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THE SCBR MODEL AS A DECISION SUPPORT TOOL TO ASSESS THE AGE OF BIOFUEL RELEASES

Camila C. Muller*, Cristina C. Nunes*, Márcio R. Schneider+, Mário do Rosário§, Henry X. Corseuil*

***Federal University of Santa Catarina, Brazil (bilamuller@gmail.com), +W2S3 Environmental Technologies, §CENPES – Petrobras Research Center**

1. INTRODUCTION

This paper addresses the necessity to understand the behavior of fuel and ethanol blends in the subsurface and the importance of considering the ethanol effects on the weathering of BTEX in computational flow models (CFM) to simulate these scenarios. With fifteen years of experience studying groundwater contamination by petroleum hydrocarbons and ethanol, the Federal University of Santa Catarina, Brazil (UFSC) and Petrobras (Petróleo Brasileiro S.A.) developed the SCBR model (Risk Based Corrective Solution), a software to assist environmental management in all steps of contaminated sites as a decision support tool.

Contaminant transport models are used for age dating, for source identification, and for cost allocation purposes [1]. Among most used CFM, SCBR stands out because it considers the ethanol effects on compounds migration and transformation as the cosolvent effect and inhibition of compounds biodegradation.

Knowledge of the contaminant's concentration over time is crucial to determine spill age. As ethanol in biofuels may alter the transport and transformation of BTEX in groundwater, the consideration of its effects on the modeling is important for an accurate investigation. Therefore, the SCBR model is becoming an important decision support tool for Petrobras to manage impacted areas in Brazil.

2. METHODOLOGY

To simulate hydrocarbon petroleum plumes in the presence of ethanol, as well as the water flow in the subsurface, SCBR uses the Boussinesq equation solved numerically to a 2D scenario, considering molecular diffusion, advection, dispersion, sorption, and biodegradation [2], as shown in Equation 1.

$$\frac{\partial}{\partial x}\left(K_x h \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y h \frac{\partial h}{\partial y}\right) + (|q_z|_0 + I) + F = S_y \frac{\partial h}{\partial t} \qquad \text{Equation 1}$$

Contaminants concentration in groundwater due to cosolvency effect is calculated according to Corseuil et al. (2004) [3], where S_m is the solubility of the solute in the water-cosolvent mixture, S_w is the solubility in pure water, f is the cosolvent volume fraction in the aqueous phase, and K_{ow} is the octanol-water partition coefficient, as shown in Equation 2.

$$\log S_m = \log S_w + f \cdot (0{,}76 \cdot \log K_{ow} - 0{,}83) \qquad \text{Equation 2}$$

The preferential degradation of ethanol in relation to BTEX is simulated by assigning zero value for the biodegradation coefficient of petroleum hydrocarbons while inhibiting concentration is less than the prescribed concentration of simulated ethanol. To avoid inconsistencies, SCBR uses finite volume method with a structured mesh, which allows the simulation of aquifer heterogeneities, multiple sources, remediation techniques, influence of rivers and lakes in the groundwater flow.

3. RESULTS

To demonstrate the use of SCBR as a decision support tool to estimate source age of a biofuel spill, the model was calibrated using ethanol and benzene data of a 14 year field experiment where 100L of Brazilian gasoline (containing 24% ethanol and 0,6% of benzene by volume) was released into a sandy aquifer. Biomass augmentation due to rapid ethanol biodegradation and increase of biodegradation rates at the source zone was observed in the field and considered in the calibration [4]. In a well 2.6 m from the source, benzene concentration starts to drop off after ethanol's migration and/or degradation (Figure 1).

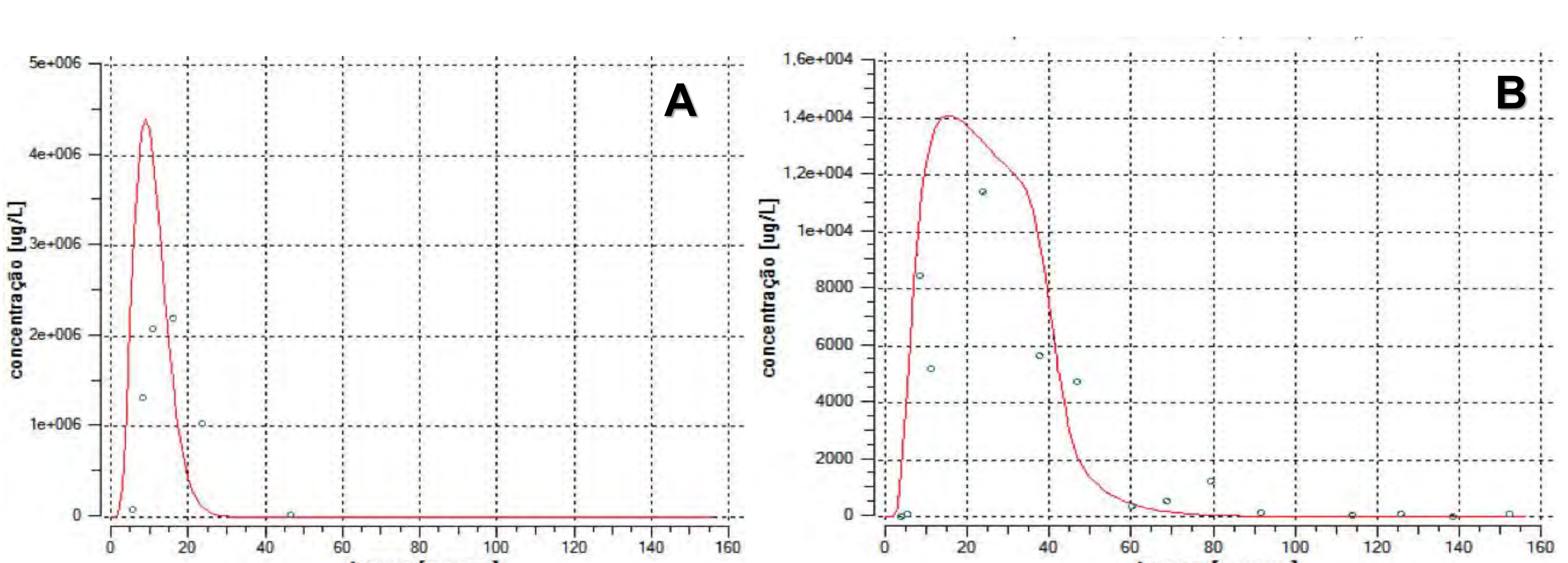

Figure 1: Ethanol (A) and benzene (B) calibration in a 100L controled released of Brazilian Gasoline

The ethanol effect on dissolved BTEX concentration may vary significantly with spill volume and groundwater velocity variation. Simulation of a 1,000 liters spill of Brazilian gasoline was performed with the same experimental conditions (v_1=3m/year) and a second simulation with one order of magnitude increase on the groundwater velocity (v_2=30 m/year). For each velocity two conditions were established, one considering and another neglecting the ethanol effects. In the simulation for the 3 m/year velocity, ethanol is present during the initial twenty-four months of the experiment, whereas for the simulation of 30 m/year, only during four months (Figure 2, Figure 3). The velocity of the groundwater flow interferes during the time period which ethanol is present in the area and hence on the inhibition time of BTEX biodegradation, i.e. the period of inhibition of biodegradation of these compounds, due to the presence of ethanol, decreases with increasing groundwater velocity.

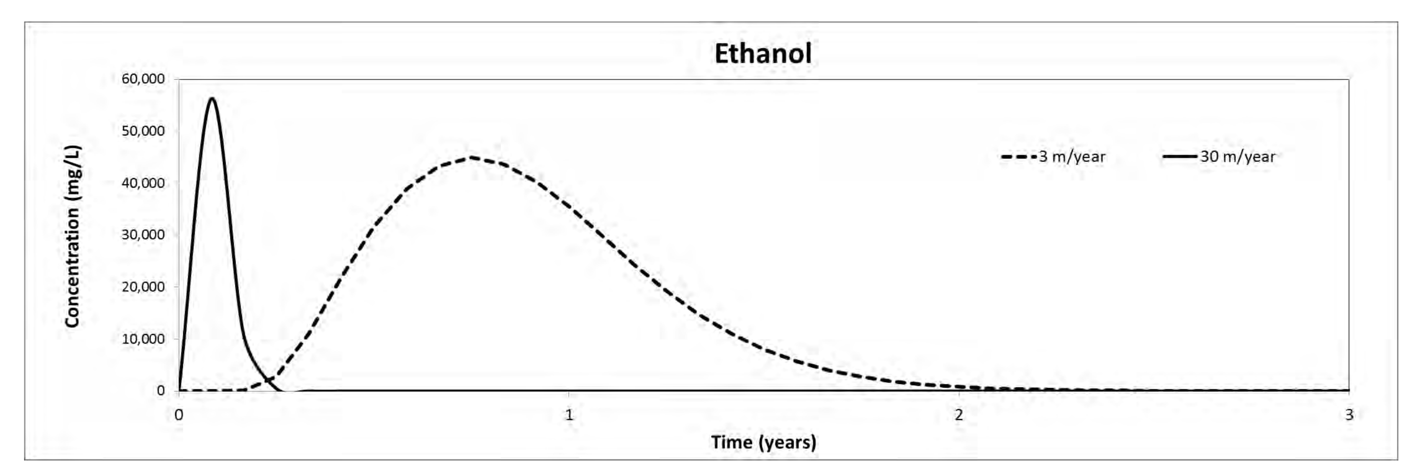

Figure 2: Ethanol concentration near the source in a simulated 1000L Brazilian gasoline spill for groundwater velocity of 3 and 30 m/year

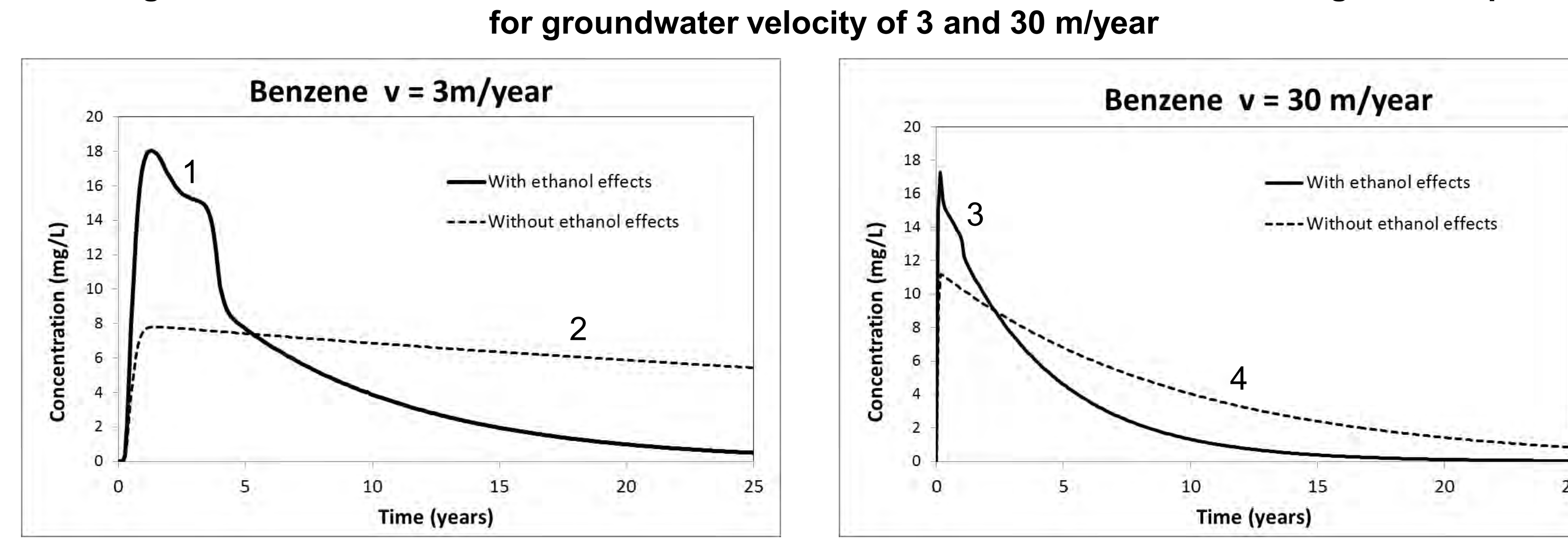

Figure 3: Simulation of 1000L Brazilian gasoline spill: 1) v_1 = 3m/year with ethanol effects, 2) v_1 = 3m/year without ethanol effects, 3) v_2 = 30m/year with ethanol effects, 4) v_2 = 30m/year without ethanol effects

4. CONCLUSIONS

Knowledge of transport and transformation processes and ethanol's interference on petroleum hydrocarbons dissolved concentrations is crucial to a realistic modeling of these compounds. Fuel composition and site specific hydrogeological parameters are also important to model plumes of dissolved compounds in groundwater. The possibility to modify fuels composition in its database (i.e.: percentage of benzene in gasoline, percentage of ethanol in biofuels) and determine the site specific weathering processes makes SCBR a flexible decision support tool to estimate fuels and biofuels source age.

Petróleo Brasileiro S.A. – Petrobras is implementing SCBR in its gas stations, refineries and terminals as a decision support tool to assist with their environmental management.

5. REFERENCES

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