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ABSTRACT

Recent interests in the transport of toxic chemicals or radionuclides in subsurface formation raise the question of the role of processes involving the interplay of fluid flow, chemical interaction and thermal effects.

The present paper reviews three examples of recent studies at Lawrence Berkeley Laboratory in this area, based on numerical modeling with a code called CPT. It is a three-dimensional chemical parcel model with a fully coupled heat and mass transport formulation for porous-fractured media with complex geometries.

The three examples are: (1) Injection and production of a denser cold fluid into a geothermal reservoir; (2) Solute transport in a two-layered aquifer; and (3) Solute transport in an aquifer with a horizontal fractured zone. The studies show a number of interesting features which may be of interest to the interpretation of field data.

INTRODUCTION

Recent interests in transport of toxic chemical and radionuclides in subsurface formations raise the question of the role of processes involving the interplay of fluid flow, chemical interactions and thermal effects. Thermal effects are especially important for radionuclide transport because of the significant heat release from nuclear wastes emplaced in geological repositories. These coupled thermo-hydro-chemical processes are also of interest to studies of tracer transport in geothermal systems. Table 1 lists some of the processes with such coupling effects.

The present paper reviews some of the recent results obtained by Lawrence Berkeley Laboratory in this area of study. Three examples are discussed below, which are studied using a numerical model called CPT (Mangold and Tsang, 1983). This is based on an earlier three-dimensional numerical code PT (Bodvarsson, 1982) developed to calculate fluid and heat flow through a porous medium with or without a few discrete fractures. The formulation includes the temperature dependence of density and viscosity of the fluid; gravitational or buoyancy effects; aquifer heterogeneity and complex boundary conditions. The numerical solution scheme in PT is based on the Integrated-Finite-Difference method. It has been verified against nine analytic and semianalytic solutions (Bodvarsson, 1982) and validated against a series of field experiments (Tsang et al., 1981; Buscheck et al., 1983). By adding to the code PT chemical transport and reactions as parcels moving with flow lines, the numerical code CPT was developed. In terms of parcel steps, chemical transport and precipitation and dissolution can be considered. We have attempted to limit numerical dispersion to acceptable levels for a given problem by reducing mesh sizes and time steps.

TABLE 1

Coupled Process-Examples

	T = Thermal H = Hydro C = Chemical
T - H	e.g. Buoyancy flow - thermal convection Hydrothermal systems
T - C	e.g. Temperature dependence of reaction rates
H - C	e.g. Toxic chemical transport Rock-water interactions
T /\ H—C	e.g. Tracer transport in geothermal systems Near-canister behavior in a nuclear waste repository Precipitation and dissolutin due to temperature change with resulting changes in permeability

Case 1: Injection and production of a denser cold fluid into a geothermal reservoir

The fluid injected into a geothermal reservoir usually is different from the reservoir fluid. In addition to a temperature difference, the injected fluid may have a greater density, since spent geothermal brine after flashing has a greater concentration of chemical constituents. For a well which partially penetrates the upper portion of the reservoir this may lead to less recovery during the succeeding production period. A colder fluid tends to sink in a warm reservoir due to differences in density caused by temperature differences. However, the cooler injected water will be gradually warmed by the reservoir heat as it advances into the reservoir, which slows the downward movement. However, such a temperature-dependent process does not account for density differences due to chemical composition which may be equally great.

For this injection test the differences in water density between the reservoir temperature of 200°C (392°F) and the injected water at 100°C (212°F) is approximately 10%. In this case in our exploratory study, the concentration of the solutes in the injected water was increased enough to increase the density of the injected fluid by another 10%. The injection was performed for 3 months through a well penetrating the upper 100 m of a 300 m thick geothermal reservoir at the rate of 20 kg/s (~300 gal/min). After this period, the well was produced for three months at the same rate. A list of properties used for the reservoir in this case is given in Table 2. A homogeneous reservoir bounded vertically by less permeable confining layers is modeled with a radially symmetric mesh.

TABLE 2

Reservoir Properties

Permeability	5×10^{-14} m^2 (50 md)
Porosity	0.20
Compressibility	2×10^{-10} Pa^{-1} (1.4×10^{-6} psi^{-1})
Thermal Conductivity	2.0 W/m.k (1.16 Btu/h·ft^2·°F/ft)
Heat Capacity	1000 J/kg·k (240 Btu/lbm·°F)
Density	2650 kg/m^3 (166 lbm/ft^3)

Caprock and bedrock have 10 times less permeability than the reservoir, with other properties the same.

The results after injection and production are shown in Figures 1 and 2. In Figure 1, the solid lines indicate the temperature contours in increments of 20°C (36°F) and the dashed lines indicate the concentration contours in increments of 20% of the initial injection concentration. It is apparent that the fluid moves downward more rapidly due to chemical concentration effects on density than due to temperature effects alone. Figure 2 illustrates the same contours after the production period: the downward movement of the denser fluid is clearly shown, despite the production of much of the cooler water injected in the first 3 months. This means that an examination of the recovery of the injected chemicals during the production period might lead to a misinterpretation of the significance of the test. The chemical substances in the injected water are causing some of this water to sink deeper than predicted with temperature-induced density changes alone. This shows that low recovery of the chemical constituents of the injected fluid may be due to the effect of chemical concentration on density in conjunction with a partially penetrating well rather than to chemical reactions, adsorption, or permeability inhomogeneities such as fractures.

Case 2: Solute transport in a two-layered aquifer

In this case we consider a contaminant plume that has infiltrated into the top of a two-layered aquifer, over a 24-m diameter area (see top figure in Fig. 3). The lower layer of the aquifer is twice as permeable as the upper. The rest of the parameters are given in Table 3.

After contaminant infiltration is stopped, an attempt is made to clean it up by extraction through a pumping well from the upper 38% of the aquifer. In Figure 3, the top graph shows contaminant concentration just before extraction begins. The increased plume flow into the higher permeability lower layer is apparent. During extraction, fluid again moves faster in the lower part of the aquifer allowing the timely extraction of

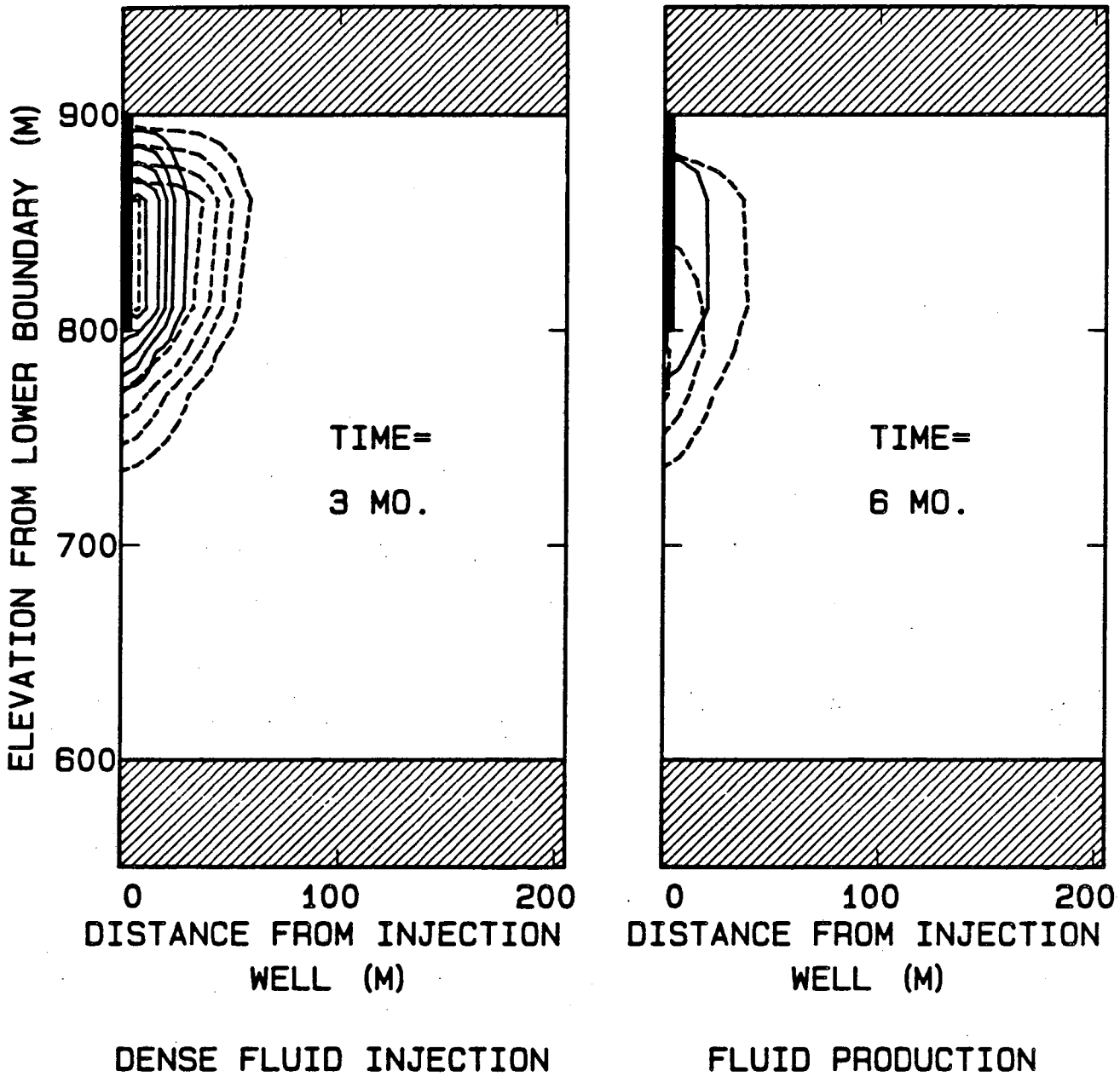

Figure 1. Temperature (solid) and concentration (dashed) contours after 3 months of injection of 100°C (212°F) water into a 200°C (392°F) reservoir from a partially penetrating well.

Figure 2. Temperature (solid) and concentration (dashed) contours after 3 months of production following 3 months of injection from a partially penetrating well.

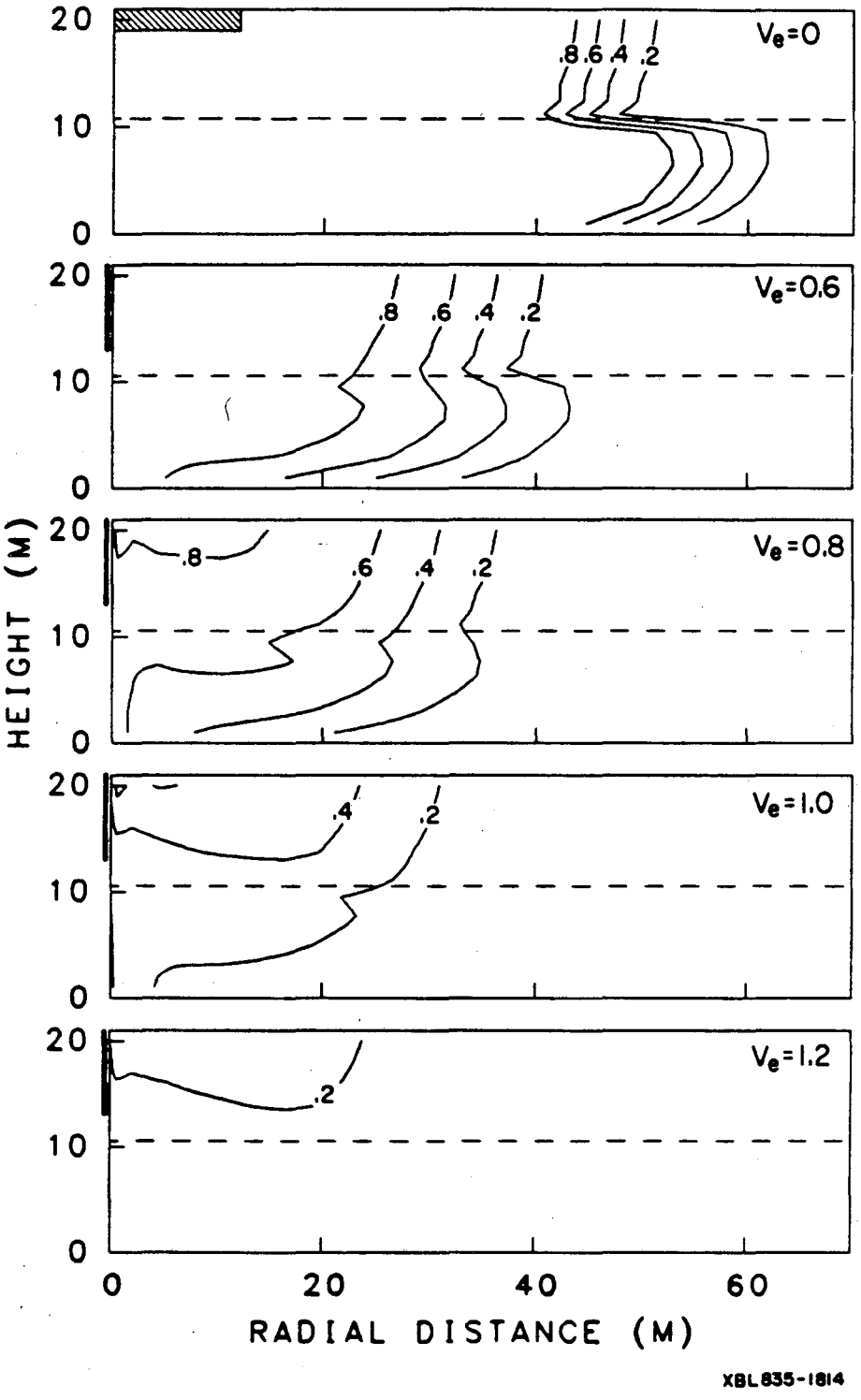

Figure 3. A time sequence showing the extraction of a contaminant plume from a two-layer aquifer. The permeability below the dashed line is double that above it. The infiltration zone is shaded; the extraction well screen is marked by the vertical segment.

TABLE 3

Physical Properties for Case 2

Aquifer Thickness = 21 m
Closed boundaries above and below the aquifer (except for infiltration zone)
Hydrostatic pressure boundary at r = 16 km

Contaminant Plume Formation

Infiltration rate	= 1.38 kg/sec	= 22 gpm
Infiltration period	= 1 year	
Infiltration zone, radius	= 0-12 m	

Aquifer Properties

Porosity	= 0.20	
Compressibility	= 1 x 10^{-8} Pa^{-1}	
Isotropic material		
Permeability of upper layer	= 2 x 10^{-11} m^2	= 20 darcies
Permeability of lower layer	= 4 x 10^{-11} m^2	= 40 darcies

a large portion of the plume there. After one year of extraction (Case: V_e = 1), a volume of water equal to original infiltrated contaminated water has been produced, and 89% of the contaminant is recovered. Here V_e is defined as the volume of water produced divided by the volume of contaminated water originally infiltrated into the aquifer. The calculation was also done for extraction locations of the well at different depths in the aquifer. Figure 4 shows the contaminant remaining in the aquifer after one year of extraction for cases A, B and C, corresponding to extraction from the full aquifer thickness, from the lower (high permeability) part of the aquifer, and from the upper (low permeability) part of the aquifer, respectively. The maximum contaminant concentration is lowest for case B; this result is contrary to the commonly held belief that extraction from high permeability zones of layered aquifers is best.

Case 3: Effects of a high permeability fracture zone

This case is the same as in Case 2, except for the fractured zone, which is assumed to have a thickness of 1 m with permeability of 2 x 10^{-10} m^2 or 200 darcies. Also, the lower layer has the same permeability as the upper one. The fracture zone acts as a fast path for the plume, as shown in Figure 5. The top graph in Figure 5 shows the calculated concentration contours just before extraction; the lower two graphs show the contaminant concentration after extraction from the upper part of the aquifer and from near the fracture zone level. The recovery effectiveness for the two cases is about the same. It is interesting to note in the figure the "concentration island" that is left behind after extraction of one year.

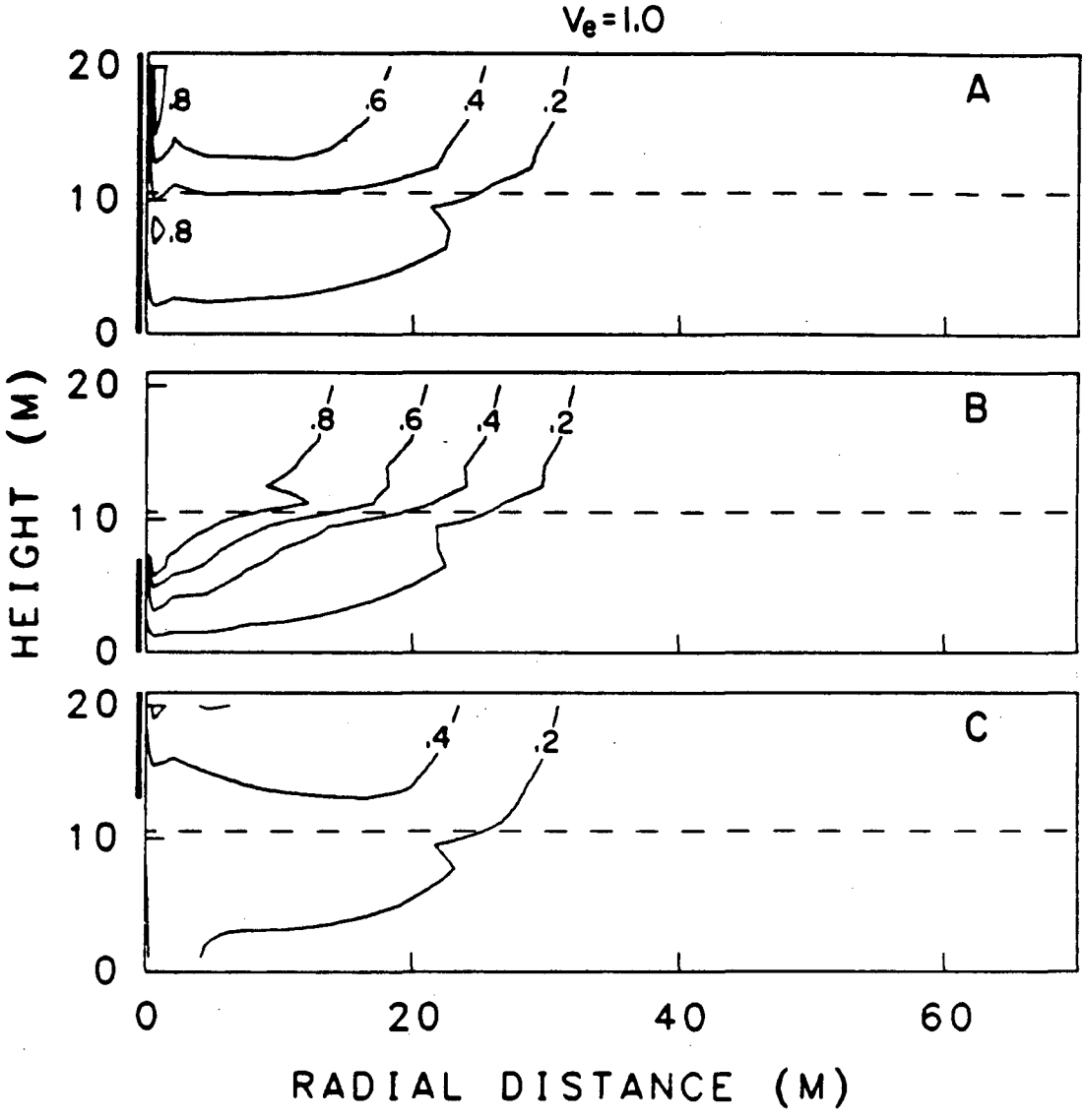

Figure 4. The concentration contours in a two-layer aquifer after plume extraction (V_e = 1) for three different extraction wells (Cases A, B, C). The original plume (V_e = 0) was shown in the top graph of Figure 3. The vertical segments on the left vertical axis show the location of each extraction well screen.

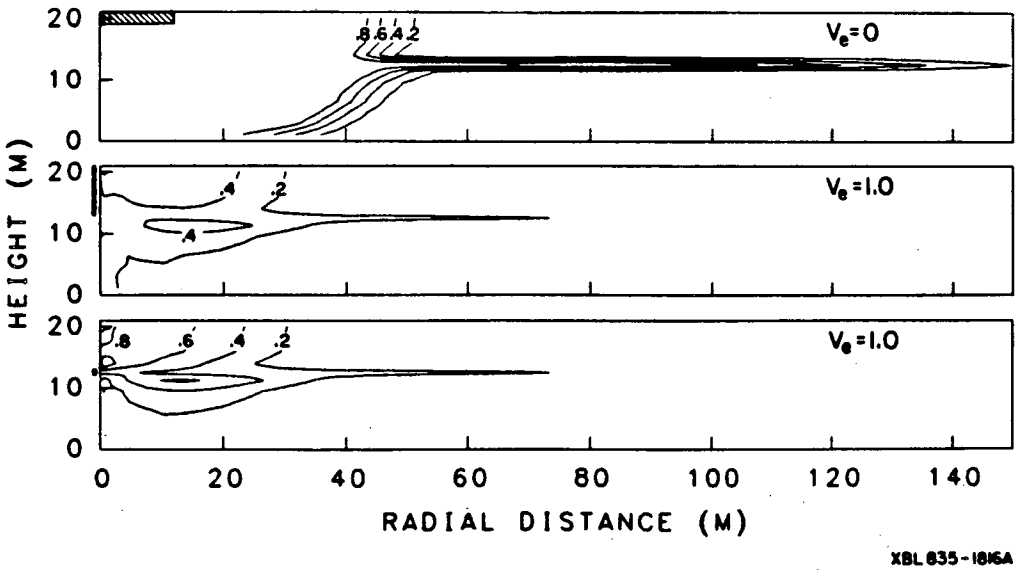

Figure 5. The top graph shows concentration contours after 1 year of contaminant infiltration into an aquifer with a horizontal fracture. The lower graphs show the contaminant contours after extraction (V_e = 1) for two different extraction well screen locations, one at the upper part of the aquifer and the other at the level of the fractured zone.

CONCLUSION

The interplay of the three effects, thermal, hydraulic and chemical results in a number of interesting processes. Some of these processes, such as buoyancy and convection, have been well studied. Many, especially those involving chemical precipitation, dissolution and transport, deserve further investigation. Three examples are discussed in this paper. The results may have an impact on the analysis and interpretation of field data. For the simulation and prediction of field behavior, an understanding of all relevant coupled processes is essential.

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