

Reliability of models for isothermal and non-isothermal multiphase processes in porous media

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Abstract Flow and transport processes in the subsurface are characterized by the presence of phases that are not miscible with each other. The phases may be water, gas, and an organic liquid phase, which may have entered the ground from disposal dumps, industrial sites, or via accidental spills. The description of the remediation of such contaminated sites by soil vapour extraction is an example of the use of a multiphase model in a porous medium. In this paper, we point at the needs of isothermal and non-isothermal multiphase multicomponent models. We present a model concept and discuss the reliability of the numerical simulations, focusing on some key input parameters of the model.

INTRODUCTION

Numerical modelling of multiphase processes in porous media is an important basis for decisions concerning the interest of environmental protection. For example, groundwater quality is endangered by a multitude of contaminants that may enter the ground from leaking disposal dumps, from the disposal of industrial waste products, or via accidental spills. These contaminants are organic substances, which are present in the subsurface as separate phases—NAPLs, Non-Aqueous Phase Liquids—with a low solubility in water. The technique of soil vapour extraction is a possible means to remediate NAPL contaminated sites. The relevant physical processes can be described by a three-phase three-component model concept. If in addition energy exchange processes play a role, we need a non-isothermal model concept that is also capable of accounting for mass and energy transfer between the phases (dissolution, evaporation, condensation). A practical application is thermally enhanced soil vapour extraction (Fig. 1).

Improved effectiveness of soil vapour extraction is achieved by injection of thermal energy via steam into the subsurface. This mobilizes NAPL in residual saturation by increasing the NAPL vapour pressure, which enhances the mass transfer of contaminants from liquid into the gas phase, and by a decrease of capillary forces, which enables a remobilization of residual NAPL. Helmig *et al.* (1998a) describe a comparison of steam injection experiments into sand filled columns with numerical simulations. Based on that, Class (1999) gives an example of the numerical simulation of a steam injection experiment into a column that was contaminated with xylene in residual saturation. Numerical modelling as a supplementary tool to the experiments contributes to better quantitative understanding of the physical processes. It enables the coupling of several processes investigated in small-scale laboratory experiments and

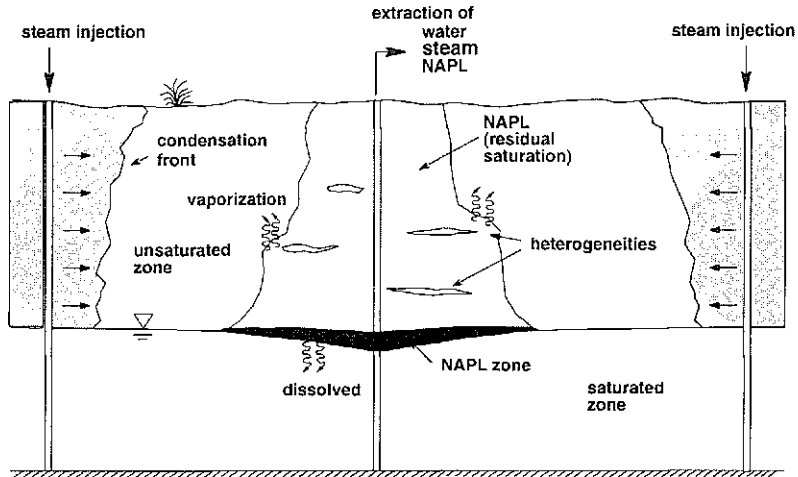


Fig. 1 Schematic of thermally enhanced soil vapour extraction.

the comparison of numerical simulations with experiments on larger scales, and, finally, enables upscaling to field-scale applications. The mathematical description of the flow and transport processes in a porous medium yields a set of strongly nonlinear partial differential equations. The nonlinearity mainly results from the relations between capillary pressure and saturation, and between relative permeability and saturation. The correct formulation of these relationships for a multiphase system in a porous medium is key to a reliable reproduction of the physical processes in the numerical model.

MODEL CONCEPT

An abstraction of the complex coupled processes in a non-isothermal multiphase multicomponent system is necessary to obtain a model concept that describes the physical system adequately. For example, the assumption of local thermodynamic equilibrium is a simplification of the system that reduces the number of unknown parameters. Figure 2 shows the possibilities of mass and energy transfer between the fluid phases, water, gas, and NAPL, and the solid phase, which is given by the porous matrix. Processes like evaporation, condensation, dissolution, and sorption must be considered in the numerical model.

The phases consist of several components. The ratio of the components can be determined by equilibrium conditions. For example, the mole fraction of water vapour in the gas phase for a certain temperature is determined by the equilibrium between liquid water and water vapour, which is described by the saturation vapour pressure. However, variation of pressure or temperature can change the thermodynamic state of a system such that a coupled mass and energy transfer process like evaporation or condensation yields a new state of thermodynamic equilibrium. To account for these processes in the model, we have to implement quantitative descriptions, e.g. of the specific internal energy and the specific enthalpy of the phases. Since the fluid properties are normally well known, their quantitative description can be reliably provided in the model.

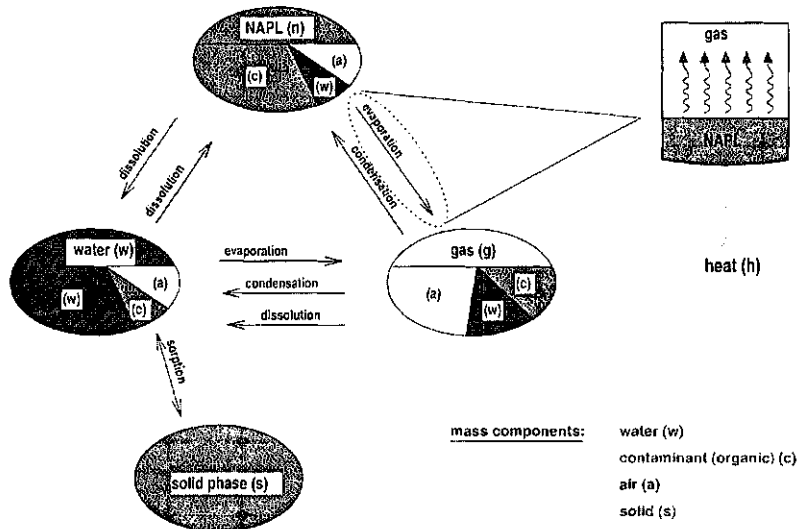


Fig. 2 Mass and energy transfer between phases.

Another key to successful modelling of flow and transport in a porous medium is the description of the properties of the porous medium itself. The relationships between capillary pressure and saturation and between relative permeability and saturation are strongly dependent upon the pore space geometry. In particular, it is impossible to determine analytically the pore size distribution and the interconnectivity of the pore space for a given porous medium. Many approaches have been derived that describe a functional correlation between capillary pressure, relative permeability, and the saturations of the fluids present in the pore space.

For example, one of the most famous models that gives a functional between capillary pressure and saturation in an air–water system is the approach of Brooks & Corey (1964):

$$p_c(S_w) = p_d S_e^{-1/\lambda} \quad (1)$$

p_d and λ are fitting parameters of the functional. The parameter λ usually lies between values of 0.2 and 3.0. A very small λ represents a single pore size distribution, whereas a very large value indicates a highly non-uniform material. p_d is the entry pressure, which is required to displace a wetting fluid from the pore space. S_e is the effective saturation. Parker *et al.* (1987) extended the approach of two-phase capillary pressure-saturation to a three-phase system: water, NAPL, and gas. Assuming that due to the order of wettability, interfaces only exist between water and NAPL and between NAPL and gas, the three-phase capillary pressures can be obtained from a combination of the two-phase systems water–NAPL and NAPL–gas.

Effects of hysteresis and the presence of heterogeneities in the porous medium make the problem of finding an appropriate functional for the capillary pressure-saturation relationship even more complicated (Sheta, 1999). Its behaviour during an imbibition process differs from that during drainage. Sheta (1999) also shows that the effects of fluid entrapment caused by hysteresis play a significant role in multiphase systems.

Like capillary pressure, the relative permeability of the fluid phases in a porous medium can also be described by parameterizations. The approach of Brooks & Corey (1964) for a two-phase system gives the wetting phase relative permeability as follows:

$$k_{rw} = S_e^{\frac{2+3\lambda}{\lambda}} \quad (2)$$

In a three-phase system the relative permeability of the water phase depends only on its own saturation. Water is the most wetting fluid in a water-NAPL-gas system and therefore preferentially fills the smallest pores. The relative permeabilities of NAPL and gas in a three-phase system depend on the saturation of all three phases. The method of Parker *et al.* (1987) is one of the most common approaches to describing three-phase relative permeabilities.

RELIABILITY OF THE NUMERICAL MODEL

The numerical simulator MUFTE_UG (Helmig *et al.*, 1998b), which is based on a modern software architecture and allows for multigrid computations on unstructured grids, contains modules for isothermal and non-isothermal multiphase multicomponent flow. The non-isothermal module was verified by numerically reproducing a semi-analytical solution of the “heatpipe effect” (Udell & Fitch, 1985) (Fig. 3).

Figure 3 shows that the simulations could match the solutions of Udell & Fitch very well. This proves that the model—presuming that the relations for relative permeability and capillary pressure are known—is able to reproduce the non-isothermal flow and transport processes correctly.

A different case of checking a numerical model’s reliability is the simulation of experiments. In the VEGAS research facility at the University of Stuttgart, a number of laboratory experiments concerning steam injection into sand were conducted in order to develop and optimize the remediation technique of thermally enhanced soil vapour extraction. A schematic of one of these experiments is shown in Fig. 4.

Steam was injected into a vertical sand-filled column from the top, to clean up the sand, which was initially contaminated with xylene. Temperature measurements were taken at different locations to monitor the steam front and the disappearance of the xylene. Modelling the processes occurring during this experiment requires that a number of parameters be determined in order to get functionals for calculating capillary pressures and relative permeabilities. These parameters are extremely difficult to determine by measurement, particularly in three-phase systems when hysteresis also has to be considered. Furthermore, even in an apparently homogeneous sand small-scale heterogeneities exist, which are impossible to determine and therefore provide an additional uncertainty.

Figure 5 shows a comparison of the temperature measurements in the column experiment with numerical simulations conducted with MUFTE_UG.

When the steam front passes a temperature sensor, it first causes a temperature increase up to a plateau at the boiling temperature of the water-xylene mixture. The temperature remains almost constant until all the xylene has disappeared, and then increases to the boiling temperature of pure water. While the arrival of the front and the plateau temperature could be matched well by the model, the calculated plateau is

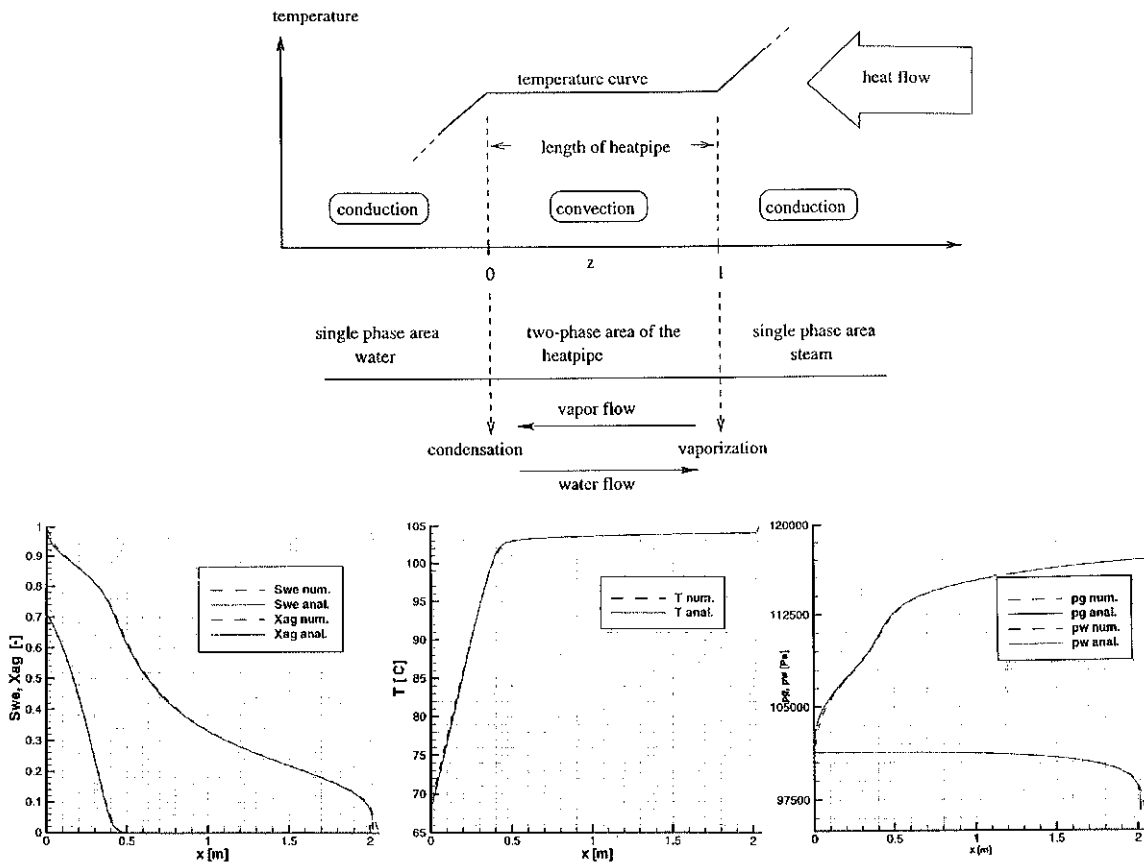


Fig. 3 The heatpipe effect: schematic sketch and comparisons between numerical and analytical results

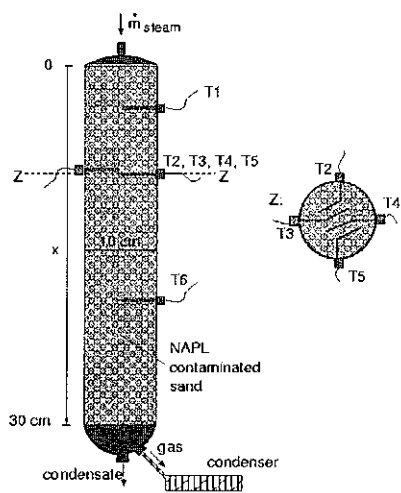


Fig. 4 Steam injection experiment in a xylene contaminated laboratory column.

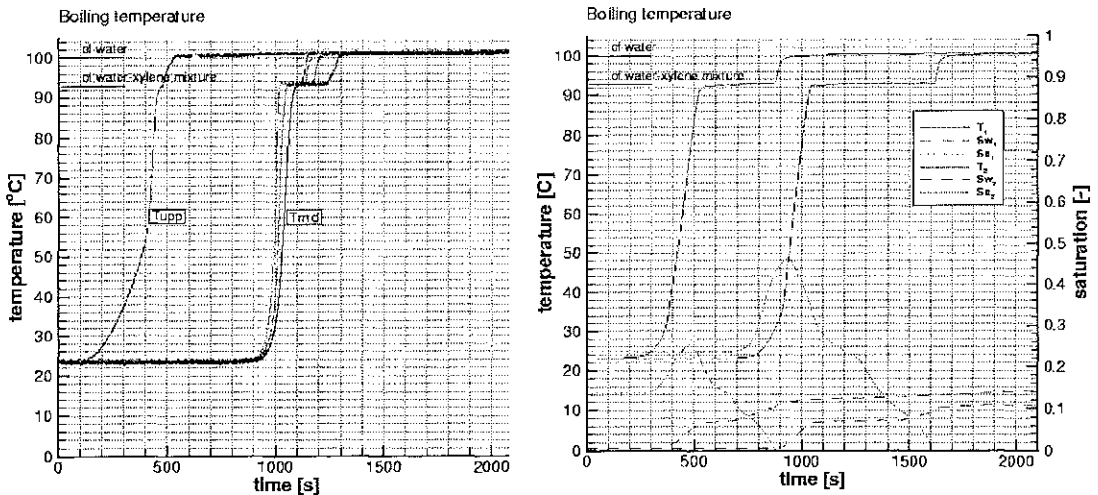


Fig. 5 VEGAS column experiments with xylene contaminated sand: comparisons between measurements (left) and numerical results (right) at 6 cm (T_1) and 14.5 cm (T_2) from the top.

significantly longer than that of the measurements. The length of the plateau depends on different factors, e.g. on the amount of NAPL present in the pore space, on the rate of mass and enthalpy during the steam injection, and on the effective permeability of the fluid-porous medium system. Condensing xylene vapour causes an increase of the liquid xylene saturation at the front. The higher the effective permeability for the xylene-absolute permeability of the porous medium times the relative permeability of xylene, the more xylene can be displaced by gravitational forces. This means that less xylene has to be evaporated resulting in a shorter plateau. The process of evaporation is dominated by the steam rate and the fluid properties, which are both known relatively well. The displacement of xylene by gravitational forces is a process that provides more uncertainties for numerical modelling in this case. Class *et al.* (1999) tried to estimate the absolute permeability of the sand and the relative permeability-saturation relationship for the column experiment. It became clear that both have significant influence on the modelling results, particularly on the length of the plateau. Thus, the uncertainty of the curve fitting parameters used to describe capillary pressure and relative permeability strongly affects the results of the numerical simulation. In this experiment the xylene saturation before the steam injection was obtained by drainage of the fully xylene-saturated column. Later, during the steam injection, condensing xylene causes an increase of the xylene saturation at the steam front and with that an increase of the xylene relative permeability. The flow of xylene reverses from drainage to imbibition, which leaves the suspicion that the parameterization for the curves before the steam front passes a sensor is different to that after it has passed.

CONCLUSIONS

Numerical modelling of multiphase flow and transport processes is useful for a better understanding of complex correlations like the strongly coupled transfer and transport of mass and energy. Fluid properties and thermodynamic states are well known. Their accurate calculation is ensured by a multitude of tables and functions in the literature. We have shown that the numerical simulator MUFTE_UG could match a semi-analytical solution of the heatpipe effect almost exactly. The main difficulties for the numerical modelling results from the mathematical description of the interaction of the fluid phases with the porous medium, namely the relationships between capillary pressure and saturation and between relative permeability and saturation. The reliability of a numerical model strongly depends on the determination of appropriate functionals for these relationships, and on the influence of small-scale heterogeneities that are impossible to determine for simulation on larger scales.

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