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RELIABILITY OF MODELLING METHODS FOR SIMULATION OF LNAPL LENS SPREADING ON GROUNDWATER TABLE

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Abstract: Light Nonaqueous Phase Liquids (LNAPL) are mineral oil products which, due to accidents can lead again and again during storage, transport, and processing to strong contamination of groundwater. Consequently, it is of interest to investigate the spreading transport behavior of these substances in the subsurface. It will be shown that the usually applied averaging method for linearization leads to large errors.

The main objective of this paper is precisely verified if the simplified linearized Bussinesq'sc equation-based modelling usually applied to solve groundwater flow problems also reliable for simulation of LNAPL lens spreading on the groundwater table.

To achieve this objective, comparative numerical calculation was performed for a particular spreading case, namely a radially symmetric spread of an LNAPL lens for which there is an exact analytical solution of nonlinear equation.

To reduce the errors a new averaging method-based linearization of Bussinesq'sc equation is proposed which significantly reduces the errors. This is confirmed with relevant numerical examples of LNAPL lens spreading on the groundwater table.

Keywords: LNAPL spread, groundwater modelling, linearization of Bussinesq's equation

1. INTRODUCTION

Light Non-Aqueous Phase Liquids (LNAPL) are a class of environmentally polluting substances that, due to their insolubility in water, can exist and flow as a separate phase in the soil over the groundwater table in form of a lens (pancake) [1,2,3]. The calculation and simulation of convective - dispersive propagation processes of light water-insoluble pollutants in phase (i.e., LNAPL) is an essential part of different engineering disciplines and is particularly used in environmental technology at the depollution of groundwater.

The spread of LNAPL in soil and thus in groundwater depends on several different physical processes, which are viewed differently in various transport models. The governing equations that must be used for a realistic description of the propagation processes are mostly complex, nonlinear partial differential equations (NL-PDGL). The initial and boundary conditions which must be used for a realistic description of LNAPL spreading are also complex due to arbitrary entry form and expansion, inhomogeneities of aquifer etc. [1], [2].

The main and primary objective of the correct and adequate choice of technical measures to reduce or even eliminate the pollution caused by LNAPL lens is to know its extension, i.e., its evolution in space and time (e.g., sketched in Figure 1). This can be achieved only by simulation of the dispersive-convective transport processes of LNAPL on the groundwater surface, taking into account the boundary and initial conditions as close as possible to reality as well as the physical characteristics of LNAPL and the aquifer: delimitation of the studied domain, boundary conditions on the domain contour, zonal inhomogeneities in the domain specified by the hydraulic conductivity of the aquifer (k_{fi}), the initial form at time t_0 of LNAPL – lens, its density and the hydraulic conductivity

A sketch for a representative LNAPL spreading is in Figure 1. depicted

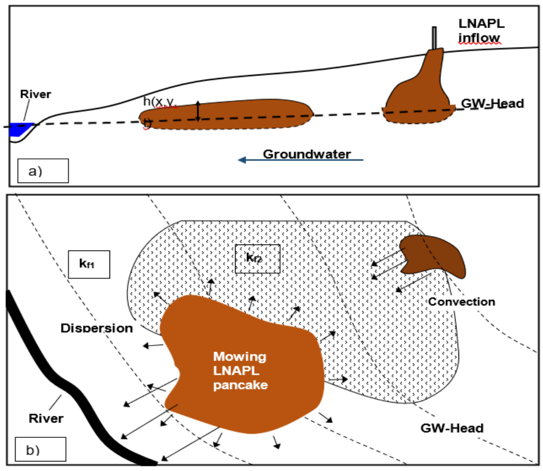

Figure 1. Scheme of LNAPL inflow and propagation on the groundwater table through convective and dispersive transport processes – a) Cross section; b) Top view

Of course, the simulation presupposes first the knowledge of the basic equations of the dispersive-convective transport process, the correct mathematical formulation of the boundary and initial problems, and the adequate methods for solving them. These aspects are briefly presented in the next paragraph.

2. BASIC EQUATIONS AND SOLUTION METHODS

For derivation of basic equations of convective-dispersive spreading of an LNAPL-lens on the groundwater table a simplified scheme sketched in Figure 2 will be considered.

Usually the LNAPL/water interface coincides approximately with the ambient groundwater table (i.e.,

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h_{lu}<<h_l). With this assumption the governing equation of the LNAPL – lens convective-dispersive spreading in term of its entire thickness h_l above of the ambient groundwater table has the form [1], [6]:

$$n_l \frac{\partial h_l}{\partial t} + \vec{q}_w \nabla\left(\frac{k_l}{k_w} h_l\right) - \nabla.(k_l h_l \nabla h_l) = q_l \qquad (1)$$

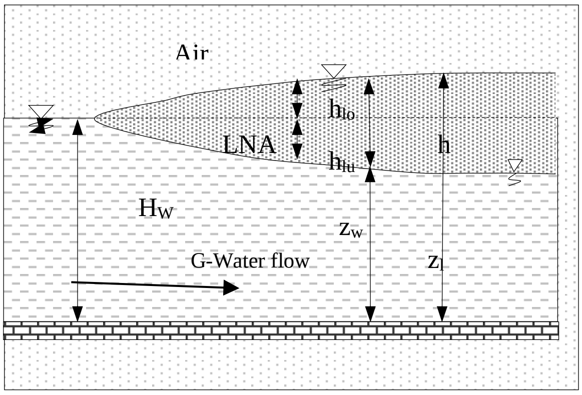

Figure 2. Sketch of a LNAPL lens on the groundwater table

Notations:

$\vec{q}_w$ = Darcy velocity of the groundwater flow

k_l, k_w = hydraulic conductivity for LNAPL and water respectively

z_l,, z_{wl} = LNAPL table and LNAPL/water interface elevation

H_{GW}= Thickness (piezometer head) of the ambient groundwater

h_{lo}, h_{lu} = LNAPL thickness over/below of the ambient groundwater table

h_l = entire thickness of the LNAPL

q_l = specific LNAPL leak

It can be seen, that the obtained governing equation (1) of convective-dispersive spreading of LNAPL -lens on the ambient groundwater table is in term of LNAPL lens thickness h_l (x,y,t). a *nonlinear partially differential equation* (NL-PDGL) second order.

For the proposed reliability analyzes it is enough to consider the simplified case of a homogeneous aquifer (i.e., k_l and k_w are constant) and a constant volume of the mowing LNAPL – lens (i.e., the spreading of an initial existing LNAPL lens). In this case the basic equation (1) can be written in the following form:

$$\frac{\partial h_l}{\partial t} + \vec{u}\nabla(h_l) - \frac{k_l}{n_l}\nabla.(h_l \nabla h_l) = 0 \qquad (2)$$

The first term in (2) describes the change over time of LNAPL thickness.

The second term modelled the convective transport of LNAPL lens on the groundwater table having a towing speed generated of groundwater flow:

$$\vec{u} = \vec{q}_w \frac{k_l}{k_w n_l} \qquad (3)$$

The last term describes the dispersive spreading of the LNAPL lens and is the *non-linear term of the governing equation.*

If q_w=0 equation (2) become:

$$\frac{\partial h_l}{\partial t} - \frac{k_l}{n_l}\nabla.(h_l \nabla h_l) = 0 \qquad (2')$$

This equation describes the LNAPL-lens spreading on the groundwater reservoir (i.e., the convective effect be dropped).

The solution of LNAPL lens convective-dispersive spreading on the groundwater table requires the knowledge of groundwater velocity q_w. Therefore, the groundwater flow problem must be solved beforehand: determination of the free groundwater water table i.e. the piezometric head function H_w(x.y.t). This means that the first step for modelling of NAPL lens convective-dispersive spreading is the solution of an initial and boundary value problem for the governing equation of the groundwater flow. The governing equation which describe the unsteady groundwater flow in unconfined aquifer in term of the entire groundwater depth H_w *(x,y,t)* is the well-known Boussinesq's [2], [6],[7]:

$$\frac{\partial H_w}{\partial t} - \frac{k_w}{n_w}\nabla.(H_w \nabla H_w) = 0 \qquad (4)$$

This will be solved considering additionally the given initial and boundary conditions corresponding to the considered ambient groundwater flow domain.

Summarizing, the simulation of an LNAPL convective-dispersive spreading on the groundwater table requires the coupled solution of basic equations (2) and (4), both nonlinear partially differential equations. In the case of dispersive spreading must be resolved the equation (2') only which is nonlinear as well.

Given the difficulties that arise in solving nonlinear partial differential equation (NL-PDE), it is important to discuss the possibilities of finding simplifications of these equations such as linearization. Related to this a first observation would be, that in both equations (NL-PDE) (2) for LNAPL lens spreading and (4) for groundwater flow the nonlinear term is of same type. On this basis, it would be possible to apply the same simplifications such linearization for example. This would be an advantage for modelling equation of LNAPL lens spreading, less studied, through transposing the solving methods of groundwater flow modelling that is widely studied and verified on numerous practical problems [2.]

To examine this possibility, we will further discuss equation (4) of unsteady groundwater flow modelling. For this purpose, in Figure 3 a representative vertical cross section of groundwater flow is depicted.

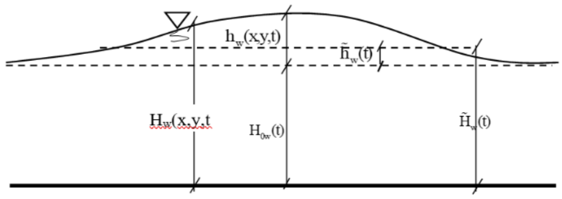

Figure 3. Sketch of vertical cross section of an unsteady groundwater flow in an unconfined aquifer

- $H_{0w}(t)$ is a basic height of the groundwater in flow domain Ω
- $h_w(x,y,t)$ is the deviating height of the ground water table in relation of $H_{0w}(t)$
- $\tilde{H}_w(t)$ and $\tilde{h}_w(t)$ are averaged heights whose meaning will be specified below

For numerous common technical tasks usually is satisfied the following condition:

$$h_w(x,y,t) << H_{0w}(t) \tag{5}$$

Between the highest in Fig. 3 take also place, the following relationships:

(6)

$$\tilde{h}_w(t) = \frac{1}{\Omega}\iint_{\Omega} h_w(x,y,t)d\Omega \tag{7}$$

The basic equation for modelling unsteady groundwater flow is the equation (4). Due to nonlinearity of this equation, there are relatively few exact analytical solutions, and the application of numerical methods is also leading to difficulties as well.

To obtain solutions for a wide range of applications a very effective approach is his linearization. The most widely used linearization technique is the replace of the water depth $H_w(x,y,t)$ in the second term of equation (4) through one averaged value in relation to the horizontal flow domain surface Ω defined as [2], [3], [6]:

$$\tilde{H}_w(t) = \frac{1}{\Omega}\iint_{\Omega} H_w(x,y,t)d\Omega = \left(\frac{V_{olw}}{\Omega}\right) \tag{8}$$

It should be noted that this average technic denoted as **Av1,** has the significance of an average height of groundwater $\frac{\partial H_w}{\partial t} - \frac{k_w\tilde{H}_w}{n_w}\nabla.\nabla H_w = 0$ on flow domain Ω calculated so that the volume of $\Omega \cdot \tilde{H}_w(t)$ be equal to the real volume V_{volw} of groundwater limited by Ω and the free surface of groundwater. Replacing the relationships (6), (7) in (8) results:

$$\tilde{H}_w(t) = H_{0w}(t) + \frac{1}{\Omega}\iint_{\Omega} h_w(x,y,t)d\Omega \tag{9}$$

Comparing (7) and (9) results averaged height

$$\tilde{H}_w(t) \tag{10}$$

This average technic for the heights $\tilde{H}_w(t)$ and $\tilde{h}_w(t)$ will further to be named as average of 1st order (**Av 1**.).

Replacing the first height $H_w(x,y,t)$ of the second term of equation (4) with the averaged height, we obtain the following usually linearized version of the governing equation for modelling unconfined groundwater flow [2], [7]:

$$\begin{aligned} H_w(x,y,t) &= H_{0w}(t) + h_w(x,y,t) \\ \tilde{H}_w(t) &= H_{0w}(t) + \tilde{h}_w(t) \end{aligned} \tag{11}$$

This *linearized form of the governing equation* is currently applied for groundwater flow modelling using different analytically and numerical methods and standard software as well obtaining reliable results for many practical applications in groundwater management [2],[6], [7].

It is however to be noted that this simplified form of the governing equations allows a reliable simulation of groundwater flow problems only when the groundwater table has relatively small deviation in relation to a flat surface (i.e., the condition (5) is satisfied). This flow condition is currently satisfied for several practical groundwater flows and so, the linearized (L-PDEQ) (9) can be applied to solve most technical problems of groundwater management using also standard software such as MODFLOW, PMWIN as well [10].

For modelling LNAPL -lens spreading on free surface of a groundwater reservoir on observe that equation (2') has the same expression as the basic equation (4) of groundwater flow modelling. Therefore, the first idea would be to use the same linearization method for LNAPL as in the case of ground water flow modelling discussed above. In this case the averaged thickness can be calculated also using the relation (10) in which the index "*w"* will be replaced with *"l"*.

$$\tilde{h}_l(t) = \frac{1}{\Omega}\iint_{\Omega} h_l(x,y,t)d\Omega \tag{12}$$

So, the linearized governing equation of LNAPL lens spreading on the free groundwater reservoir surface has the expression as:

$$\frac{\partial h_l}{\partial t} - \frac{k_l\tilde{h}_l}{n_l}\nabla.\nabla h_l = 0 \tag{13}$$

It is also to mention that in (13)

$$\frac{k_l\tilde{h}_l}{n_l} = \tilde{D}(t) \tag{14}$$

has the meaning of a dispersion coefficient.

Compared to the groundwater flow discussed above in this case $H_{0l}(t) = 0$ and so, the condition (5) is not satisfied. Consequently, an important question can be put namely if this linearized equation using averaging 1st order (i.e., Av 1) is reliable or not for simulation of LNAPL lens spreading on the groundwater table.

To analyze more correctly and completely the answer to this question, another variant of averaging of the LNAPL lens height is proposed. This was presented in a previous paper [6] and gave better results as Av1. The proposed new averaging technique is called average second order and notate Av2 is defined by the expression:

$$\begin{aligned} &\tilde{h}_l(t) = \frac{1}{V_{ol(l)}}\iint_{\Omega} h_l(x,y,t)dV_l \\ &where \\ &dV_l = h_l(x,y,t)d\Omega \end{aligned} \tag{15}$$

It should be mentioned that this average *technic Av2 is related to the volume weight centre of* LNAPL lens.

To check the reliability of the two variants, an example of LNAPL lens spreading will be considering for which there are an exact analytical solution. It will be performed comparative calculus using several numerical methods [11], [12]. The obtained results and answers to the question regarding the reliability of the linearized governing equation will be presented in the next paragraph.

3. RESULTS AND DISCUSSIONS

To check the reliability of both average technics Av1 and Av2 defined above a practical example was considered, namely the spreading of an existing radial symmetrical LNAPL lens which at the time t=0 has o form depicted in Figure 4.

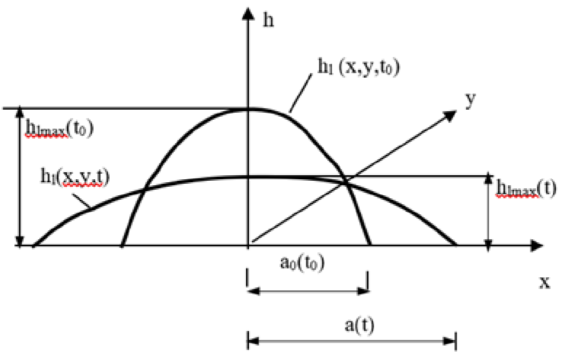

Figure 4. Calculus scheme of the LNAPL lens

The values of the geometrical and material parameters of the considered example depicted in Figure 3 are: h_{l0max}=0.30m; $a_0(t_0)$ =5.00m; n_l=0.25; k_l=4m/day; V_{l0}=11,7 m^3

One assumes also that the LNAPL lens volume remains constant during the spreading equal to initial volume (V_{lo}).

For the considered radial symmetric lens spreading (Fig. 4) there are an exact analytical solution [2], [6] expressed as:

$$h_l(x,y,t) = h_o \cdot \left[\frac{\left(1+\frac{8\cdot k_l \cdot h_o \cdot t}{n_l \cdot a_o^2}\right)^{0,5} - \frac{r^2}{a_0^2}}{\left(1+\frac{8\cdot k_l \cdot h_o \cdot t}{n_l \cdot a_o^2}\right)} \right] \qquad (16)$$

$$r = \sqrt{x^2 + y^2}$$

To simplify the notations, h_l is still used without the index's "*l" (i.e, h).*

The horizontal expansion at the basis of the lens can be calculated using the expression:

$$a(t) = a_o \left(1 + \frac{8\cdot k_f \cdot h_o \cdot t}{n_e \cdot a_o^2}\right)^{\frac{1}{4}} \qquad (17)$$

For the numerical solutions of the linearized equation (13) were used the explicit finite difference method upwind (EAS-UPW) and the MacCormack predictor-corrector method (MCV) [11], [12]. To calculate the average thickness the simple average technique Av1 (12) was used. For the numerical calculation of the averaged thickness a break condition was introduced ς at each time step namely (V_{lo}-V_{lt})/V_{lo}[10^{-4}. The obtained results for the maximum thickness using the exact solution (16) (EAS) and the above-mentioned numerical methods based on the averaging **Av1** (UPW and MCV) for discretization steps Δx=Δy=1.0 m, Δt= 0.1 day are presented in Table 1.

It is noticed that the errors of the numerical solutions (NS-A1: UPW and MCV) compared to the exact solution (EAS) are relatively large, about 30-80%.

For the same numerical data in the Table 2 the results obtained with average technique **Av2** formula (15) are presented.

It is noticed that the errors of the numerical solutions (NS-A2: UPW and MCV) compared to the exact solution (EAS) are relatively small under 3%.

Table 1. Comparative results and errors

Time [Day]	h_{max} EAS [m]	Num. Method	h_{max} (Av 1.) [m] (SC:10^{-4})	Error (Δh/h) [%]
1	0,187	UPW	0,241	-29,0
5	0,101		0,167	-65,5
10	0,073		0,129	-76,3
1	0,187	MCV	0,248	-32,7
5	0,101		0,172	-70,8
10	0,073		0,133	-80,8

EAS, UPW and MCV (**Av 1**. Ordner)
Discretization: Δx=Δy = 1 m, Δt = 0,1 day

Table 2. Comparative result and errors

Time [Day]	h_{max} EAS [m]	Num. Method	h_{max} (Av 2.) [m]	Error (Δh/h) [%]
1	0,187	UPW	0,197	-5,1
5	0,101		0,104	-2,6
10	0,073		0,075	-1,9
20	0,053		0,053	-1,5
1	0,187	MCV	0,199	-6,2
5	0,101		0,104	-3,5
10	0,073		0,075	-2,4
20	0,053		0,054	-1,7

EAS, UPW and MCV (Av 2. Ord.)
Discretization: Δx=Δy = 1 m, Δt = 0,1 day

The numerical calculus-results are presented in Figure 5, for a radial symmetrical LNAPL lens spreading using numerical methods UPW and MCV and the averaging techniques Av1(NS-A1) and Av2 (NS-A2), compared to those calculated with the exact analytical solution.

It can be clearly seen that the results obtained with the averaging techniques Av1 and Av2 respectively are significant different and the Av2 averaging method leads to results that are very close to the exact analytical solution.

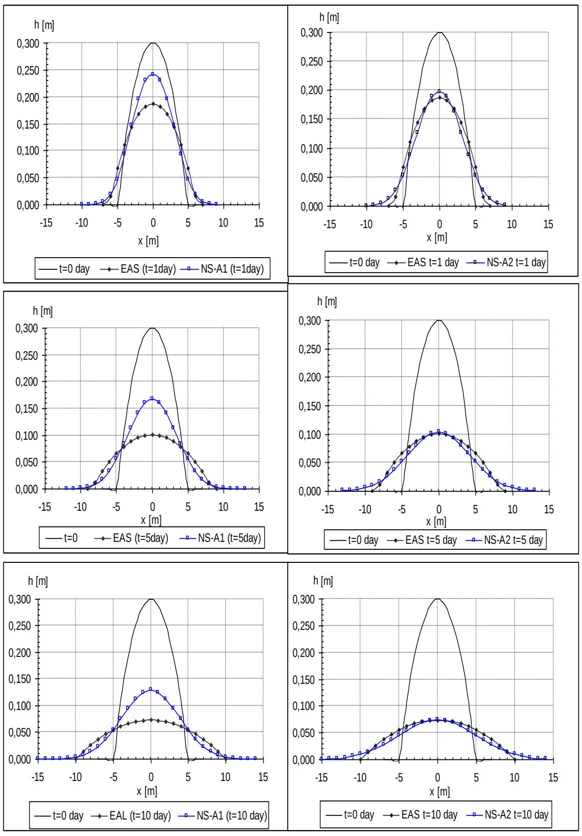

Figure 5. Results for the spreading of a radial symmetrical LNAPL lens using the averaging techniques
a) Averaging 1. Order (Av 1.) and
b) Averaging 2. Order (Av 2.)

Another example of a numerical simulation of a convective-dispersive LNAMPL lens spreading on the table of moving groundwater is sketched in Figure 6. The flow domain contains three subdomains having different hydraulic conductivities (zone 1, 2 and 3).

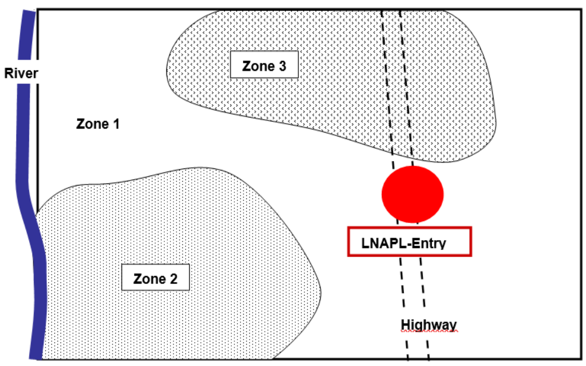

Figure 6. Sketch of the groundwater flow domain for the numerical simulation of LNAPL lens on the groundwater table

Parameters of the considered groundwater flow domain to perform the given LNAPL lens spread on the moving groundwater table:

LNAPL volume 13 m³

Dimensions of the model area
x direction 150 m; y-direction 100 m

Discretization:
Δx= 2 m, Δy= 2 m, Δt= 0.1 days
Boundary conditions:
Groundwater levels in the river 5 m and
on the right side of the flow domain 10 m

Hydraulic conductivities:
Zone 1 10 m / day 1.2 * 10-4 m / s
Zone 2 8 m / day 9.3 * 10-5 m / s
Zone 3 6 m / day 6.9 * 10-5 m / s

Such examples are very important because protective or remedial measures can only be used sensibly if the extent of the LNAPL spread is known or the position of the LNAPL lens is fully recorded.

The first step to solve this problem is groundwater flow modelling which delivers the groundwater velocity which further are necessary to model the convective-dispersive spread of LNAPL lens (see equations 2 and 3). Groundwater modelling was performed using PMWIN [13]. The results of the groundwater flow simulation can be shown in Figure 7.

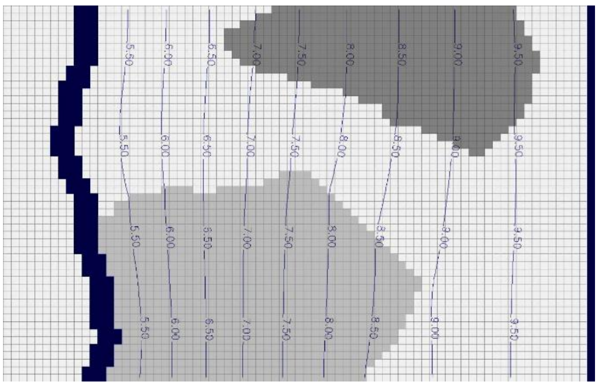

Figure 7. Results of the groundwater flow simulation

The LNAPL lens spread was performed using the Lax-Wendroff (LMV) numerical method which differs from the ERV used in previously examples only in the convective term of the difference equation. In the LWV, a central difference scheme is used for the convective term which delivers stable results. The groundwater flow speed was taken over by groundwater flow modeling presented above.

The results are presented in Figure 8 and show the LNAPL lens spreading on the groundwater table using the two averaging techniques:

a) Averaging 1. Order (Av 1.) and
b) Averaging 2. Order (Av 2.)

It can be clearly seen in this case also, that the results obtained with the averaging techniques Av1 and Av2 respectively are significant different, both in terms of lens thickness values and the extension through dispersion of the polluted area.

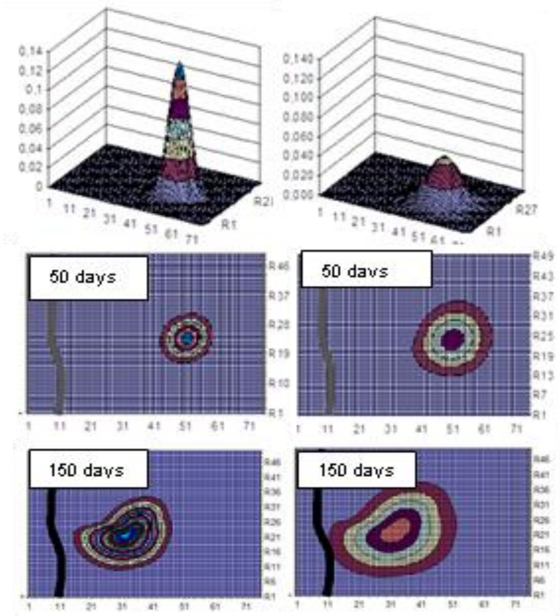

Figure 8. Results of the convective-dispersive LNAPL lens spreading

4. CONCLUSIONS

Based on results presented in the article, it can be concluded that the use of the classical average technique **Av1** (formula (10)) to linearize the Businesq's equation for modelling of LNAPL lens spread leads to relatively large errors of LNAPL lens thickness profiles (errors of *30-80 %*, Table 1.). Unlike this, the use of the proposed average technique **Av2 (**formula (15)) leads to small errors (3-4% for t >1 day, Table 2).

The comparative presentation of the results in Figure 8 regarding the convective-dispersive spread of the LNAPL lens on the moving groundwater table also confirms the reliability of proposed averaging method Av2 in comparison to the classical method Av1 (see comparative LNAPL lens expansion in Figure 8).

It can be concluded, therefore, that the average Av2 technique proposed is indisputably better than the classic one and it is recommended to use for LNAPL lens spreading simulation.

We consider also that the Av2 method can be extended successfully to the unsteady groundwater flow modeling, substituting successfully the classical averaging technique Av1 usually applied in groundwater modelling.

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