Conceptual real-time multiphase flow modeling for complex NAPL remediation systems

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ABSTRACT: Groundwater data collection is done under statutory supervision and control in catchment. The storage, evaluation and utilization of groundwater and geo-strata information are of importance to the protection of the quality of water for industrial and other uses. The contamination of groundwater sources through immiscible fluids, including NAPLs, is of interest to current research. Equally important is the demand to quickly locate, demarcate and visualize these contaminated areas. This paper provides a structured modelling strategy for digital groundwater data assessment system (DGWDAS) for the 2D/3D visualisation of contaminated areas. This conceptual model forms a basis for a visualization tool for solutions to free-hydrocarbon recovery systems. The tool helps to visualize results of simulations on coupled stratified immiscible fluid flows of NAPL, that satisfy PDEs with coupling conditions on the sharp interface under steady-state flow, based on the assumption of vertical equilibrium. An informative visualization tool based on DGWDAS may also allow evaluation of the discharge, the heads, etc of the recovery system by given heads or discharges in the wells respectively. Additionally, the visualization tool, which is based on the n-Tier Software Architecture, may assist in environmental planning and management in the early stages of assessment of sensitive contaminated areas.

1 INTRODUCTION

The contamination of aquifer, especially with Non-Aqueous Phase Liquids (NAPL), may lead to environmental risks to aligning settlements and protected zones. Relatively accurate groundwater (GW) models for environmental impact assessments may help in early decision making. The source, and accurate use of qualified field data for the parameterization of groundwater models, determines the practical significance of simulation results [Portugal / Den Haag].

The modelling of the coupled flow of free-phase NAPL in groundwater and their remediation using complex multiple well recovery systems (MWNRS) has been discussed elsewhere [1, 2].

Optimizing solutions of the coupled flow and transport processes lead to non-linear and non-convex objective functions with multiple local minima and both nonlinear models and nonlinear constraints. The presence of local minima has implications for the performance and results obtained by optimization algorithms.

The development of these algorithms, however, may have to be preceded by descriptive site-related parameter sensitivity assessments of different remediation scenarios. This procedure for the estimation of the aquifer response for the most important factors of influence, leads to a more suitable definition of the objective functions, scope and constraints required for the optimization of the remediation systems. Achieving a real-time simulation and visualization must take these complexities into consideration.

The paper presents the follow-up steps and methodologies for modeling, simulating and optimizing of multiphase flow and transport of mobile plumes of NAPL in porous media at real-time. Adequate insight is also given on the method of reflection and of superposition of potentials used in the new so-called Bounded Cell Multi-Wells Method for the simulation of NAPL remediation with a grid-based well-field. In particular, emphasis is placed on the various concepts and technologies for handling client-side output, as employed in current on-going research. Practical examples are discussed to underpin the methods discussed in this paper, which may form benchmark solutions for the hydraulic remediation of NAPL-contaminated sites.

2 ESTIMATING GW-MODELING PARAMETERS

The phenomenological approach for modeling GW flow and transport is the assumption of a homogenized structure for continuum models that neglects the microstructure. These superimposed continua provide abstraction of the geometrical model and field data for preliminary simulation purposes. The sources of data for the parameterization of these models, however, are through well-targeted site characterization or baseline studies - and standard field measurements using environmental data collection wells or boreholes [1,2]. The spatially weighted averaging method for estimating GW modeling parameters is described in [3]. Hydro-Geological databases are another source of reliable information on soil morphology, especially in inaccessible areas [2, 4, 5, 6, 11].

3 SOIL PROFILES DIAGRAMS WITH CUBIC SPLINE INTERPOLATION ALGORITHMS

A cubic spline is a spline constructed of piecewise third-order polynomials which pass through a set of ***n*** control points. A cubic spline is a spline constructed of piecewise third-order polynomials which pass through a set of m control points. This means that between each two points, there is a piecewise cubic curve. When we string these curves together, we set the second and first derivatives at the endpoints of each piecewise cubic curve equal to that of the adjacent cubic curve's second and first derivatives thus providing for a continuous second derivative. This gives a smooth curve that passes through each point, thus interpolating them.

A polynomial fitted to many data points exhibit erratic behaviour. Splines are smooth and continuous across the interval [16].

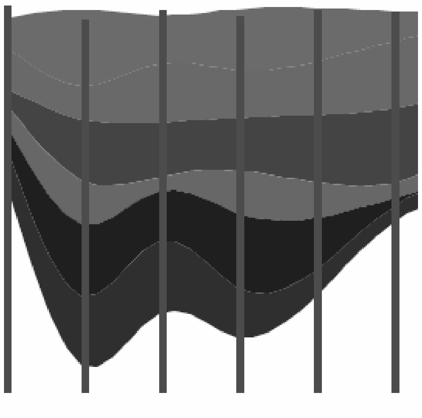

Figure 1. Soil profile interpolation using cubic spline algorithms and SVG.

The use of cubic splines for 2- and 3D Interpolation and graphical visualizations is most suitable, as the resulting soil layers provide the closest approximations to the natural flow of soil layers.

4 REMEDIATION OF NAPL WITH COMPLEX WELL FIELDS

The scheme of the contamination scenario is shown in Figure 1, in which a flow domain of defined boundaries is contaminated with a mobile plume of LNAPL.

Two methods for modeling and simulating the recovery of free-phase NAPL in aquifer are discussed under 4.1 and 4.2. Both methods are suitable for modeling flow and recovery in large domains[1, 12]. While the first method can incorporate the dimensioning of a flexible well-placement regiment of the recovery system [1], the second method allows the more usual practice of well-placements on predefined grids.

4.1 *Remediation of extended domains*

[1] and [2] discussed the theory and implementation of free-phase hydrocarbons on extended domains. On the basis of the practical application demonstrated in these publications, it was shown that most remediation cases may be formulated and modeled.

On the basis of this calculation method, and with the data in Table 1: and Table 2:, it can be shown that the very accurate rasterized piezometric surfaces can be obtained for all nodes(Figure 10ff). Additionally the extraction rates for each well can also be calculated for each time step.

Table 1: Model parameters for LNAPL remediation

Parameter	Value	Unit
Hydr. Cond., light phase (LP), k_{fl}	2,62E-5	[m/s]
Hydr. Cond., dense phase (DP), k_{fd}	9,81E-5	[m/s]
Density, LP	800	[kg/m3]
Density DP	1000	[kg/m3]
Eff. Porosity, n_e	0,2	[-]
Boundary Conditions		
Thickness, DP	11,2	[m]
Groundwater level	12,0	[m]
Thickness LP	1,0	[m]
Domain		
Diskretization	1,0	[m]
Length	100	[m]
Breadth	100	[m]
Wells		
Radius	0,2	Fully penetrating
Type	-	Skimmer well

Table 2: Coordinates of recovery wells W_i

Well-Point	X	Y
1	30	70
2	35	30
3	45	40
4	60	40
5	65	60
6	70	30

4.2 *Basic formulations of the Bounded Cell Method*

Figure 4 shows a scheme of the so-called Bounded Cell Method (BCM). The concept of this method is to demarcate grid-based areas of influence (cells) for each well in a recovery system (Figure 4), for each of which the boundary conditions can be determined. The number of cells determines the number of wells in the recovery system. Determining the governing equations for this method is done through the super positioning and mirroring of the potentials at discharge point (wells) in the domain on the boundary of the reference cell (Figure 2 and Figure 4).

Potential at a Point M:

The hydraulic potential in the flow domain at any given point is defined as:

$$\varphi = -k_{fl} \cdot \frac{h^2}{2} + c \qquad \text{(Eq.1)}$$

Initial / Boundary Conditions:

From Figure 3, we can define the following initial conditions:

$$\begin{aligned} h_{li} &= h_{la}, \quad i = 1,\ldots,n \\ h_{l0} &= h_{lw} \\ Q_i &= Q\ , \quad \textit{where} \quad i = 0,\ldots,n \end{aligned} \qquad \text{(Eq.2)}$$

where:

Q : Discharge in the Well *i* (*i* = 0,….,n), in [l/s]

To demonstrate the calculation method, an equivalent, constant discharge rate Q is assumed for all all wells in the recovery system.

Generated / Induce Potential:

The generated or induced potential at any point of extraction or infiltration is defined as:

$$\varphi_l = -\frac{Q}{2\pi} \ln E \qquad \text{(Eq.3)}$$

where ***E*** is the planar distance between two Well positions in a multiple well recovery system.

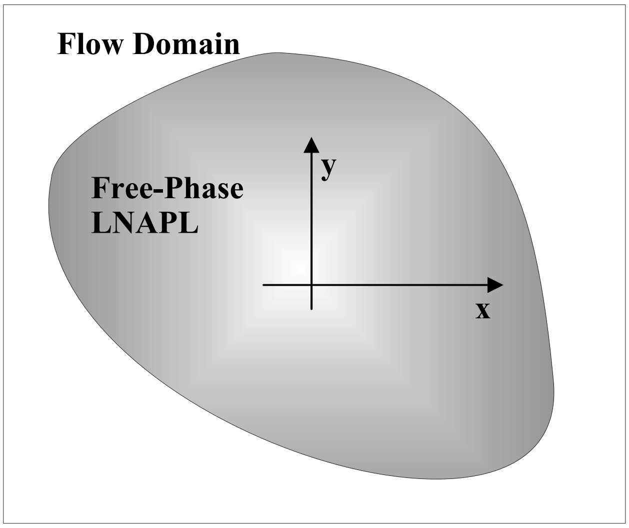

Figure 2. Scheme of the NAPL-contaminated flow domain.

For each of the Wells W_i,th induced potential can be written as follows:

$$\varphi_0 = -\frac{Q}{2\pi} \ln \sqrt{x^2 + y^2} \qquad \text{(Eq.4)}$$

$$\varphi_1 = -\frac{Q}{2\pi} \ln \sqrt{(x-2a)^2 + y^2} \qquad \text{(Eq.5)}$$

$$\varphi_2 = -\frac{Q}{2\pi} \ln \sqrt{(x+2a)^2 + y^2} \qquad \text{(Eq.6)}$$

$$\varphi_8 = -\frac{Q}{2\pi} \ln \sqrt{(x-2a)^2 + (y+2a)^2} \qquad \text{(Eq.7)}$$

The sum of the discharge potentials for ***n*** Wells in the flow domain is:

$$\Phi = \varphi_0 + \sum_{i=1}^{n} \varphi_i \quad ; \quad n = 8 \qquad \text{(Eq.8)}$$

This leads to a general expression for any discharge point, relative to a reference well to be written in the form:

$$\begin{aligned} \Phi = -\frac{Q}{2\pi} \ln \Big[& \sqrt{x^2+y^2} \cdot \\ & \sqrt{(x-2a)^2+y^2} \cdot \sqrt{(x+2a)^2+y^2} \cdot \\ & \sqrt{x^2+(y+2a)^2} \cdot \sqrt{x^2+(y-2a)^2} \cdot \\ & \sqrt{(x+2a)^2+(y-2a)^2} \cdot \sqrt{(x-2a)^2+(y-2a)^2} \cdot \\ & \sqrt{(x+2a)^2+(y+2a)^2} \cdot \sqrt{(x-2a)^2+(y+2a)^2} \Big] \end{aligned} \qquad \text{(Eq.9)}$$

Piezometric head at any point M:

The hydraulic potential at any point on the piezometric surface of the domain is defined as:

$$\Phi = -k_{fl}\frac{h^2}{2} + c \qquad \text{(Eq.10)}$$

where $h = h(x, y)$, the piezometric head

4.2.1 *Multiphase extraction of only the Light Phase*

To determine the equation for the extraction rates of the light/dense phase (LNAPL/G-Water) and the elevation at any point M on the domain, existing points of known potential and boundary conditions, such as at P_1 and the reference well W_0 may be used. Alternatively, any two points of reflection on the boundary, such P_1 and P_5, satisfy the conditions of equipotentials in the reference Cell (Figure 4).

Equipotentials as Boundary Condition at P_i:

From the Boundary Conditions, the superimposition of the potentials of all wells W_i in the domain on the point P_1 can be expressed as.

$$-k_{fl}\frac{h_{la}^2}{2} + c = -\frac{Q}{2\pi}\ln(975 \cdot a^9) \qquad \text{(Eq.11)}$$

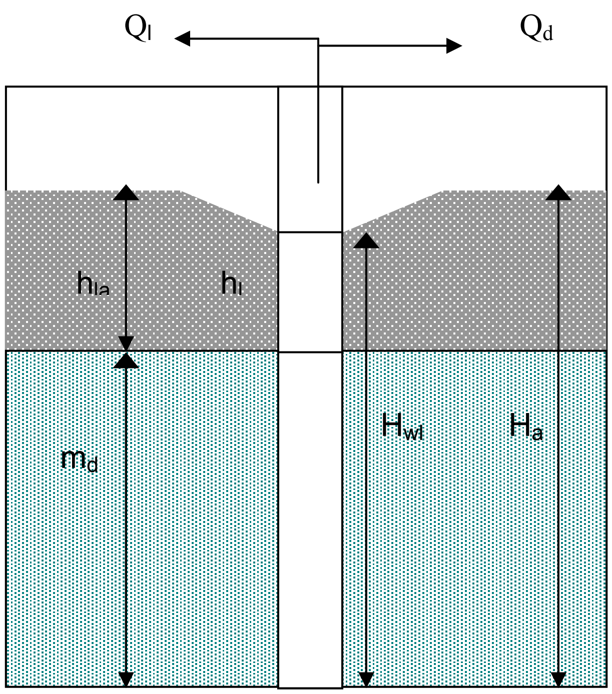

Figure 3. Cross-section of extraction well W_i.

Potentials at the reference Well W_0:

At the reference Well $\boldsymbol{W_0}$, the pressure head h_l can be calculated through:

$$-k_{fl}\frac{h_{lw}^2}{2} + c = -\frac{Q}{2\pi}\ln(1024 \cdot a^8 \cdot r_w) \qquad \text{(Eq.12)}$$

Discharge equation at the reference Well W_0:

At any point on the Boundary, the hydraulic and discharge potentials are equivalent and Equations (9) and (10) are equal:

$$\Phi_\Omega = const \qquad \text{(Eq.13)}$$

Subtracting Eq. 11 from Eq. 12, we obtain:

$$Q = \frac{\pi k_{fl} \cdot (h_{la}^2 - h_{lw}^2)}{\ln \dfrac{a}{1,05 \cdot r_w}} \qquad \text{(Eq.14)}$$

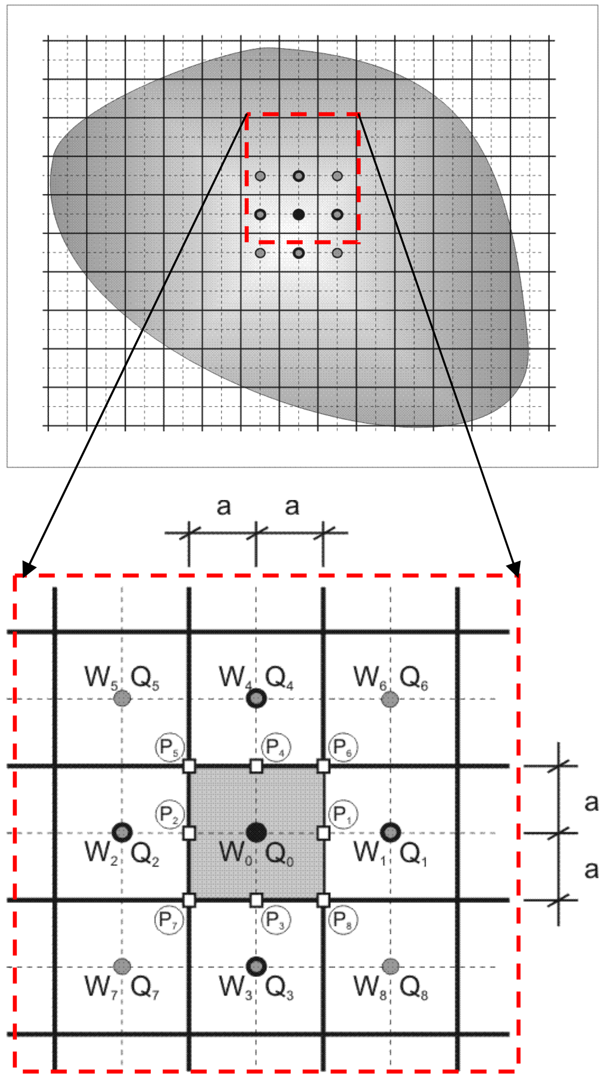

Figure 4. Bounded Cells with Boundary Points P_i.

4.2.2 *Multiphase extraction of both Phases*

As described in [1, 2, 3], it may be essential to simultaneously extract both phases (LNAPL/G-Water).

From the figure above, it can be deduced that the discharge rate of dense phase can be expressed as:

$$Q = \frac{2\pi k_{fd} m_d \cdot \frac{\rho_l}{\rho_d}(H_a - H_{wl})}{\ln \frac{a}{1,05 \cdot r_w}} \qquad \text{(Eq.15)}$$

where

$$A = \frac{H_{lR} - H_{lS}}{H_{dR} - H_{dS}} = \frac{H_a - H_{wl}}{m_d - H_{wd}} \quad \rightarrow \infty$$

i.e, $m_d = H_{wl}$ at each time step throughout the duration of the pumping/recovery.

The extraction region is carried out under the prerequisite that the groundwater level remains at constant at m_d in the well.

The simulation results, which compares well with previous bench mark solutions [1, 2], are shown in Figure 6 to Figure 8. By considering the investment and running costs on Figure 8, a break even point for an optimal selection of design configuration of the recovery well can be determined.

5 MODELING TOOLS AND FRAMEWORK

Conception ally, the design of the software components for the visualization of NAPL contaminants should provide functionalities that emulate the procedures and tools used by environmental damage control engineers for planning immediate to long-term remediation work. Increasingly, Geographic Information Systems (GIS) software is providing the functions and tools needed to store, analyze, and display environmentally-relevant information [2].

On the other hand, and to avoid the integration of proprietary modules in existing n-Ter systems (Figure 5), the more platform-independent XML-based libraries such as Scalable Vector Graphics (SVG) provide state-of-the-art cutting-edge methods for most development needs.

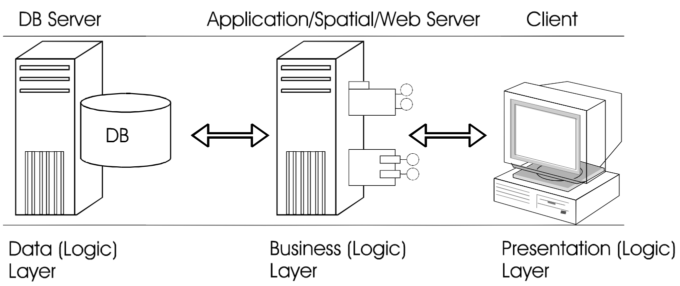

Figure 5. 3-Tier Geosoftware Architecture [2]

For raster-based digital geo-referenced systems (e.g. based on GIS), both multi-well calculation methods (see 4.1 and 4.2) may be suitable for the visual modeling of the contaminated site, and for the 2D/3D graphical output of the simulation and the optimization results on NAPL flow and migration results.

6 AQUIFER RESPONSE TO SENSITIVE PARAMETERS

Results were obtained for *q* in the following situations:

a) Values for *q* for all allowable values of h_d at constant values of h_l.
b) Values for *q* for all allowable values of h_d and h_l for varying influence radii, R.
c) Values for *q* for all allowable values of h_d and h_l, at varying positions of the wells.
d) Maximum and minimum values for *q* for all allowable values of h_d and h_l on different hydraulic coefficients, k_{fl}.

Results from field data in (David et al, 2004, Urban et al, 2004) show significant accuracy for HGPCs through the Spatially Weighted Average Parameter (SWAP) method presented in this Paper. While conventional methods only consider soil layers of relatively large thicknesses, SWAP incorporates all soil layers, thus making the result more representative of the natural flow domain. Confining estimates to only the bandwidth of soil layers directly affected by the contamination can further improve their accuracy through SWAP [2].

7 SIMULATORS AND OPTIMIZERS

The mathematical model described in the foregoing sections of this submission provides the basis for modelling any combination of real world physical contaminant management problems involving NAPL in aquifer. The constraints on the recovery system must include the aspects of cost to the objective function, either as a separate formulation for their optimization, or in conjunction with others. The strategy leads to the formulation of multi-objective functions that require complex optimization algorithms to solve.

Modelers must input data on contamination management models into Simulators such as MODFLOW. Simulators predict how a physical system will respond to an input strategy. The interplay between Simulators and Optimizers may produce management strategy of an assumed management problem.

Aquifer response is measured through the sensitivity analysis for set proplems. Sensitivity analysis techniques give a way to compute solution uncertainties by using information on the sensitivities of the solution to various parameters. These sensitivities are just the solution derivative with respect to the parameter in question, and equation for them can be derived by differentiating the original model problem. The resulting sensitivity equation is linear and can be solved in tandem with the model equations. First order estimates of solution uncertainties can be developed from these sensitivities with a straightforward additional calculation [8].

8 RESULTS

The results obtained for the two methods of simulating recovery of LNAPL with complex well-fields are shown to demonstrate the effectiveness, and the suitability of the methods, among others, for real-time simulation and visualization purposes. The data are based on bench mark values and parameters discussed elsewhere [1, 2].

8.1 *Results on using the Bounded Cell Method*

Using a well radius of 0,2m and an LNAPL thickness of 1.0m, the following results were obtained for a cell size of 20m (Figures 6ff).

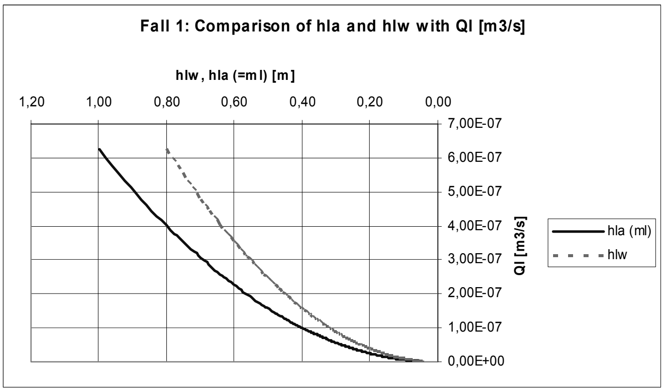

Figure 6. Comparing the effects of the thickness on extraction rates of LNAPL.

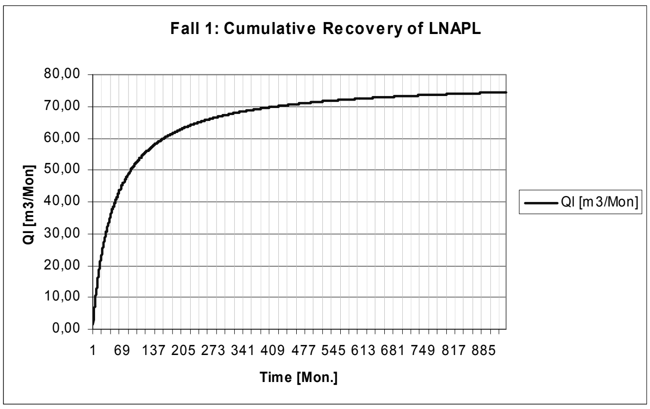

Figure 7. The cumulative recoeverable LNAPL curve shows 80% recovery within 210 months.

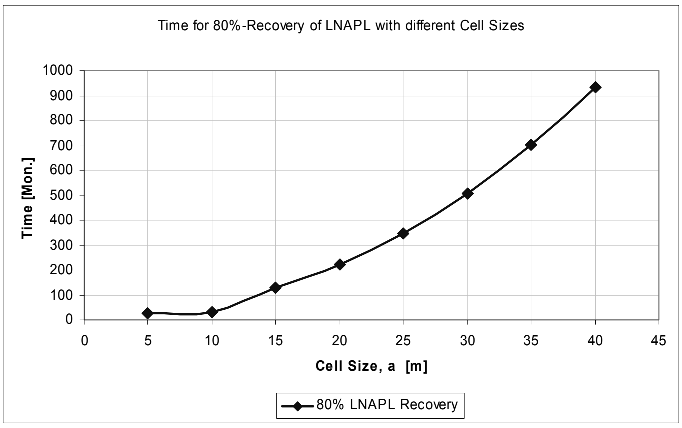

Figure 8. The effects of cell size on total pumping time, yield and well placement.

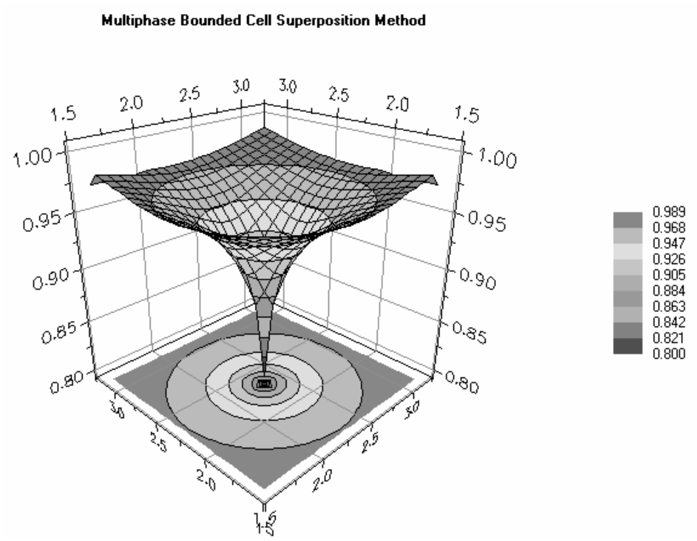

Figure 9. Extraction funnel on simulation of one Well in a bounded cell.

8.2 *Results on using Extended Domain Method*

The simulation of the LNAPL recovery with the system configuration shown in Table 1: and Table 2: yields a minimum discharge rate of 115 [l/d] in Well 4 and a maximum discharge of 207 [l/d] in Well 1. The maximum yield per day is 728 [l/d]. Well 6 remains dry within the initial time step. These values compare favorably with previous results [1,2].

Figure 10 and Figure 11 show the 2D elevation profiles generated by a six well skimmer recovery system for LNAPL. The performance of individual wells can therefore be tracked and regulated externally Figure 11 during the operation. The wells are numbered form 1 to 6 from left to write in Figure 10ff.

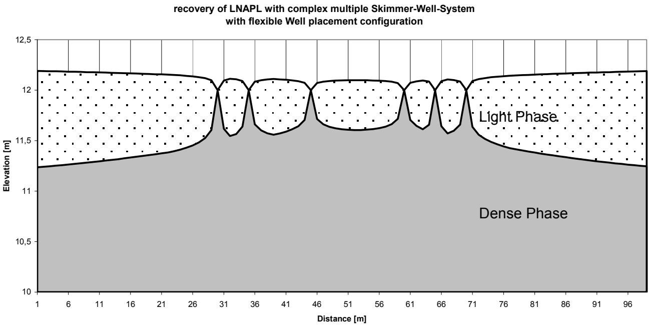

Figure 10. Elevation profile with 6 Wells (Well 1-Well 6, left to right).

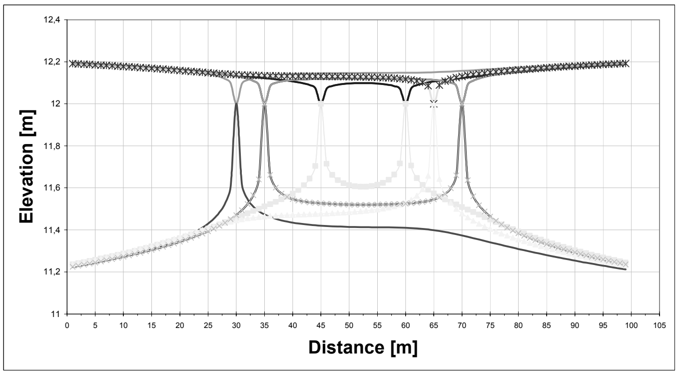

Figure 11. Extractions of individual wells.

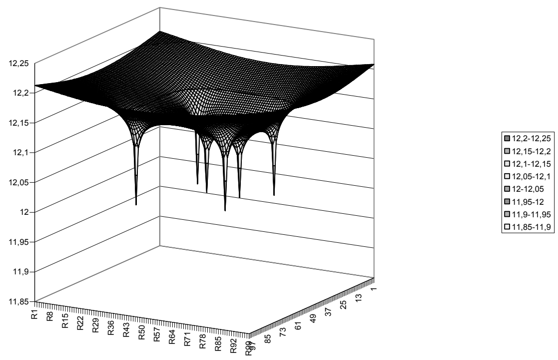

Figure 12. Spatial visualization of LNAPL surface profiles at run-time.

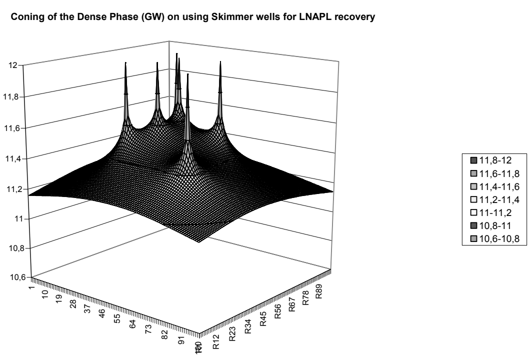

Figure 13. Coned surface profile of the dense phase at run-time.

9 CONCLUSION

This paper has discussed an overview of the underlying methods for real-time modelling of complex coupled multiphase flow and recovery of free.phase contaminants such as NAPL.

Spatially weighted average parameter estimation for groundwater modelling (SWAP4GWM), which is based on qualified source data and Voronoi algorithms, can assist the configuration of mathematical models for first-hand estimates [2, 7, 8, 9, 10].

The simulation of the free-phase NAPL migration and recovery on domains with known boundary conditions on fixed bounded cells or through flexible well arrangements has also been discussed. The simulation results from both methods compare well with other numerical results.

Scalable Vector Graphics (SVG), when combined with the natural smoothening performance of the cubic spline algorithm, provides a state-of-the-art technology for a platform-independent visualization of simulation results in real-time, especially for n-Tier software solutions.

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