SPE 35851

Validation of a General 3-D Numerical Model for Simulating Organic Pollutants Migration and Application to Site Remediation

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Abstract

This paper presents a general numerical model able to simulate both organic pollutants migration (3-phase compositional flows, mass transfer, transport) in soils and aquifers and decontamination techniques such as pumping, skimming, venting, hot venting, steam injection, surfactant injection and biodegradation.

To validate the simulator, a 3-D experiment in a large pilot (25 m x 12 m x 4 m) was carried out. A total of 0.475 m^3 of diesel oil was injected into the pilot, and numerous in-situ measurements were performed to determine pollutants location and concentrations within the vadose and saturated zones. Prior to the pilot test, a predictive simulation computed the extent of the contaminated zone and the oil saturations. Numerical results showed good agreement between experiment and simulation.

To demonstrate the simulator abilities to improve remediation operations, a soil vapor extraction (venting) of weathered gasoline in the vadose zone under a service station was simulated. Fourteen wells were drilled on the site and extraction took nine months. The simulation closely matches the field data. Further simulations show the possibility of venting optimization for this site.

Introduction

Groundwater contamination by organic compounds such as hydrocarbons or chlorinated solvents has become a major environmental concern. To help in understanding of the complex phenomena associated with the migration of non-aqueous-phase liquids (NAPL) and the design of remediation operations, specific numerical tools have been introduced.

Understanding the evolution of NAPL in the subsurface requires knowledge of the migration of the contaminants (advection and dispersion) in both the vadose and saturated zone, transfer of components from NAPL to water and gas phases. Prediction of long-term evolution of the contamination may also require knowledge of interactions between organic pollutants and the porous matrix and biodegradation of both dissolved pollutants and residual NAPL trapped in the pores. Good comprehension of the above mechanisms will allow numerical simulators to be efficient tools for risk assessment purposes.

Remediation processes aimed at removing NAPL from the subsurface. Different technologies are available or under development:

- direct mobilization of NAPL, e.g. pumping, surfactant injection;
- partitioning of contaminants from either the aqueous phase or oil phase into the gas phase, e.g. in situ stripping, vacuum extraction (venting), steam injection;
- biodegradation of dissolved pollutants and of residual NAPL.

While these various methods of remediation have been studied on the laboratory scale and have been used in field conditions, the design of an operation is often based on empirical guidelines or previous experience. Use of a comprehensive numerical tool may significantly increase our capability of optimizing such remediation operations.

Numerous numerical models have been applied to oil-spill problems and decontamination processes as reviewed by Pinder and Abriola[1] (1986), Corapcioglu and Panday[2] (1991) and Panday et al.[3] (1995). Compositional models developed to examine groundwater contamination scenarios include those by Abriola and Pinder[4], Corapcioglu and Panday[2], Forsyth and Shao[5,] Sleep and Sykes[6], Falta et al.[7], Le Thiez and Ducreux[8], and Unger et al.[9]

The goal of this work is to present two simulations cases performed with the SIMUSCOPP numerical model[8] and the comparison between computed results and field observations.

The first case consists of the migration of 0.475 m^3 of diesel oil into a large pilot (25 m x 12 m x 4 m) filled with clean sand. Numerous in-situ measurements were performed to determine pollutant location and concentrations within the vadose and saturated zones. The second case consists of a gasoline station contaminated by 15 m^3 of weathered gasoline. A soil vapor extraction (venting) was performed during nine months by fourteen air extraction wells. Simulation of this case is presented and further simulations show the possibility of venting optimization for the site.

Model description

The SIMUSCOPP model is a general 3-D simulator, dedicated to pollution / decontamination problems derived from reservoir engineering models SARIP[10] (thermal applications) and ATHOS. ATHOS is an extremely flexible, state-of-the-art reservoir simulator, capable of handling a wide variety of fluid compositional models, reservoir geometry and PVT conditions. This latter simulator was used as the software basis for developing the SIMUSCOPP model. SIMUSCOPP can solve problems of 1, 2 or 3-phase flow, compositional or not, from the laboratory scale to the site scale. Concerning decontamination, SIMUSCOPP is able to simulate most of the processes described above, including biodegradation, steam injection and surfactant injection. Its code is portable between most common computers: PC, Unix workstations and also vector computers. Geometry can be described by cartesian coordinates or radial coordinates, with possible local mesh refinement.

Governing equations. The mathematical description of compositional multiphase flow in porous media is based on equations of mass conservation for each component and of momentum conservation for each phase. Any number of components can be accounted for, depending on the processes to be simulated. These components represent organic pollutants (partitioned between oil, water, air phases and adsorbed), water (in water and gas phases), air (may be dissolved in water phase for biodegradation problems), surfactant (water and oil phases, and adsorbed), tracers (in water phase only). The general mass conservation equation for a component i existing in the three fluid phases (p) and adsorbed on the rock (r) is:

$$\frac{\partial}{\partial t}\left[\phi\left(\sum_{p=1}^{N_p}\rho_p \cdot S_p \cdot x_i^p\right)+\left(1-\phi\right)\cdot\rho_r\cdot q_i^r\right]$$
$$+\mathrm{div}\left(\sum_{p=1}^{N_p}\rho_p \cdot x_i^p \cdot \alpha_i^p \cdot \vec{u}_p + \vec{J}_i^p\right)+R_i+Q_i=0 \qquad (1)$$

As written above, the equation of conservation assumes local thermodynamical equilibrium (local = within a grid-element). Compositions of various phases are then linked

through K-values. Judging from the abundant literature concerning mass partitioning of hydrocarbon between the oil phase and the water phase, it seems obvious that hydrocarbon concentrations in water are not properly described by dissolution equilibrium for both laboratory experiments and field cases. On the contrary, oil reservoir engineering applications generally consider local equilibrium to calculate compositions in the different phases. A good review of nonequilibrium dissolution can be found in an article by Powers et al.[11] Consequently, dissolution kinetics has to be introduced in the mathematical formulation. To avoid the increase of equations to be solved simultaneously by using such transfer kinetics, SIMUSCOPP uses flux modifiers in the transport equation, as described before. These "α-factors" (α_i^p in Eq. 1) were initially proposed by Baker and Fayers[12] to simulate heterogeneity effects associated with coarse grids in reservoir simulations. For nonequilibrium dissolution of hydrocarbons in water, "α-factors" in water (α_i^w) have to be defined. For values lower than unity the flux of a dissolved hydrocarbon will be lower than the average water flux. Consequently, its apparent dissolution rate will be lower than the equilibrium dissolution rate, leading to a slower elimination of soluble compounds from residual oil. This empirical formulation was tested in SIMUSCOPP and calibrated by laboratory experiment of gasoline and diesel-oil dissolution in water (Le Thiez et al.[8]). These flux modifiers can also be used for nonequilibrium volatilization of hydrocarbons during a venting operation. "α-factors" for components in the gas phase can be defined (α_i^g) for limiting transfer from the residual oil to the gas phase.

For thermal applications (e.g. migration of hot pollutants, hot venting, steam injection), an equation must be written for energy conservation:

$$\frac{\partial}{\partial t}\left[\phi\left(\sum_{p=1}^{N_p}\rho_p \cdot S_p \cdot U_p\right)+\left(1-\phi\right)\cdot\rho_r\cdot U_r\right]$$
$$+\mathrm{div}\left(\lambda^* \cdot \overline{\mathrm{grad}}\,T + \sum_{p=1}^{N_p}\rho_p \cdot H_p \cdot \vec{u}_p\right)+\sum_{p=1}^{Np}H_p \cdot Q_p=0 \qquad (2)$$

The momentum equation for each fluid phase is reduced to Darcy's generalized law.

Constitutive equations. To close the system of equations, constitutive equations must be written for:
- phase densities and viscosities and equilibrium constants as functions of pressure, temperature and compositions (use of analytical expressions or equation of state),
- relative permeabilities and capillary pressures,

- molecular diffusion and hydrodynamic dispersion,
- sorption isotherm,
- biodegradation reaction rates.

Hydrodynamic dispersion and biodegradation kinetics, not used in the present paper, will not be described. On the contrary, three-phase relative permeabilities and capillary pressures play key roles in the simulation of diesel-oil migration in unsaturated and saturated zones, as described hereunder.

Relative permeabilities and capillary pressures. In our simulator, relative permeabilities are input via two two-phase tables (water-oil and air-oil) obtained from laboratory experiments or computed with Parker et al.[13] analytical equations. Oil relative permeabilities in three-phase flow are then obtained with either Stone's first method modified by Fayers[14] or Stone's second method[15]. In petroleum applications it is assumed that no water-gas exists in the oil-zone, i.e. only two capillary curves are needed to describe three-phase flow: water-oil curve and oil-gas curve. For a pollution case, a continuous oil phase everywhere in the porous medium cannot be assumed. The following equations given by Forsyth[16] have proven to be effective for simulating NAPL migration as described in a previous paper[8]:

$$P_g = P_o + \beta \cdot P_{cgo} + \left(1 - \beta\right) \cdot \left(P_{cgw} - P_{cow}^{min}\right) \qquad (3)$$

$$P_o = P_w + \beta \cdot P_{cow} + \left(1 - \beta\right) \cdot P_{cow}^{min} \qquad (4)$$

$$\beta = \min\left(1, \frac{S_o}{S_o^*}\right) \qquad (5)$$

S_o^* represents the "critical oil saturation". When the oil phase is absent from the system (uncontaminated zones), water and air pressures are linked via the water-air capillary pressure. For oil saturations above critical saturation, the oil phase is assumed to be continuous and no more water-air contact exists in this case. Pressures in the three phases are then expressed via the conventional approach using water-oil and air-oil capillary pressures. The β–parameter used in Eqs. 3 and 4 performs a smooth interpolation between the pure two-phase water-air system and the three-phase one in which the oil phase is present.

Phase equilibrium. Component molar fractions in oil, gas and water phases are computed via equilibrium constants as functions of pressure and temperature. Oil-gas equilibrium may also be computed directly by the Peng-Robinson equation of state. For three-phase equilibrium, K-values may be generated by an equation of state proposed by Soreide and Whiston[17], derived from the Peng-Robinson equation and able to compute equilibrium between oil, gas and water phases. This equation is also able to take into account the salinity effect on hydrocarbon dissolution in water. The adsorption of organic pollutants dissolved in the water phase is described by a simple linear isotherm or by a Langmuir isotherm.

Boundary and initial conditions. Two kinds of boundary conditions are implemented in SIMUSCOPP:
- wells: injecting and pumping wells as in reservoir engineering applications; radial flow is assumed;
- boundaries: simulating aquifer influx and outflux, recharges, rain, NAPL spill, link with the atmosphere, etc.; linear flow is assumed.

The bound working conditions are the imposed flow rate or the imposed pressure. For this latter condition, fluids may enter or exit, depending on the pressure difference between the bound and the concerned grid-block centers. As the considered domain is not necessarily confined like in an oil reservoir, bounds may consider a continuity, including capillary pressures, between the model and the outer medium.

The initial state is computed automatically by knowing location of the water table, its slope and the water-air capillary pressure curve.

Space and time discretization. The system of equations is discretized using a finite-volume method for both regular grids or locally refined grids. Time discretization uses a fully implicit scheme or an IMPES scheme. Nonlinearities are linearized by Newton's method. Linear systems are solved by direct methods or by a conjugate gradient with various preconditioning techniques.

Diesel-oil migration in a large-scale basin

Pilot description. The simulation results discussed here were performed by simulating 3-D diesel oil infiltration on a pilot scale. This pilot (SCERES basin), located at the CNRS-Campus of Strasbourg (France), is a large impervious concrete basin (25 m long x 12 m wide x 4 m deep) packed with quartz sand. The porosity of the sand is 40%, and its hydraulic conductivity is 8.10^{-4} m/s (intrinsic permeability = 80 darcy). This pilot was build for testing some decontamination processes such as surfactant-aided recovery and in-situ bioremediation[18,19]. Figure 1 gives a schematic representation of the SCERES facility. During the summer of 1994, the basin was contaminated by 475 liters of diesel oil through a limited area of 1.8 m², 3 m above the water table. After a few months of stabilization, core-drill investigations were performed in order to determine the shape and extent of the residual contaminated zone and pollutant concentrations (i.e. oil-phase saturations) in the various parts of this contaminated zone. The diameter of the oil-impregnation body in the unsaturated zone was about 1.85 m. The horizontal extent of the oil phase in the capillary fringe was in the range of 5.60 m to 5.90 m, with a mean thickness of 10 to 15 cm. Residual oil saturations were close to 5% of pore volume in the unsaturated zone and in the range of 21 to 24% in the capillary fringe[20].

In a second stage, an elevation of 0.5 m of the water table was performed in order to vertically displace the oil phase initially trapped in the capillary fringe. New measurements gave a value of 10% for the residual oil saturation in the saturated zone after the rise of the water table.

Pilot simulation. The purpose of this numerical modeling was to reproduce the migration of diesel oil in the SCERES basin and the shape and the final extent of the contamination. For this, we performed simulations with three-phase non-compositional flow. Only three components were taken into account: oil, water and air, without any mass transfer. The SCERES basin was discretized with 12000 grid-blocks (25 x 24 x 20). Three-phase relative permeabilities for the oil, water and air phases were obtained by laboratory experiments. The water-air capillary pressure curve was obtained by inversion of the vertical water saturation profile measured in the basin by a neutron probe before the oil spill. Water-oil and air-oil capillary pressure curves were then obtained by scaling the water-air curve according to their respective interfacial tensions. The main data used for the simulations are given in Table 1. Four boundary conditions were used for this simulation:

1. aquifer influx: pressure in the water phase was fixed at 1 atmosphere at the top of the water level, and water was injected between -3 and -4 m;
2. aquifer outflux: pressure was fixed at 1 atmosphere at -3.125 m, corresponding to the slope of the water table (0.5%),and water was produced between -3.125 and -4 m;
3. pollution infiltration: area at the top of the model ($z = 0$) where diesel oil was injected at a constant rate of 9 liters per minute (475 liters injected);
4. surface of the model: pressure in the gas phase was fixed at 1 atmosphere, allowing air to get out of the system when oil was infiltrating.

Figure 2 gives the shape of the contaminated zone and the oil saturations on a cross-section for two times: at the end of the diesel-oil injection (1 hour), and 2 months later, and an areal view at the top of the water table after 2 months. As shown in the figure, the horizontal extent of the oil lens calculated by the simulator is close to 5.50 m, which is in very good agreement with the value observed. Concerning the spreading of oil in the unsaturated zone, the calculated extent of the contamination is greater than the observed one. As shown in Fig. 2, The main cylinder of residual oil centered under the injection zone has a diameter of 2 m, which is in good agreement with the observations. Oil saturation in this zone is 5%. Around this main cylinder, the numerical model computed very low oil saturations, which have not been observed in the pilot. This is probably due to numerical dispersion in this zone or to excessive air-oil capillary forces leading to a lateral spreading of the contamination zone. Fig. 3 gives the vertical profile of oil saturations under the surface of pollution injection after 1 hour (end of injection), after 2 months and after the 0.5 m rise of the water table. As shown in Fig. 3, injected diesel-oil migrated vertically through the unsaturated zone and spread within the water-air capillary fringe. A vertical equilibrium was then reached, where the maximum of oil saturation was 28% (an average value of 24% was measured in the basin). The rise of the water table

displaced this oil lens vertically and trapped the pollutant at its residual saturation of 10%. Calculated saturation profiles before and after the rise of the water table effectively reproduce the observations of the pilot.

Soil-vapor extraction from a service station
Site description. The site described here consists of a service station located in the Paris area. A spill of gasoline occurred and polluted the unsaturated zone above the water table, located 4 m below the surface. The porous medium consisted of a sand with 10^{-4} m/s of hydraulic conductivity. Analyses performed with contaminated soil samples demonstrated that the pollutant consisted of a mixture of weathered gasoline and diesel oil. This latter product is not removable by venting because of its low volatility at low temperature. The total volume of pollutants within the soil was estimated to be close to 15 m³. Fourteen extraction wells were drilled and linked to a vacuum extraction pump able to pump 1200 m³/hour of air. These wells were grouped in 3 sectors in order to perform alternate pumping (V1 to V10, V13 to V15, and V16 - see Fig. 4). After 6 months of pumping, 9.1 m³ of gasoline was recovered. At the end of the operation (9 months), 11.3 m³ was recovered. Analyses performed after the venting operation showed that the gasoline fraction was totally removed from the polluted zone and that heavier hydrocarbons remained unextracted.

Simulation of the venting operation. For this purpose the compositional option of SIMUSCOPP was used. The pollutant was split into 3 pseudo-components: C_7-C_8, C_9-C_{10}, C_{11+}. The two first components correspond to the gasoline fraction and the last one represents the heavier fraction of hydrocarbons detected in the soil and corresponds to diesel oil. The fluid properties used for the simulations are given in Table 2. The domain was discretized into 850 grid-blocks (25 x 17 x 2). The length and width of each block were 2 m. Two layers were defined. The first at the top of the model was 2.75 m high and the second at the bottom of the model (top of the water table) was 1.25 m high. This latter layer corresponds to the contaminated zone as measured on the site. Without a precise delineation of the contaminated area, the 15 m³ of pollutants were initially equally distributed in the grid-blocks concerned. This schematic contaminated zone was located in layer 2, from blocks 1 to 25 in x-direction and 1 to 12 in y-direction. As the ground surface of the station was impervious, air was assumed to enter the model by edges. Four boundaries working at an imposed pressure of 1 atmosphere and at a temperature of 15 °C were defined. The simulation considered local equilibrium between residual oil and air. In their study concerning in-situ soil venting, Johnson et al.[21] confirmed this assumption by providing calculations showing that the distance in the porous medium to reach equilibrium was not greater than 0.2 cm for typical conditions. Concerning the air pumping rates actually applied during the operation, exploitation of the results of the pilot showed that the average air pumping rate during the 9 months

of operation was around 800 m^3/h. This is due to the alternate pumping of the 3 sectors of extraction wells. For example, with sectors 2 (3 wells) and 3 (1 well), the maximum rate should have led to pressure drops impossible to reach in this case. During the simulation, the air flow rate was adjusted to match pressure-drop measurement in the wells.

Figure 5 gives the comparison between observed and calculated cumulative oil production. For the simulated results a recovery of 9.7 m^3 was obtained after 6 months of venting, and 11.2 m^3 after 9 months.

Optimization of the basic case. New simulations were carried out in order to calculate the effect of new operating conditions by means of (1) extraction without cycles, (2) horizontal well, and (3) coupling venting with hot-air injection.

Simulation of venting without cycles. To avoid the limitation of the air pumping rate, air could be pumped at a constant rate of 1200 m^3/hour, equally distributed between the 14 wells. This new simulation showed that the average pressure drop in the wells was close to 30000 Pa, which is compatible with values observed on the site. Fig. 6 shows that recovery rates increased compared to the initial case with cycles, due mainly to the greater air volume flowing within the contaminated zone.

Simulation of venting with a horizontal well. The aim of this simulation was to check the potential of extraction with an horizontal well for venting purposes. A simulation was performed using a horizontal well located in layer 2 (within the contaminated zone) and 32 m long (from blocks 5 to 20 in x and 6 in y). Other wells were closed, and the extraction rate was kept at 1200 m^3/hour. Cumulative production described in Fig. 6 shows that oil was more rapidly removed from the site by extraction with a horizontal well than with conventional vertical wells. 11 m^3 of gasoline was recovered in 5 months, instead of 9 months with 14 vertical wells. Due to its location within the contaminated zone and its better drainage efficiency, a horizontal well could be a good technique to improve venting.

Simulation of venting coupled with hot-air injection. For this simulation, five wells of the initial scheme (V3, V5, V7, V9 and V15 in Fig. 4) were converted into hot-air injectors. Air was injected at 300°C at a constant rate of 300 m^3/hour. The 9 other wells were still pumping air at a total rate of 1200 m^3/hour, without any cycles and 900 m^3/hour of cold air at 15°C was coming from the boundaries of the model. Cumulative hydrocarbon production for this case is given in Fig. 6. Comparatively to cold-air pumping without cycles, the rate of removal was not increased by hot-air injection. As shown in Fig. 7, the temperature after 9 months remained lower than 75°C in the contaminated zone, except around the hot-air injection wells. This average temperature was not high enough to significantly increase the vaporization rate of the mixture of weathered gasoline and diesel oil. Nevertheless, high temperatures around the injectors (close to 200°C) were able to vaporize heavier fractions (diesel oil), and 1 extra m^3 of hydrocarbons was recovered.

Conclusions

A general numerical model has been developed, dedicated to the simulation of organic pollutant migration in soils and aquifers, and of most in situ remediation techniques. Numerous validation cases from the laboratory scale to the real-site scale have been studied with this simulator. A special effort was devoted to describing three-phase flow and mass transfer under non-equilibrium conditions, as described in a previous paper[8]. Among the validation cases performed, two are described here: (1) migration of diesel oil within a large-scale basin (noncompositional simulation), and (2) depollution of a gas station by venting (compositional simulation). This study shows that:

(1) good agreement between simulated results and observations for both cases given here was obtained,

(2) the SIMUSCOPP model has the capability of handling complex problems of risk assessment by means of three-phase flow (compositional or not),

(3) compositional modeling can be an effective and useful tool for designing and optimizing a conventional remediation technique, such as venting.

Nomenclature

H_p = phase p internal energy, J/mol

$\bar{J}_i^p$ = diffusion-dispersion flux of i in phase p, mol/s

P = phase pressure, Pa

Pc = two-phase capillary pressure, Pa

P_{cow}^{min} = minimum water-oil capillary pressure

q_i^r = mole fraction of i adsorbed on the rock phase

Q_i = component i injection/production source term, mol/s

R_i = component i biodegradation source term, mol/s

S_o^* = critical oil saturation

S_p = phase p saturation

t = time

T = temperature, °C

$\bar{u}_p$ = darcy velocity of phase p, m/s

U_p = phase p internal energy, J/mol

x_i^p = molar fraction of i in phase p

α_i^p = "α-factor" of i in phase p

β = interpolation parameter in three-phase capillary pressure equations

λ^* = equivalent thermal conductivity, W/m/K

ϕ = porosity

$$\rho_p \quad = \quad \text{phase } p \text{ molar density, mol/m}^3$$

Subscripts

g = gas phase
i = component
o = oil phase
p = fluid phase (g, o, w)
r = rock phase
w = water phase

Acknowledgments

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TABLE 1 - DATA FOR SCERES BASIN SIMULATIONS	
oil density	$=$ 838 kg/m^3
oil viscosity	$=$ 3.91 mPa.s
irrdeducible water saturation	$=$ 0.2
residual oil saturation (air-oil flow)	$=$ 0.05
residual oil saturation (water-oil flow)	$=$ 0.1
max. air-water capillary pressure	$=$ 5000 Pa
max. water-oil capillary pressure	$=$ 1700 Pa
max. air-oil capillary pressure	$=$ 1200 Pa

TABLE 2 - DATA FOR VENTING SIMULATIONS	
irreducible water saturation	$=$ 0.1
initial mole fraction of C_7-C_8	$=$ 0.1
initial mole fraction of C_9-C_{10}	$=$ 0.7
initial mole fraction of C_{11+}	$=$ 0.2
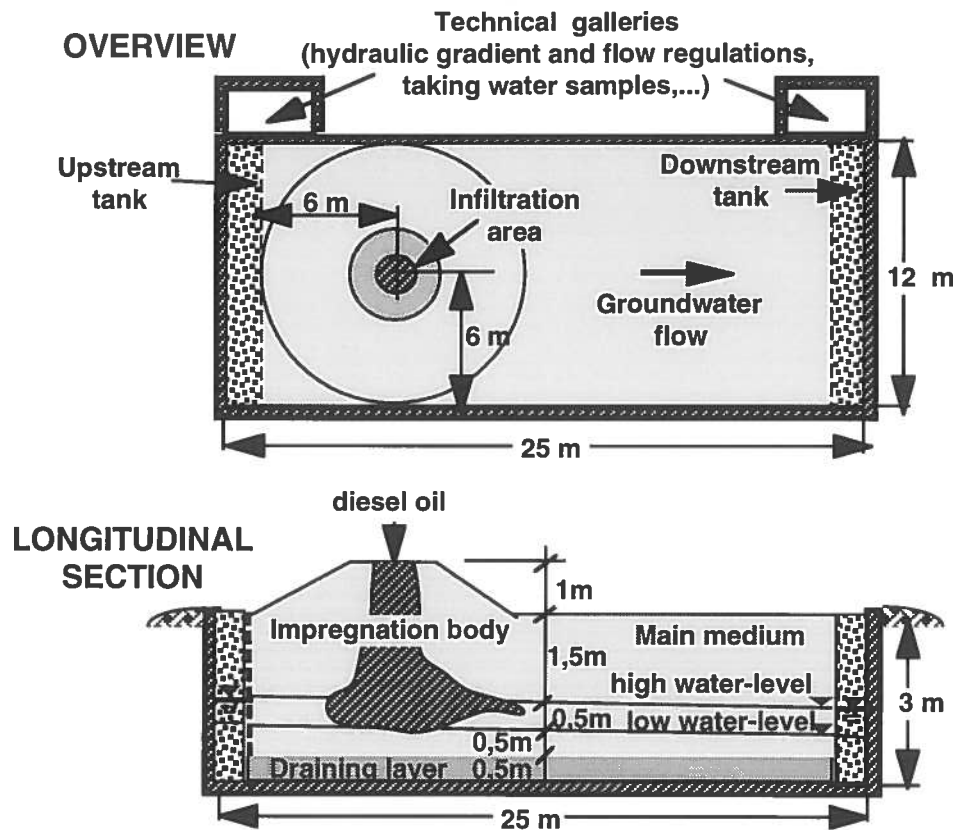
Fig.1 - Schematic representation of the SCERES facility.
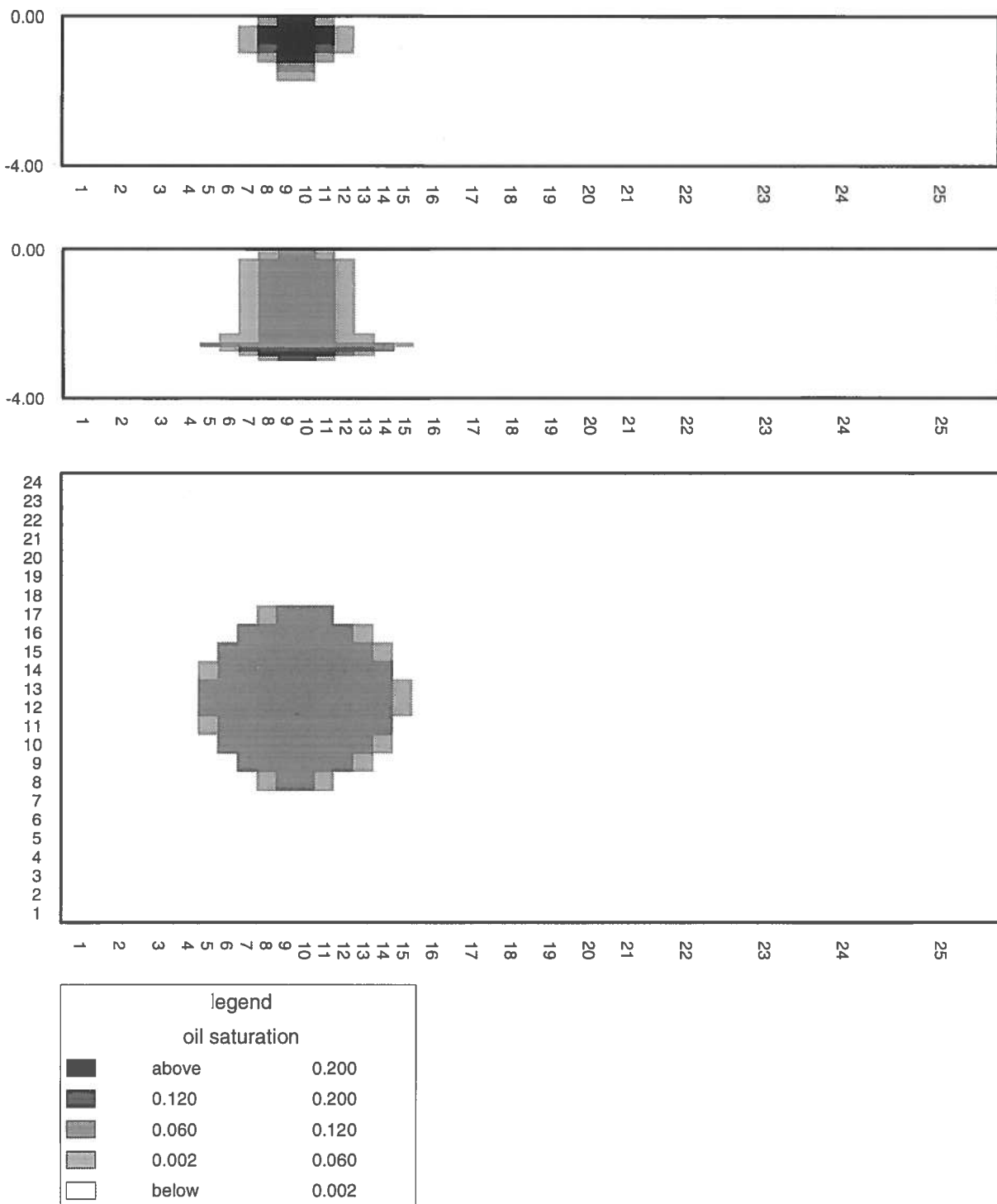
Fig. 2 - Oil saturations in the SCERES basin: (a) cross-section after 1 hour, (b) cross-section after 2 months, (c) top of the water table after 2 months.
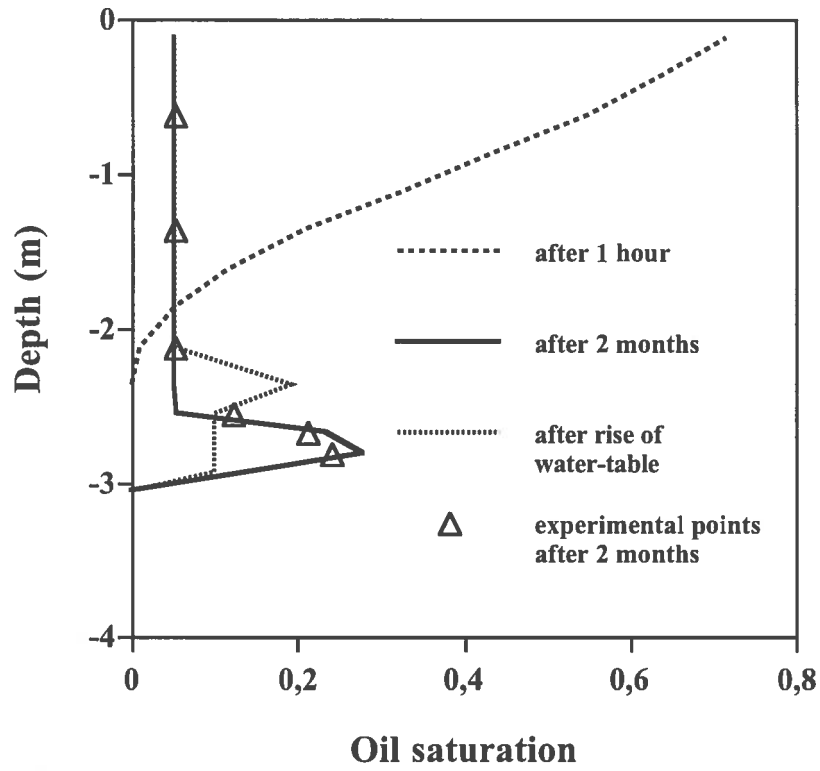
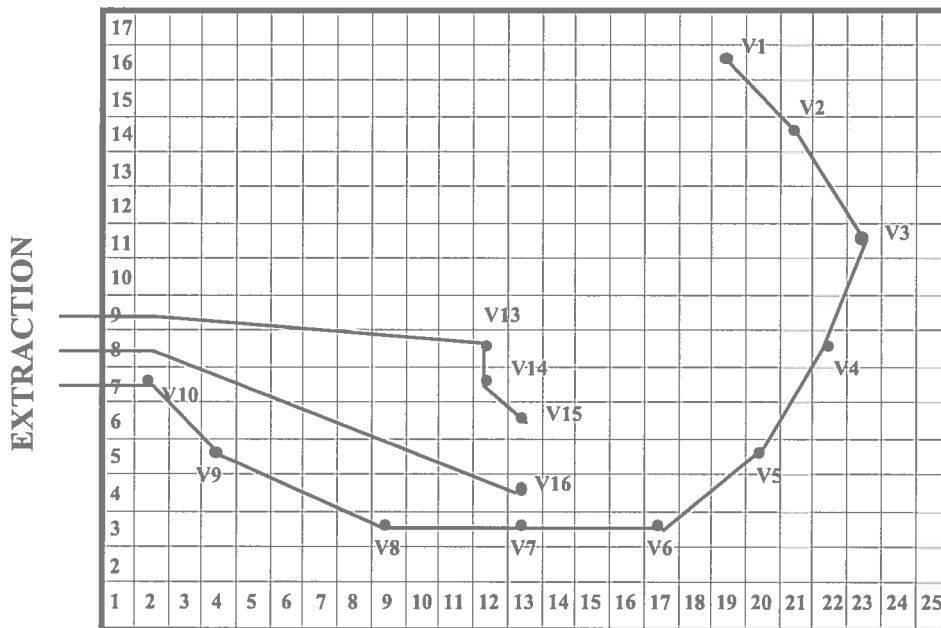Fig. 3 - Computed oil saturation profiles in the SCERES basin.

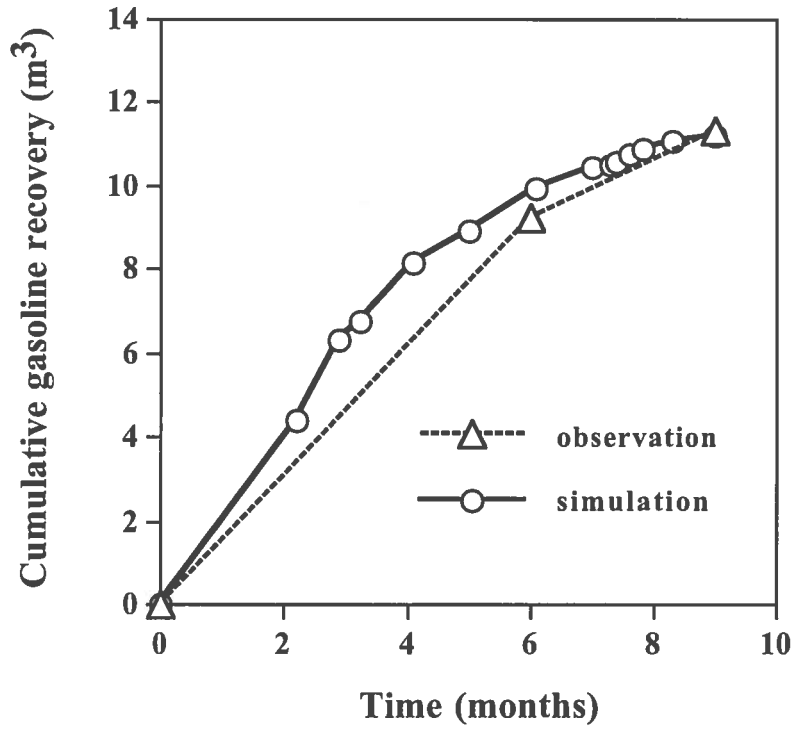Fig. 4 - Gridding and wells location for venting simulations.

Fig. 5 - Cumulative oil recoveries for the venting case - comparison between simulation and on-site observations.
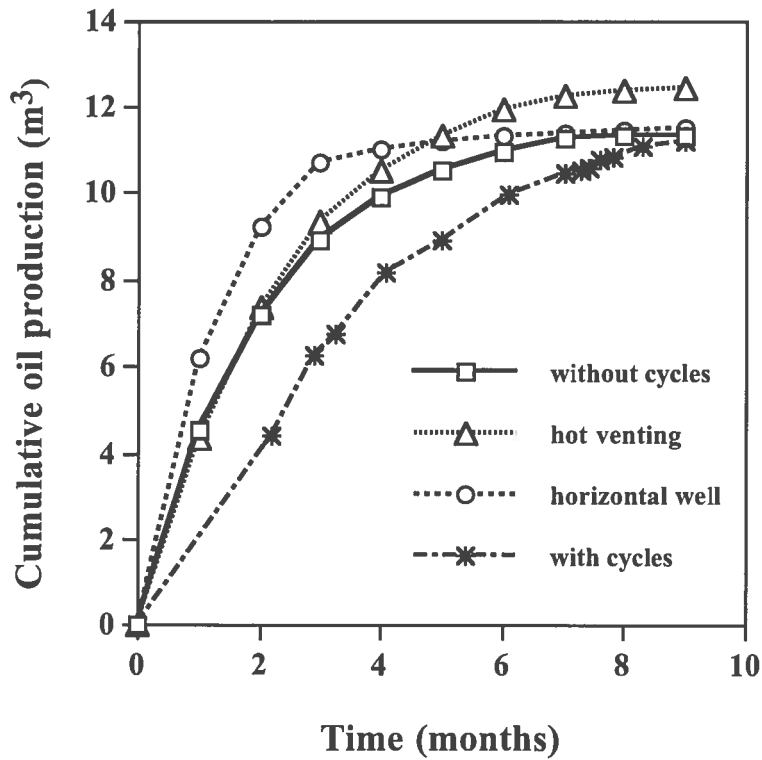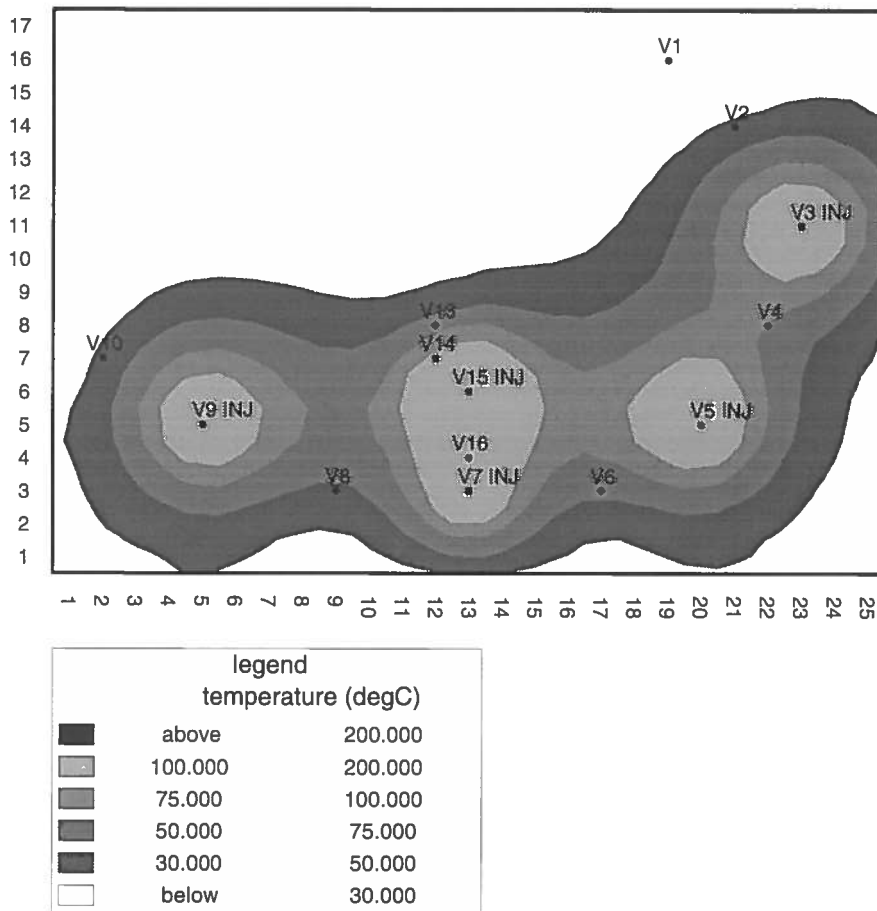

Fig. 6 - Cumulative oil recoveries for the optimization runs.

Fig. 7 - Temperature map after 9 months of hot-air injection.