two separate transport equations allows the turbulent velocity and length scales to be independently determined. The standard k-ε model in STAR-CD falls within this class of turbulence model and has become the most widely used software in the practical engineering flow calculations. Robustness, economy, and reasonable accuracy for a wide range of turbulent flows explain its popularity in industrial flow and heat transfer simulations. It is a semi-empirical model, and the derivation of the model equations relies on phenomenological considerations and empiricism.

### 2.2.1 GEOMETRIC MODELING FOR THE NUMERICAL ANALYSIS

In our numerical analysis the transient viscous flow about the filtration reactor having baffles and porous filters as shown in Fig. 2 is simulated to investigate the flow phenomena inside the reactor. As transient RANSE/VOF calculations for such models need tremendous computer resources and extensive computation time, several restrictions should be observed, e.g. the total number of nodes should be as small as possible so long as it resolves the local flow phenomena. As a consequence, unstructured grid methods are recommended, i.e. a fine grid in the near field of the porous media filter.

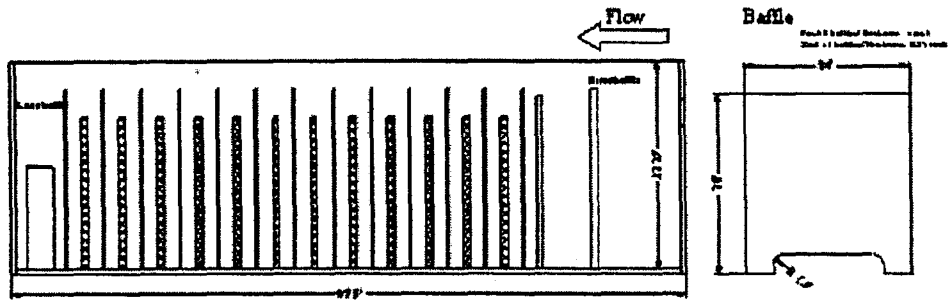



**Fig. 2 Schematic of a filtration reactor with baffles and porous media filters**

### 2.2.2 GRID GENERATION

As the fluid flow is solved in three dimensional, hexagonal domain a 3D hexahedral grid is used. The mostly orthogonal 270,000 computational cells are arranged as shown in figure 3. Unstructured grid generation is used for high resolution near the filter with a reasonable number of nodes in all regions of the solution domain. For the porous filter, actual holes are modeled in the present study as shown in figure 4. Local meshes in the area simulating narrow flow passages are refined to house more computational meshes to resolve the flow. The size of the passage need to be determined via experiment.

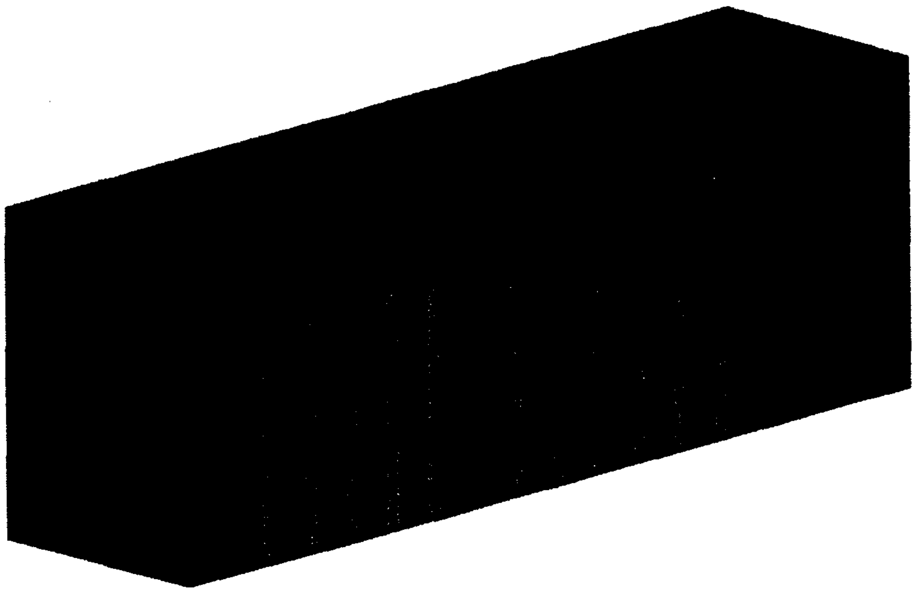


**Fig. 3 Computational grid of a filtration reactor**

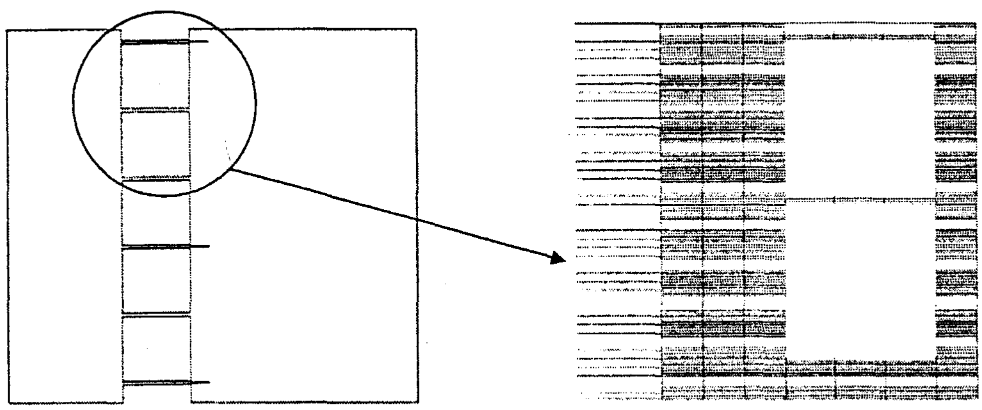


**Fig. 4 Filter modeling of a filtration reactor**

### 2.2.3 BOUNDARY CONDITIONS

Many boundary conditions can be used in STAR-CD and the boundary types used in the present simulation are as follows (see Fig. 5):

Inlet: most information, such as velocity, temperature and characteristics are known and can be defined. This boundary type is given at the water inlet at top of the shed with constant flow rate of 30gal/min.

Outlet: fluid flows outwards and not many information are needed but it cannot be used in areas of recirculations. The exit where the water flows out of the shed is given this boundary type.
Wall: Velocities are set to zero when laminar but special treatment is needed when the flow is turbulent. The walls contacting the flow are given this type of boundary.

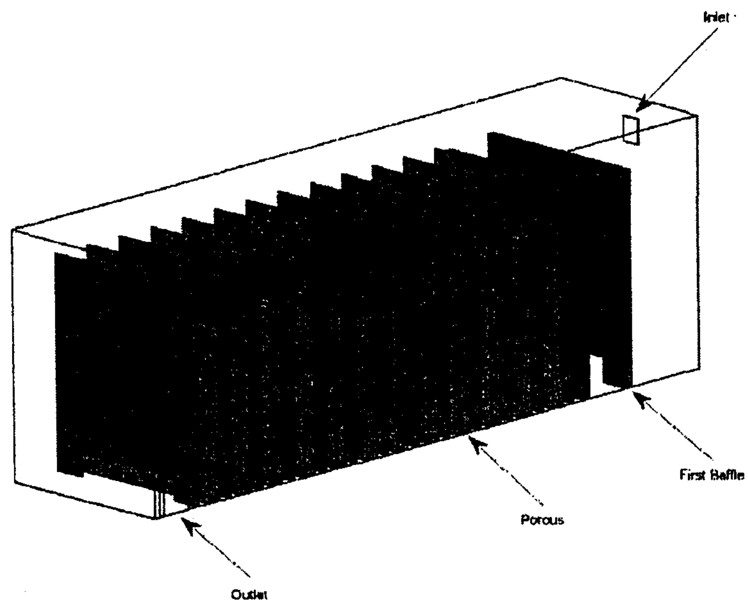



**Fig. 5 Computational domain showing boundary conditions and baffles and refined porous filters**

### 2.2.4 PROPERTIES AND SOLUTION CONTROLS

As the free surface is included in the computations, the fluid material properties for both water and air are supplied. Properties at standard temperature and atmospheric condition are selected for all computations. The PISO (Pressure Implicit with Splitting of Operands) solution algorithm is activated instead of the SIMPLE(Semi Implicit Pressure Linked Equations) algorithm, because better convergence performance is expected generally for transient computations. For getting a sharp interface at the boundary between water and air the VOF method together with the CICSAM (Ubink,1997) differencing scheme is used[]. Since the quality of the computational results is highly dependent on the Courant Number, an automatic time step control routine is activated to hold the value of the Courant Number below 0.3.

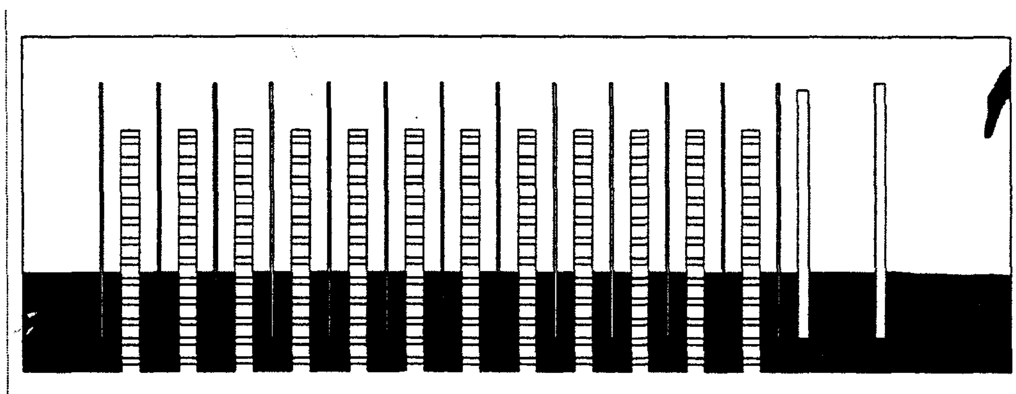
The computations are carried out on a LINUX PC cluster based on Intel Pentium □ 850 MHz processors. By using 1 CPU the present transient computation took 270 hours of CPU time to simulate 10 seconds of flow. If more CPUs are used in the computation with parallel processing, the computation time can be reduced almost proportionally to the numbers of CPU used.

## 3. RESULTS AND DISCUSSION

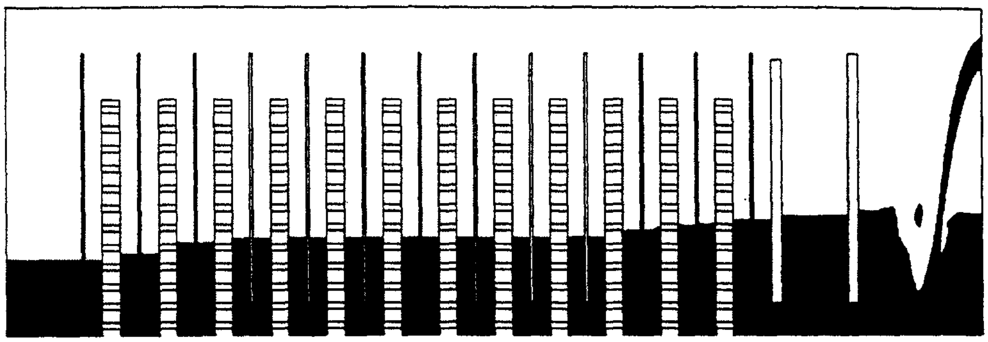
The computation was started from the partially filled initial condition. Figure 6 shows free surface locations at various times after filling and draining is started. One can observe the level of water rising with splashing at the region where the water enters the shed and falling at drain region. In between due to the flow resistances, the water level is continuously decreasing with waves propagating on it. For this particular case, the height of the flow was increasing to the moment at time of 30 sec and reached to the steady state with the rate of 30 gal/min. Thus, this filtration reactor can treat the flow of 30 gal/min based on the simulation.

By changing the shape of the shed and porosity of the filter, one can have different flow characteristics. For example, if the porosity of the filter is very low then one might have flooding over the baffles. On the other hand, if highly porous material is used for the filter, then the flow is maintained at lower level of the shed with high flow velocity. And hence the residence time of the water in the shed is highly reduced, which results in lower reaction time.

In the present study, the possibility of CFD simulation on performance of watershed was demonstrated based on the design drawings. In the future, various characteristics for the design can be simulated with more realistic conditions of the shed, which may help final design.

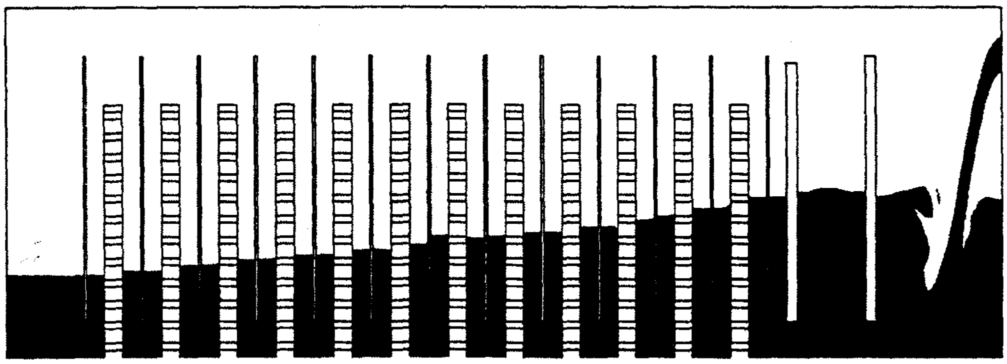


t = 0.2 sec

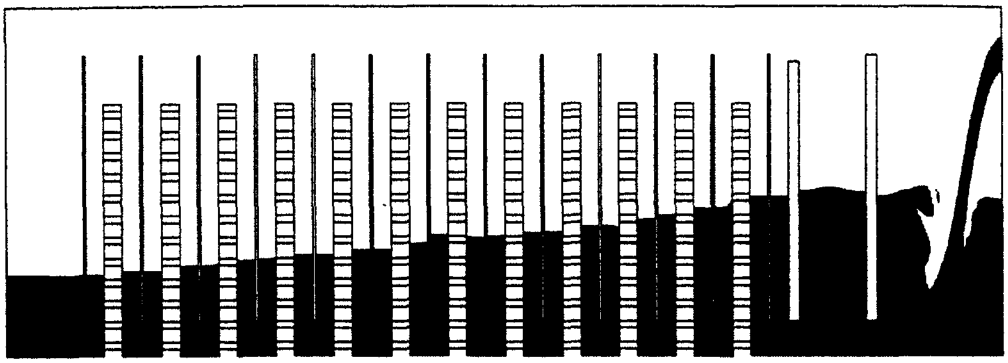


t = 10 sec

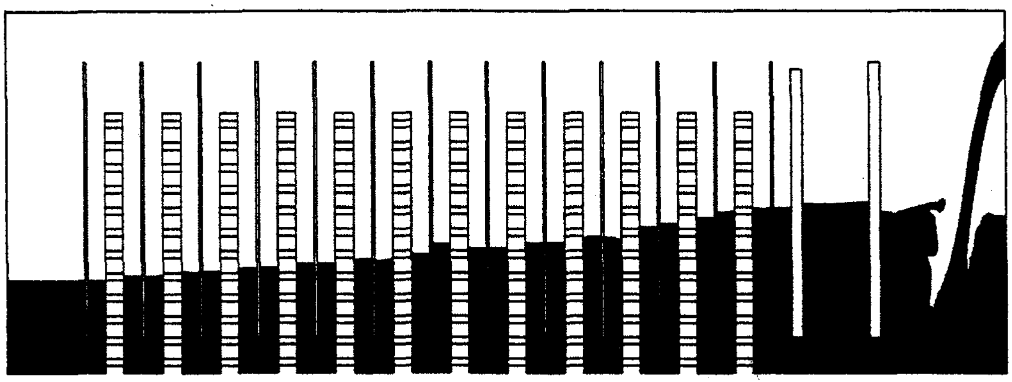
t = 20 sec



t = 30 sec



t = 40 sec



t = 50s

**Fig.6: Simulation Results showing free surface locations at various times after initial partially filled condition**

## 4. CONCLUSION

The filtration reactor was designed at the Forest Products Laboratory and made of fiberglass. Lignocellulosic filter mats were placed in the reactor. After the filter mats were installed, samples were taken from the inlet and outlet of the filtration reactor. The possibility of CFD simulation on performance of the reactor was demonstrated. The reactor was proved to treat the flow of 30 gal/min based on the computer calculation. Due to the flow resistances between the filters, the water level was continuously decreasing with waves propagating on it. The aim of this study is to provide information on flows inside the system to aid the design of an ideal reactor. The major influential parameters such as porosity, height, width, number of filters, and distances between the baffles were investigated. Different flow characteristics can be obtained by changing the shape of the reactor and porosity of the filter. For realistic flow simulation, pressure drop characteristics of the filter need to be obtained through experiment. In the future, various characteristics for the design can be simulated with more realistic conditions of the reactor, which may help final design.

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