SOIL REMEDIATON BY HEAT INJECTION: EXPERIMENTS AND NUMERICAL MODELLING

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Abstract. In order to understand physical processes of thermally enhanced soil vapor extraction methods in porous media the isothermal, multiphase formulation of the numerical model MUFTE will be extended by a non-isothermal, multiphase-multicomponent formulation. In order to verify the numerical model, comparison with analytical solutions for well defined problems will be carried out. To identify relevant processes and their interactions, the results of the simulation will be compared with well controlled experiments with sophisticated measurement equipment in three different scales. The aim is to compare the different numerical solution techniques namely Finite Element versus Integral Finite Difference technique as implemented in MUFTE and TOUGH2 [9] respectively.

1 Introduction

During the last years, actual and potential contamination of air, soil and groundwater with organic substances became a field of increasing environmental interest in Germany. The focus is on the huge number of abandonned landfill sites, where organic liquid components often infiltrate the unsaturated zone. Since non-aqueous phase liquids (NAPL) - for example mineral oil or chlorinated hydrocarbons - are rather immobile if the NAPL-content of the soil is less than 10 % contaminant spills with NAPL stay as long term contaminant source. They evaporate in the soil air and will be transported by diffusion processes into the atmosphere, or they dissolve into the groundwater as organic solvents. For remediation the traditional "pump and treat" methods are inefficient because mass extraction depends on the solubility, sorption and vaporisation of the contaminant which can be rate limited processes.

To work on remediation technologies, the experimental hall VEGAS (research facility for subsurface remediation) [7] was built at the Institute for Hydraulics at University of Stuttgart/Germany. The aim of the investigations in VEGAS is to optimize existing and to develop new, improved technologies for in-situ remediation and exploration techniques by means of large scale laboratory experiments. One of the ongoing studies in VEGAS concerns soil venting, which is an established technology for the remediation of organic contaminants in the vadose zone. Additional injection of heat will enhance some physical processes, which are dominant for the remediation, e.g. increasing of vapor pressure and decreasing of capillary forces.

The aim of the study is to develop a better understanding of the physical processes in respect to the optimization of existing thermally enhanced methods. Therefore the study consists of two main parts. The experimental part investigates the remediation of contaminated soils in different scales. The numerical model would provide a quantitative description of the relevant processes and mechanisms based on the results of the experiments.

2 Experimental Setup

The experimental part consists of setups in three different scales, which represent 1-, 2- and 3-dimensional modes.

The 1-d-experimental column scale setup consists of a DURAN-glass column, 90 cm high and 10 cm wide. The 2-d-setup, the so called bench scale experiment, measures 75 x 140 x 10 cm and is produced of TEMPAX-glass plates isolated with laminated wood and is fixed in a frame of stainless steel. These both laboratory setups are filled with quartz sand. The experiments will be conducted both in homogeneous and in distinct heterogeneous layers.

The laboratory offers many technical and methodical possibilities thus allowing to investigate the specific differences of hot air and steam as media carrying heat and of different contaminants. For these experiments a lot of measurement equipment is needed. The temperature and the fluid-phase saturation for two phase flow will be measured at five (for 1-d) respectively 52 (for 2-d) positions. At selected points the pressure will be recorded. The outflux of the extracted fluid phase as well as the fluxes of the injected and extracted gas will be recorded by integral measurement. The measurement of the saturation (principle: gammaabsorbtion), of temperatures (Pt-100), pressure (piezo-electrical sensor with numerical temperature-compensation) and bulk-flow (heated floating- body flow-meter with a magnetic servo system and a electropneumatical control-valve) requests an extended system of control and regulation. All signals from measuring and controling devices are recorded and evaluated with a data aquisition system via 4 interfaces with a total number of 66 channels.

In a first set experiments are conducted without contaminants, only with the components water and air. The aim is to develop a better understanding for the physical processes of flow and heat transport in this two phase system as well as to study the possibilities of process control and management. In a second set of experiments, contaminants and their material properties are included. In particular five different kinds of contaminants will be regarded: the pure compounds xylene, n-octan, dichlorobenzene and naphtalene. Kerosene, which often represents the main part of contaminations in air ports and gasoline-stations will be used as a mixture (C11-C13). The experiments focus particularly on understanding the physics of three phase flow including phase changes if steam is injected. Of special interest is the different behaviour of the five contaminants with respect to mass balance and mobility with respect to time.

The 3d-experiments will be performed in the large stainless steel VEGAS-container (h x b x l : 4.70 x 5.70 x 6.00 m). The experimental setup is shown schematicaly in Fig.1. The container is filled with well-defined homogeneous sand, later with several homogeneous layers of sand. For the remediation-experiments in the container kerosene will be used as contaminant. The media carrying heat will be injected into the porous media via six injection-wells arranged circularly around the contaminated area. From the central extraction well soil vapour is extracted so that the evaporating contaminants flow along the potential gradient towards the extraction well. In order to check the contaminant concentration in the saturated zone, groundwater will also be pumped for analysis. Temperatures will be recorded at about 200 selected positions to obtain the movement of the temperature front.

The comparison of the small-scale experiments conducted in the laboratory with the large-scale experiment in the VEGAS-container permits to understand possible scale-effects.

3 Numerical Model

A numerical model concept for simulating multiphase flow processes (MUFTE) [5] is presented. Up to now MUFTE is capable to simulate isothermal three phase flow (no partitioning of components from one phase in an other phase). Because the pressure formulation usually is unsuitable as a mathematical basis for investigating heterogeneous porous media because of negligably small capillary pressure, a pressure/saturation formulation involving the unknowns p_1, S_2, S_3, which is valid for an arbitrary capillary pressure, was chosen.

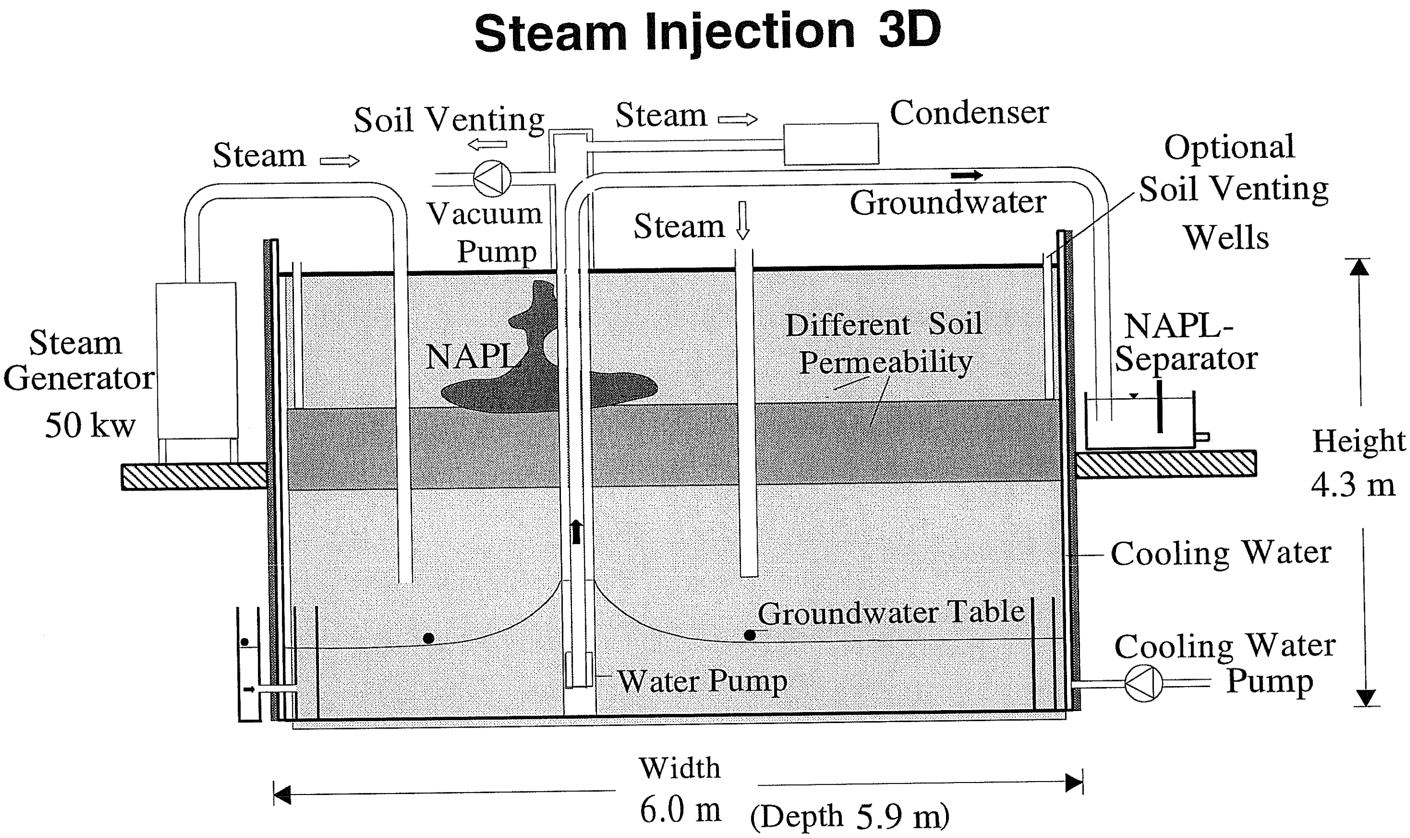

Fig. 1: Experimental setup for 3-D experiments

The system of equations presented is solved with the aid of a modified Petrov-Galerkin method. In discretizing the transient problem, it is appropriate to formulate the time discetization on the basis of an iterative concept. An implicit two-point algorithm developed for this purpose is incorporated into the Newton-type iterative concept for the consistent linearized multiphase problem. In order to describe various complicated geological structures (flow channels, fractures, rock matrix, highly heterogeneous media), it is necessary to employ arbitrary combinations of finite elements of different dimensions. Moreover, the finite elements must be capable of correctly describing the problem defined by the multiphase flow process.

Experience has shown ([10],[8]) that the following elements are especially suitable for modelling flow and transport processes in fractured porous media:

- isoparametric hexahedral elements;
  these may be applied to represent a continuum in three-dimensional models;

- plane isoparametric rectangular elements; these may be used to represent fractures in three-dimensional models and a continuum in two-dimensional models;

- line elements;
  these are suitable for representing well-defined flow channels or boreholes in three-dimensional models and for approximating fractures in two-dimensional models.

As the solutions are computed for each element in turn, the geological parameters may vary from one element to the next. The aforementioned combinations of different element types may be applied in a single model; the spatial orientation of the elements is arbitrary. By this means, it is possible to simulate complex geological structures [11].

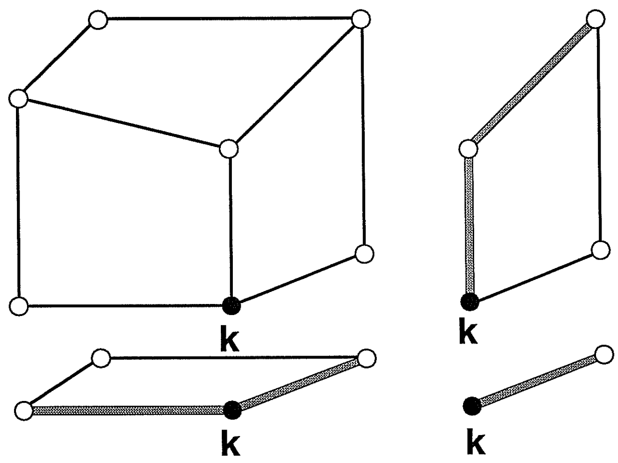

Fig. 2: Arbitrary coupling of 1-D, 2-D and 3-D elements

In order to ensure convergence of the numerical solution, a modified PETROV–GALERKIN method [4] was developed in which the test functions are up to two polynomial degrees higher than the base function (shape function). As a supplement to this, a lumped finite element formulation was also prepared. It should be noted that Hackbusch (1988) [3] was able to show that with regard to the conservation of mass for a patch, the PETROV–GALERKIN method in combination with the lumped finite difference formulation is equivalent to a finite volume formulation (e.g. TOUGH2).

Further development: Based on the isothermal part of MUFTE, the goal is to substitute the multiphase formulation by a multiphase-multicomponent formulation for the components air and water. In addition the energy equation has to be implemented to be able to simulate phase transitions from one phase to two phase and the opposite way. As primary variables, pressure, gas saturation and temperature were chosen for two phase conditions. When phase switching from two phase to one phase conditions occurs, the saturation is replaced by the air mass fraction as primary variable. The secondary variables like density, viscosity, enthalpy, internal energy and mass fractions are calculated from the primary variable set. For water and steam, all properties were calculated after International Formulation Committee [2]. For air ideal gas law was assumed. The governing equations for the conservation of mass of a component K and of energy in the gas and liquid phase $(\alpha = l, g)$ are:

For component mass:

$$
\begin{aligned}
L_{1,2}(p_g, S_g, T) :=& \\
& n \sum_{\alpha=l,g} \frac{\partial(\varrho_\alpha X_\alpha^K S_\alpha)}{\partial t} \\
& - \sum_{\alpha=l,g} \operatorname{div} \{\mathbf{K}\frac{k_{r\alpha}}{\mu_\alpha}\varrho_\alpha X_\alpha^K (\mathbf{grad}\, p_g - \varrho_\alpha\, \mathbf{g})\} \\
& - \operatorname{div} \{\mathbf{K}\frac{k_{rl}}{\mu_l}\varrho_l X_l^K \frac{dp_c}{dS_l}\mathbf{grad}\, S_g\} \\
& - \operatorname{div} \{ D_{AV}\, \varrho_g\, \mathbf{grad}\, X_g^K \} - m^K = 0
\end{aligned}
$$

For energy:

$$
\begin{aligned}
L_3(p_g, S_g, T) :=& \\
& (1-n)\,\varrho_s c_s \frac{\partial T}{\partial t} + n \sum_{\alpha=l,g} \frac{\partial(\varrho_\alpha u_\alpha S_\alpha)}{\partial t} \\
& - \sum_{\alpha=l,g} \operatorname{div} \{\mathbf{K}\frac{k_{r\alpha}}{\mu_\alpha}\varrho_\alpha h_\alpha (\mathbf{grad}\, p_g - \varrho_\alpha\, \mathbf{g})\} \\
& - \operatorname{div} \{\mathbf{K}\frac{k_{rl}}{\mu_l}\varrho_l h_l \frac{dp_c}{dS_l}\mathbf{grad}\, S_g\} \\
& - \operatorname{div} \{ D_{AV}\, \varrho_g (h_g^a - h_g^w)\, \mathbf{grad}\, X_g^a \} \\
& - \operatorname{div} \{\mathbf{K}_E\, \mathbf{grad}\, T\} - m^E = 0
\end{aligned}
$$

The Jacobian matrix for the Newton-Raphson iteration scheme is calculated using thermodynamic relationships for the pressure-, saturation-, air mass fraction- and temperature-derivatives. To avoid excessive computing time, the implementation of the robust multigrid program "ug" [1] on unstructured grids on a parallel computer is planed. By the aid of the well controlled experiments a further goal is to compare this simulator with TOUGH2 with respect to e.g. accuracy of the solution of isothermal/nonisothermal processes, numerical solution of sharp front problems, how fast convergence criteria can be achieved with FE/IFD methods and to verify and – if possible to validate – the program system by comparison with well controlled experiments, e.g. VEGAS (see fig. 2).

4 Joint Research

Presently no method is known or is likely to emerge in the near future, which could demonstrate the accuracy or validity of a numerical model in general final terms. This limitation calls for a cautious approach in model applications. Numerical modelling should be open to iterative refinement; models need to be complemented with engineering judgement, and provisions for monitoring and confirmation of system performance must be made. The test facility VEGAS [7] will provide new possibilities for extending the experimental data base for checking and validating multiphase flow and transport models (see Fig. 3).

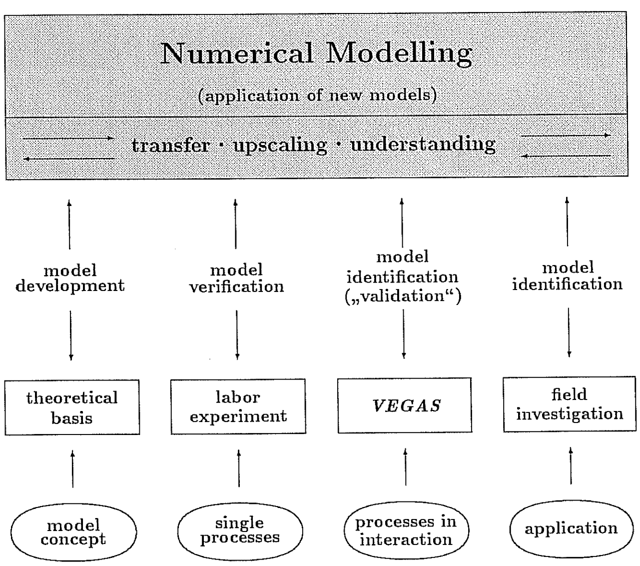

Fig. 3: Numerical modelling and upscaling [6]

The identification of processes will be achieved by the connection of physical and numerical experiments, whereby still a large amount of method- development is needed in both areas. For example from the physical point of view, this need will be covered by the introduction of innovative measurement methods like light fiber techniques and resistance tomography.

To reach this aim a joint research was founded in the framework of VEGAS. The participants and their projects follow. They are supposed to be completed in the future by basic-, technological- and use-orientated projects.

Dr. B. Barczewski, Institute for Hydraulics at University of Stuttgart: "Development of an *in-situ* method for local measurement of NAPLs in the underground": Modification and test of a fiber optical instrument for measurement of the concentration of organic substances in the subsurface. The advantage of an instrument like this compared to classical methods is the comparatively cheap measurement. The instrument will be used in other projects to measure the spatial– and time–changes of the substance concentration with high resolution.

Dr. C. Nitsche, Dresdner Grundwasserforschungszentrum: "Development of measurement– , investigation– and model–techniques for the evaluation of the status of soils, contaminated with mineraloil hydrocarbons" Modification of methods for the measurement of hysteresis state functions for the multiphase system solid–air, solid–water and hydrophobic liquid phase in small laboratory columns and use of these functions for the interpretation of an infiltration experiment on the upper next scale. The phase distribution will be measured by tomographical methods, which will be tested in a half–technical scale in this project. Such methods are quite attractive for the exploration at field scale (10 - 100 m).

Prof. Dr. K. Roth, University of Hohenheim: "Experimental pure research for the transport of organic substances (CKW, ...) in different natural soils" Experimental research of the multiphase transport in different natural structures on different scales by infiltration experiments in small (0.1 m) and big (1 m) undisturbed piles. The aim is to determine (i) the connection between processes on both scales and (ii) the distribution of the component's fluxes to the different phases. With this data, methods for upscaling and for the identification of parameters will be tested.

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