MEMORANDUM

DATE: January 26, 1999

TO: Andrew Wittner

FROM: John Vierow and Chris Long

SUBJECT: Summary of CMTP Sensitivity to Changes in Kd
EPA Contract No. 68-W-98-025, WA No.11
SAIC Project No. 06-5029-08-7436-200

Background and Summary of Results

In a meeting with Andy Wittner (EPA), SAIC, and industry stakeholders on January 20, we discussed how metals transport can be simulated using existing ground water transport models including EPACMTP and MYGRT. Both models are very similar in their modeling of arsenic, in that they assume reversible physical sorption throughout the flow path, with the magnitude of these effects constant in space and time. In the meeting we referred to this as the 'Kd approach.'

EPACMTP allows for the automatic calculation of Kd and retardation rate based on metal identity and pH. For all of our risk assessment results, such as the June draft final report, we have conducted all calculations using this method. In contrast, MYGRT allows for the direct input of retardation rate. To allow for a more direct comparison of the flexibility of the two models, we conducted a series of runs where we input Kd directly into EPACMTP, instead of specifying the metal type and the pH. We also conducted runs that allowed us to see how changes in the pH affect the well concentration, when using the EPACMTP metals isotherm data.

We have the following observations in analyzing these EPACMTP results:

- For arsenic, small changes in pH do not have much impact on the EPACMTP results. A wide range of environmental pH, from 3 to 11, produces a two-fold change in peak concentration for the impoundment case and a three-fold change in peak concentration for the landfill case. Smaller changes in pH (e.g., from 6 to 7) would have less effect.

- Increasing the Kd (i.e., higher retardation) produces a lower peak concentration; a doubling of the retardation rate results in a halving of the peak concentration. A similar quantitative relationship was observed for MYGRT version 2 when conducting runs in September 1998.

- These results should be viewed as sensitivity analysis results and not validation of any particular value of Kd.

EPACMTP Calculation of Retardation Rate

EPACMTP calculates a value for retardation rate based on Kd, bulk density, and porosity. For metals, the value for Kd may be derived based on pH and metal-specific information. For example, the derived value of Kd equals 29 cm^3/g for arsenic in all of the comanaged waste scenarios (with pH of 6.92). Alternatively, the user may directly specify the value of Kd following the steps listed below:

- Changing the 'metal flag' from true to false in the first row.
- Setting variables US10 and AS21 to the desired Kd value. These variables correspond to inputs in the unsaturated and saturated zones, respectively. Different values could be specified for each zone, however for simplicity this was not conducted.
- Leaving variable AS9, the retardation rate, as a derived variable.
- Ensuring that variables US11 and AS22 are omitted or set equal to 1. They represent exponents for adsorption algorithms. Values not equal to one correspond to non-linear cases.

Whether the user-specified or the model-derived value of Kd is chosen, the retardation rate is calculated using Equation 6.5.6 in the User's Guide:

$$R_s = 1 + \frac{\rho_b k_d}{\phi}$$

where ρ_b is bulk density of the subsurface (1.42 g/cm3 for the aquifer) and ϕ is the porosity (0.41 for the aquifer). Using these values and the pH shown above, R_s, the retardation rate, is 101.

Setting the variables in the above manner, with a Kd value of 29, gives identical results to those obtained when allowing the model to calculate Kd based on the metal type and the pH. Specifically, the following results were obtained:

Impoundment Case, allowing model calculation of Kd: Peak concentration of 0.147 mg/L at 1,570 years (initial concentration 9.64 mg/L).
Impoundment Case, with direct input of Kd=29: Peak concentration of 0.147 mg/L at 1,570 years (initial concentration 9.64 mg/L).

Landfill Case, allowing model calculation of Kd: Concentration of 0.075 mg/L at 10,000 years (initial concentration 0.24 mg/L).
Landfill Case, with direct input of Kd=29: Concentration of 0.075 mg/L at 10,000 years (initial concentration 0.24 mg/L).

Effect of Retardation Rate on Well Concentration

We conducted several runs at different retardation rates, with Kd specified by the user and with Kd calculated by the model from the metal and pH. The purpose of these runs is to better show the sensitivity of results to changes in retardation rate, rather than to imply that one of these values is 'better' than the value used for our previous runs. The following results are obtained:

EPACMTP Results for Arsenic in a Surface Impoundment, Kd Calculated by Model as a Function of pH C_0=9.64 mg/L		
pH	Peak Well Concentration, mg/L	Time of Peak Concentration, years
3	0.196	1,180
7	0.146	1,580
11	0.109	2,110

EPACMTP Results for Arsenic in a Landfill, Kd Calculated by Model as a Function of pH C_0=0.24 mg/L		
pH	Peak Well Concentration, mg/L	Time of Peak Concentration, years
3	0.113 *	10,000 *
7	0.074 *	10,000 *
11	0.031 *	10,000 *

* EPACMTP calculations are stopped after 10,000 years. The well concentration likely is still rising at this time and a true 'peak concentration' would occur after 10,000 years.

EPACMTP Results for Arsenic in a Surface Impoundment, Kd Specified Directly by User C_0=9.64 mg/L		
Kd	Peak Well Concentration, mg/L	Time of Peak Concentration, years
1	3.11	91
10	0.420	560
30	0.143	1,620
50	0.0858	2,690
100	0.0430	5,320
500	0.00003 *	10,000 *

* EPACMTP calculations are stopped after 10,000 years. The well concentration likely is still rising at this time and a true 'peak concentration' would occur after 10,000 years.

These tables show the following:

- For arsenic, small changes in pH do not have much impact on the EPACMTP results. A wide range of environmental pH, from 3 to 11, produces a two-fold change in peak concentration for the impoundment case and a three-fold change in peak concentration for the landfill case. Smaller changes in pH (e.g., from 6 to 7) would have less effect.

- A change in the Kd, over a range of 10 to 100, will produce an identical change in both the peak concentration and its time for the impoundment case. For example, increasing the Kd by an order of magnitude (from 10 to 100) increases the time to reach peak by the same amount, and decreases the peak concentration by an order of magnitude.