



## Field scale characterization and modeling of contaminant release from a coal tar source zone

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### ABSTRACT

A coal tar contaminated site was characterized using traditional and innovative investigation methods. A careful interpretation of hydrogeological and hydrogeochemical data allowed for the conceptualization of the heterogeneous coal tar distribution in the subsurface. Past and future contaminant release from the source zone was calculated using a modeling framework consisting of a three-dimensional steady-state groundwater flow model (MODFLOW) and two hydrogeochemical models (MIN3P). Computational time of long-term simulations was reduced by simplifying the coal tar composition using 3 composite and 2 individual constituents and sequential application of a 2D centerline model (for calibration and predictions) and a 3D model (only for predictions). Predictions were carried out for a period of 1000 years. The results reveal that contaminant mass flux is governed by the geometry of zones containing residual coal tar, amount of coal tar, its composition and the physicochemical properties of the constituents. The long-term predictions made using the 2D model show that even after 1000 years, source depletion will be small with respect to phenanthrene, 89% of initial mass will be still available, and for the moderately and sparingly soluble composite constituents, 60% and 98%, respectively.

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### 1. Introduction

Coal tar is a complex mixture of various aqueous-immiscible organic chemicals with density greater than that of water. In the subsurface environment, it constitutes a dense non-aqueous phase liquid (DNAPL). DNAPLs spilled into the subsurface migrate through the vadose zone and below the water table, where they are found as separate liquid phases at residual saturation or in more concentrated "pools" serving largely as persistent long-term sources of contamination. Coal tar consists of numerous compounds (BTEX, PAHs, NSO heterocycles and others) covering a large range of physical, chemical, and toxicological properties (e.g. Bundy et al., 2001; Eberhardt and Grathwohl, 2002). Though being governed by processes that often occur at a slow rate, contaminant mass transfer in the flowing groundwater may pose a risk to human health or the environment (ITRC, 2004). The field

scale estimation of contaminant mass release, also denoted as mass discharge or mass flux, is an important means to evaluate the significance of contaminants in groundwater with respect to their environmental impact (e.g. Gnanapragasam et al., 2000; Einarson and MacKay, 2001; Newell et al., 2003). Changes in contaminant mass discharge is also recommended as an appropriate metric for assessing performance and efficiency of source zone remediation techniques (e.g. US EPA, 2003; Soga et al., 2004). Rao et al. (2002) proposed contaminant release estimates for the evaluation and prioritization of site management alternatives.

Independent of whether partial source removal measures (e.g. air sparging, thermal treatment) or plume management options (e.g. pump-and-treat, monitored natural attenuation) are to be assessed, predictions of the time scales of organic contaminant release are required for the natural as well as the remedial scenario to evaluate feasibility, costs, benefits and adverse impacts of the particular measure. These predictions can be made using mathematical models. Various model approaches have been proposed, ranging from simple

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analytical models (e.g. Sale and McWhorter, 2001; Rao and Jawitz, 2003; McWhorter and Sale, 2003; Newell et al., 2003; Zhu and Sykes, 2004; Falta et al., 2005; Newell and Adamson, 2005; Fure et al., 2006) to sophisticated 3D numerical high-resolution models (e.g. Parker and Park, 2004; Christ et al., 2006; Rahbeh and Mohtar, 2006, 2007). In the case of field scale problems, the selection of the model that is most appropriate for the given problem is typically driven by the limitations in available input data and computational cost constraints.

Appropriate quantity and quality of collected data and information is therefore a crucial point in characterizing and understanding of the distribution of the subsurface contamination and its properties. Due to the significant heterogeneity of most subsurface environments, it is per se extremely difficult to quantify and assess the extent and distribution of contaminants as well as the hydraulic, chemical, and biological parameters and processes that control their migration and persistence in the subsurface (Stroo et al., 2003). As a result, model-based predictions based on an inevitably limited knowledge are uncertain. This is true even for well-characterized systems (e.g., Brahma and Harmon, 2003; Maji et al., 2003), and is likely to be more pronounced when models are applied to larger, highly variable field sites. Therefore, especially in non-research projects, which in practice typically have financial budget constraints, there is a great need for efficient and target oriented site investigations. The number and location of sampling points as well as the type of investigation techniques to be applied need to be carefully chosen in accordance to the site-specific geological conditions.

The selection can be made from numerous conventional (e.g. groundwater monitoring wells and soil borehole logging) as well as novel investigation methods (e.g. reactive tracer techniques and direct-push methods) currently available for the detection and delineation of subsurface DNAPL distribution (e.g. Jin et al., 1995; Rao et al., 2000; Kram et al., 2001a, 2002; Brusseau et al., 2007). An inexpensive and rapid in situ technique for the vertical delineation of NAPL is the laser-induced fluorescence (LIF), which in particular can detect BTEX and PAH in submerged sediments, unconsolidated materials and aqueous solution (e.g. Chen et al., 1997; Grundl et al., 2003; Sinfield et al., 2007). For the investigation of a DNAPL source zone, the LIF technique is often applied in combination with cone penetration testing (CPT) (e.g. Kram et al., 2001b; Pepper et al., 2002; Kram et al., 2004), which provides high spatial resolution data on the geological subsurface (e.g. Fukue et al., 2001; Miles et al., 2007).

The intention of this paper is to give an example of how diverse investigation techniques and mathematical modeling can be combined to create a coherent modeling framework at field scale in spite of data limitations. Starting with the building of a hydrogeological model, the distribution of the coal tar source zone was estimated on the basis of both investigation data and modeling results. The model is capable of consistently estimating the status quo as well as future contaminant release.

## 2. Site characterization

### 2.1. Background

The field site, which is located 40 km south of the city of Hamburg in Buchholz (Germany), is a former wood treatment

plant that operated from 1904 to 1986 (Fig. 1). Activities of wood impregnation caused a coal tar contamination of the local unsaturated and saturated zones. Since 1986, environmental impact assessments of the site have been conducted. Data on local geology, hydrogeology and contaminant concentrations were originally obtained through groundwater monitoring wells, borehole logs, sieve analyses, pumping tests, groundwater level measurements and groundwater and soil samples.

Based on borehole log data, the contaminated aquifer can be divided into three Quaternary glacial stratigraphical units: (i) medium sand layer (from the surface to around 43 m above sea level), (ii) fine sand layer (from around 43 m to 23 m asl) and (iii) coarse sand layer (from around 23 m to 14 m asl). These sedimentary layers were deposited upon an approximately 30 m thick silty fine sand layer, which is the main local aquitard and separates the upper contaminated aquifer from a deeper pristine aquifer, which is, therefore, not considered in this work. The overall groundwater flow direction in the contaminated aquifer is towards the Southeast and does not present significant seasonal oscillations.

Several site investigations of the dissolved phase indicated (for naphthalene) a plume length of around 450 m and a maximum width of 150 m (Fig. 1). However, the contaminant plume was not homogeneously distributed along the aquifer thickness. As the distance from the source area increases, this plume becomes increasingly restricted to the bottom of the aquifer (coarse sand layer). Furthermore, three distinct methods of investigation, i.e. signature metabolite analysis (SMA), compound-specific isotope analysis (CSIA) and redox-sensitive tapes (RST), indicated that active biodegradation takes place in the plume (Blum et al., 2006).

### 2.2. Source zone characterization

Originally, the source in the unsaturated zone was investigated through 29 percussion drillings, with a maximum depth of 12 m, while the saturated zone was explored by means of dry drillings during the installation of monitoring wells G11, G14, G15 and G16 (Fig. 1) in the core of the source zone. In all these wells coal tar was observed. However, to obtain the architecture of the residual coal tar, additional site information was required. Therefore, a comprehensive source investigation strategy was initiated, which was subdivided into three main distinct phases: (i) exploratory source zone investigation using CPT, (ii) detailed source zone investigation using CPT combined with LIF sounding, and (iii) core sampling of the source zone.

#### 2.2.1. Exploratory source investigation with CPT

Eight exploratory CPT soundings were applied to refine the geological knowledge in the source area. To delineate different sediment types, the relationship between stress and soil deformation was interpolated by measuring probe tip resistance, friction sleeve resistance and dynamic pore pressure (e.g. Robertson, 1990). A geological interpretation that combined existing borehole and CPT logs was carried out. Considering the behavior of DNAPLs in geological materials, a result of particular importance was the delineation of a continuous thin silt layer in the saturated zone, restricted mainly to the former plant area (Fig. 1).

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