ENVIRONMENTAL APPLICATIONS OF ECLIPSE - A MULTIPHASE FLOW SIMULATOR USED IN THE OIL AND GAS INDUSTRY

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ABSTRACT

The assessment and cleanup of sites contaminated with immiscible organic liquids and vapors may require simulation of multiphase flow. Current environmental modeling codes, however, suffer numerical difficulties in dealing with multiphase systems. These difficulties have been overcome by petroleum reservoir simulation codes during many years of commercial applications. This paper demonstrates the advantages of using ECLIPSE -- a petroleum reservoir simulation code -- to solve environmental problems.

INTRODUCTION

Groundwater and contaminant transport simulators are routinely used in environmental site assessment and remedial feasibility studies. Unfortunately, the existing models are limited in their capabilities to address some important environmental issues, especially in the field of multiphase flow systems.

For example, several models have been developed to simulate SVE (Soil Vapor Extraction)systems for removal of VOCs (Volatile Organic Compounds). Unfortunately, these models maybe inadequate in many practical applications because they do not consider mass transfer, and/or the effects of subsurface heterogeneities (1). In an SVE, gas flow is affected by the VOC free-product residual saturation, which varies as the mass transfer between phases proceeds. The rate of mass transfer, in turn, depends on the gas flow field. The problem can be even more complicated when considering the heterogeneous nature of the site. Stratified soils and non-uniform distribution of hydraulic properties in the soil material may generate finger-shaped contaminant plumes, and the flow field cannot be described by simple homogeneous models. Hence, the cost-effective design of an SVE system may require coupled, heterogeneous models.

Mercer (2) has pointed out that because sophisticated multiphase simulators are not presently ready for full-scale commercial operations, environmental modelers should explore the possibilities of using petroleum reservoir simulators for contaminant problems involving organic liquids and vapors. Numerical simulation was used in petroleum reservoir engineering at least a decade earlier than in environmental investigations. Over the years, model developers have made great strides in improving numerical schemes, computation efficiencies, and accuracy. We believe the experience of the oil and gas industry in modeling subsurface flow of complex, multiphase fluids can be directly applied to guide environmental cleanups.

In this paper, we demonstrate the environmental applications of ECLIPSE, a robust and field-tested numerical code developed originally for petroleum reservoir engineering simulation. Two examples are presented. First, ECLIPSE is used to model the effectiveness of SVE for removal of volatile DNAPLs (Dense Non-Aqueous Phase Liquids) in heterogeneous soils. In the second example, we use ECLIPSE to model the effectiveness and optimal placement of an interceptor ditch for removal of LNAPLs (Light Non-Aqueous Phase Liquids) in shallow groundwater systems.

THE ECLIPSE SOFTWARE PACKAGE

ECLIPSE was developed by Intera Information Technologies, Inc. in Abingdon, United Kingdom. It was developed primarily to simulate the flow of hydrocarbon fluids in porous media.The software can also be used to solve other engineering problems including petroleum production, gas recovery from coal seams, environmental assessment and remediation. ECLIPSE is the most widely used reservoir simulator in the petroleum industry. The reliability of the program has been tested through many years of commercial applications and results have been verified by actual field observations. The capabilities of ECLIPSE are constantly being enhanced and updated.

ECLIPSE simulates the simultaneous transport of water, gas, and organic phases in one-, two-, or three-dimensions. Local equilibrium, or a fixed rate, may be assumed to control mass transfer among the phases. The transport of organic vapor by advection and molecular diffusion can be simulated using ECLIPSE. ECLIPSE multiphase features include user initialization, capillary-gravity initialization (by which a capillary transition zone can be created), saturation function hysteresis, saturation end-point scaling, and surfactant flooding. With the Environmental Tracer Option, a user can model the fate of 50 different components either dissolved in water, or anorganic phase, or mixed with soil gases, and migrating by advection and diffusion, with attenuation by adsorption and biological or radioactive decay. The well-simulation capabilities in ECLIPSE include extraction and injection, operating under a fixed pressure or at a constant rate.Wells can be vertical, deviated, or horizontal. Operational cycles can be specified as well as other operational parameters.

ECLIPSE can model complex subsurface systems, such as dual-porosity and dual-permeability systems, with advanced technologies such as corner point geometry and non-neighbor connections. ECLIPSE 200 includes options such as local-grid refinement/coarsening and flux boundary conditions. ECLIPSE 300 is a compositional simulator with a choice of equations of state for a hydrocarbon mixture containing up to 50 components. ECLIPSE uses a free-format input data file. Pre- and post- processors provide a flexible user interface and interactive subsurface mapping capabilities, grid design, and analysis of results. ECLIPSE provides its users with the flexibility to control simulations using adjustable time-steps, tolerances, and iteration limits.

ECLIPSE uses fully-implicit technology to provide stability over long time steps. Care is taken to ensure that the non-linear, fully-implicit equations are solved precisely by reducing all residuals to very fine tolerances. Material balance errors (residue sums) are extremely small. Newton's method is used to solve the non-linear equations. The Jacobian matrix is fully expanded in all variables to ensure quadratic (fast) convergence. Various special methods are used to accelerate convergence in highly non-linear problems. The linear equations arising at each Newton iteration are solved simultaneously by nested factorization accelerated by Orthomin (3).

EXAMPLES

ECLIPSE's capabilities in environmental applications are demonstrated below using two examples based on the results of recent investigations (4,5). The studies involve multiphase problems that occur in many sites contaminated with organic liquids. In both examples, the fluids modeled include water, air, and NAPLs. The Stone type function (6) is used for the relative permeability of the NAPL phase in the water-air-NAPL system. A model described by Parker et al. (7) is adopted for water-air and water-NAPL capillary pressures as function of water saturation. In both studies,the adsorption and dissolution of NAPL into water are neglected. Isothermal conditions are assumed in both examples.

Example 1. Simulation of SVE for Removing VOCs in Heterogeneous Soils

An SVE system can enhance the mass transfer of organic contaminants to the vapor phase by injecting clean air and extracting the gas phase mixed with organic vapor from the soil. The contaminant in this example is assumed to be TCE (trichloroethylene), which is a volatile DNAPL(TCE has density 1462 [kg/m^3], vapor pressure 0.07196 [bar], and viscosity 0.59×10^{-3} [Pa-s]).

The effects of the stratified soil is studied using a two-dimensional model. A soil profile is chosen to resemble the main features of a contaminated area at the Savannah River Site, South Carolina. The soil in the model contains sands, clay lenses, clayey sands, and a steady-state water table as shown in Fig. 1. The hydraulic properties are listed in Table I (8). The top surface and right-hand side of the cross section are constant pressure boundaries. The bottom is a no-flow boundary. The left-hand side is a no-flow boundary because a symmetrical half domain is assumed. TCE is assumed to leak into the soil from a surface line source orientated normal to the soil cross section (Fig. 1) at a rate of one barrel per month (30 days) per meter. After continuous leakage and infiltration for ten years, a preliminary SVE plan is applied to the site using the TCE saturation and gaseous concentration plumes from the simulation results as a guide. Then, the operation of the SVE is simulated. Based on the simulation results, such as plume reduction, total contaminant removal and removal rate of each well, the SVE model is modified in terms of well locations, pressures, rates, and restart period. This is continued until an optimal SVE plan is approached. The gas injection rate in the example varies from 10 to 20 liters per second. The ratio of extraction pressure to ambient pressure varies from 0.93 to 0.95.

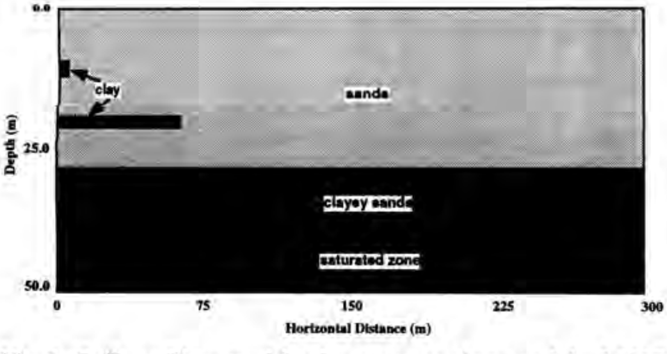


Fig. 1. Soil profiles used in the cross-section model of SVE studies.

TABLE I
Hydraulic Properties of the Soil

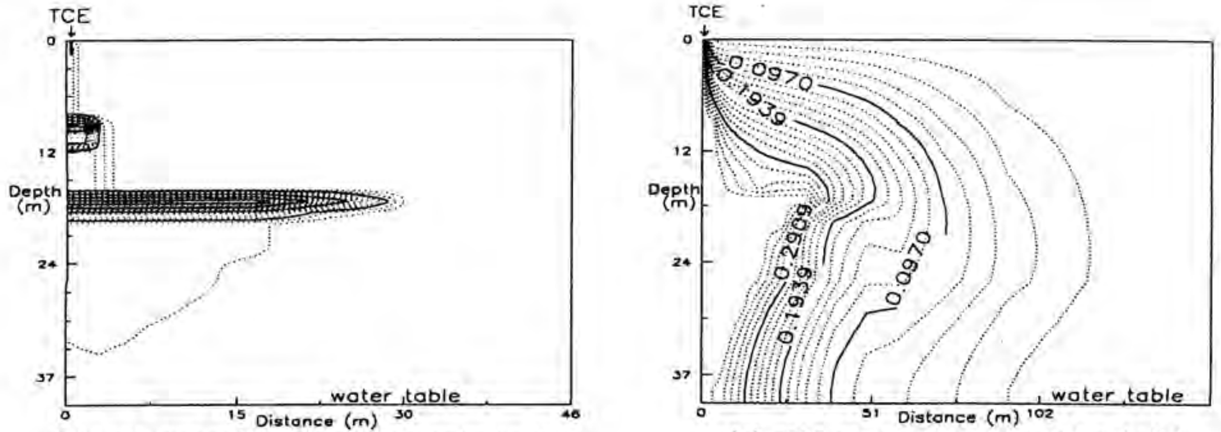
	Sands	Clayey Sands	Clay
Permeability [m^2]	10-11	10-12	10-15
Porosity	0.35	0.35	0.5
Irreducible water saturation	0.15	0.6	0.6
Irreducible gas saturation	0.001	0.001	0.001
Irreducible NAPL saturation	0.05	0.05	0.05

Figures 2(a) and 2(b) depict the TCE free-product saturation and gaseous concentration distributions after a ten-year period of release and infiltration, and prior to the application of SVE.Due to the clay lenses below the TCE source, the TCE free-product does not reach the water table at ten years. The extent of the vapor plume, however, reaches the water table and is much greater than that of the free-product plume. Figures 2(c) and 2(e) show the TCE free-product plumes at 110 and 600 days after the operation of an SVE system. Figures 2(d) and 2(f) indicate the TCE gaseous concentration plumes at 110 and 600 days.

About 30 SVE plans have been simulated for a period of 600 days. The plans vary in terms of well locations, operating pressures and rates, and operating cycles for each well. The effectiveness of a plan is measured as the total TCE removal as a function of the number of pore volumes of injected air. Figure 3 shows the effectiveness for a typical plan. From this study, we found that in stratified soils, the location of less-permeable clay lenses and clayey sand layers controls the distribution of the VOC sources, and ultimately determines the performance of the SVE system.

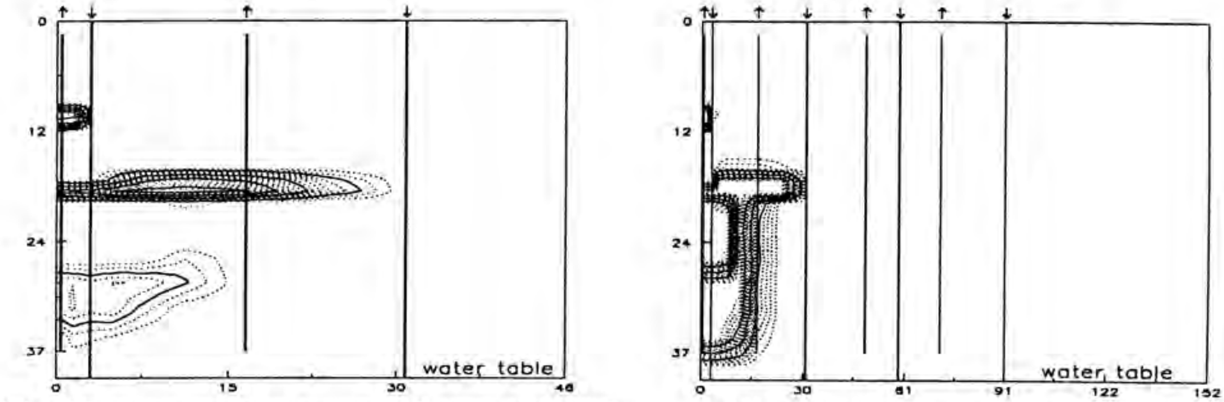
The effect of heterogeneous permeability distribution in the soil column is illustrated using a three dimensional model. The modeling area is 60 m x 60 m and the depth is 15 m. An optimized SVE plan is simulated for 60 days. One homogeneous and eleven heterogeneous distributions of permeability are simulated for the SVE. The heterogeneous distribution of permeability is generated using a random field generator (9). The variance of the log-normal distribution is unity and theme an permeability is equal to that for the homogeneous case, with the permeability assumed equal to that for the sand layer (Table I). The TCE removal at different realizations of random permeability distribution is shown in Fig.4. As can be seen, the modeling approach based on an equivalent homogeneous permeability tends to overestimate the effectiveness of the SVE system, and the range of uncertainty caused by this simplified approach may be large.

In summary, soil heterogeneity can exert a dominant control on the effectiveness of the SVE system. These results are discussed in detail by Zhou et al. (4).



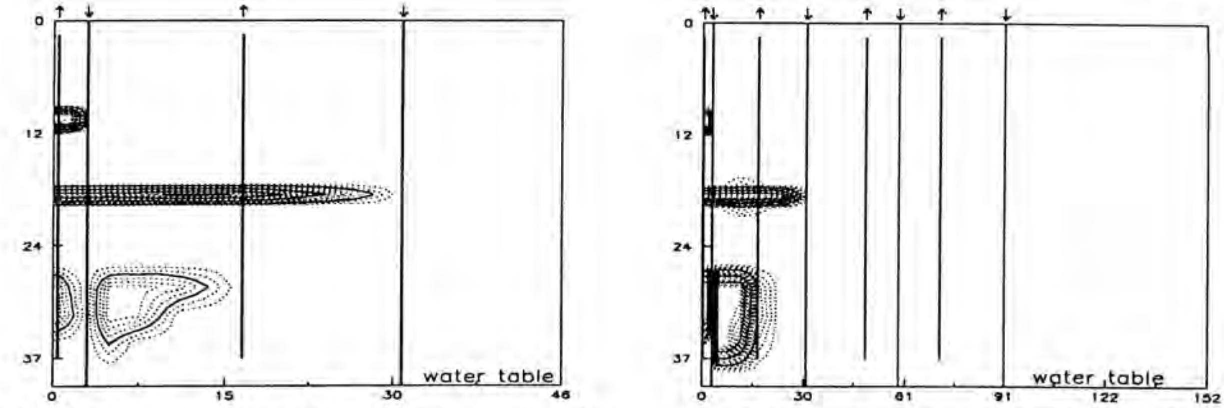
(a). TCE saturation distribution prior to SVE.

(b). TCE gaseous concentration (g/L) distribution prior to SVE.



(c). TCE saturation distribution 110 days after SVE.

(d). TCE gaseous concentration (g/L) distribution 110 days after SVE.



(e). TCE saturation distribution 600 days after SVE.

(f). TCE gaseous concentration (g/L) distribution 600 days after SVE.

Fig. 2. TCE plumes prior to and after SVE. In regions bounded by the concentration contours, the concentration decreases from center outward. Up arrows indicate extraction wells and down arrows show injection wells. Note the horizontal scales for (a), (c), and (e) are different from those for (b), (d), and (f).

Example 2. Simulating Optimal Placement of Interceptor Ditches for Removal of LNAPL in Shallow Groundwater

The concept of an interceptor ditch is derived from agricultural applications, where drainage ditches are used to remove groundwater. Recently, the concept has been extended to remediate groundwater pollution because it is simple and reliable (10,11). Such applications normally involve sites where the contaminants are dissolved in groundwater. However, interceptor ditches have also been used recently to remove LNAPLs. The effectiveness of LNAPL removal by this method has not been studied due to the complex nature of multiphase flow systems.

An LNAPL will migrate vertically in the vadose zone, and then laterally when it reaches the water table. The LNAPL

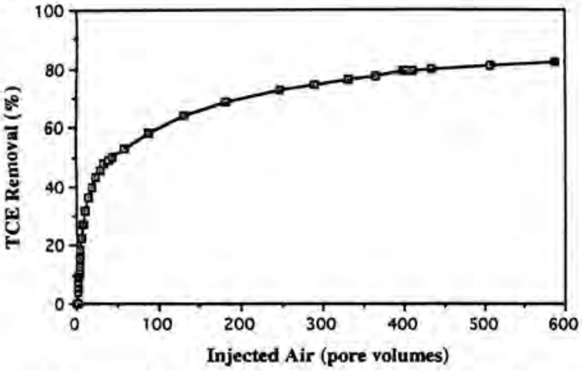


Fig. 3. TCE removal vs. number of pore volumes of injected clean air.

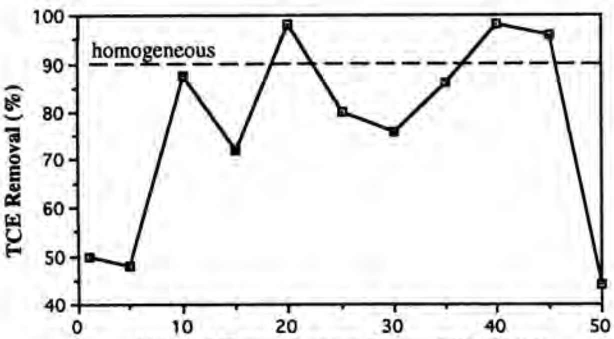


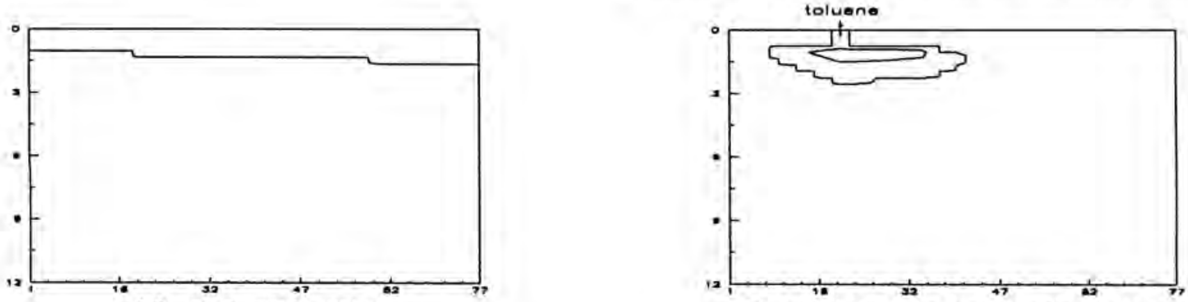
Fig. 4. TCE removal vs. realization numbers of heterogeneous permeability distribution.

plume then flows in response to the water table gradient. Figure 5 shows the scenario of LNAPL migration in a shallow groundwater, as simulated using ECLIPSE. It can be seen that LNAPL spreads laterally under the hydrostatic pressure and flows downstream under the gradient of water table. The figure also shows that due to the invasion of LNAPL, the water table is distorted.

Interceptor ditches create a hydraulic barrier, preventing the spread of contaminants further downstream. Figure 6 shows the groundwater flux distribution under the influence of a ditch, as simulated using ECLIPSE. As can be seen, a streamline exists which divides the flow field into two parts. One part involves flow into the ditch and the other part involves flow without interception by the ditch. To achieve complete LNAPL removal, the contaminant plume must be bounded by the dividing streamline.

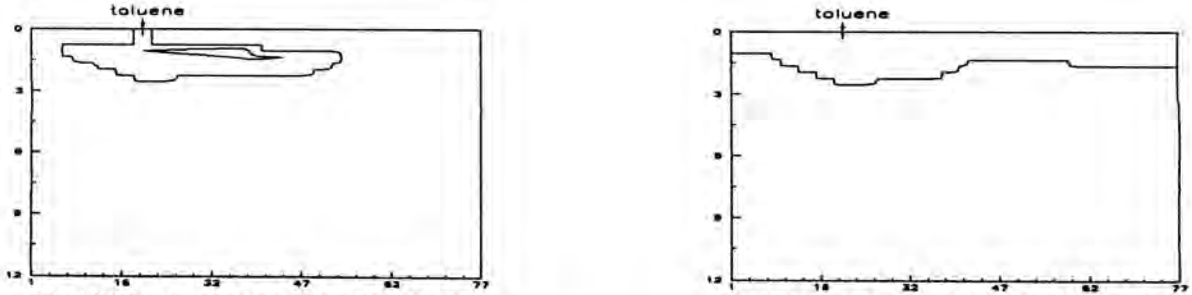
The modeling domain is a two-dimensional cross section with 80 meters horizontal length. The depth varies from 20 to 60 meters depending on the assumed water table gradient. The choice of depth is made to create a thick aquifer so that the dividing streamline can be simulated. The water table is 1.2 meters below the land surface and the aquifer is unconfined. The LNAPL in this case is toluene (density 881 [kg/m^3]; viscosity 6 x 10^{-4} [Pa-s]).

We first establish a steady state water table with a specified gradient. The hydraulic conductivity used in this model is 43.3 meter/day and the ratio of vertical to horizontal hydraulic conductivities is 1/2. Then, toluene is released from a source at the land surface and the migration of toluene is simulated. At certain times after release, the source stops and an interceptor ditch is placed at the downstream edge of the plume. The removal of both toluene and groundwater by the ditch is simulated. The effectiveness factor of the ditch, defined as the



(a). Initial water table.

(b). LNAPL plume one year after release.



(c). LNAPL plume two years after release.

(d). Water table one year after LNAPL release.

Fig. 5. Scenario of LNAPL release and migration in shallow groundwater simulated by ECLIPSE.

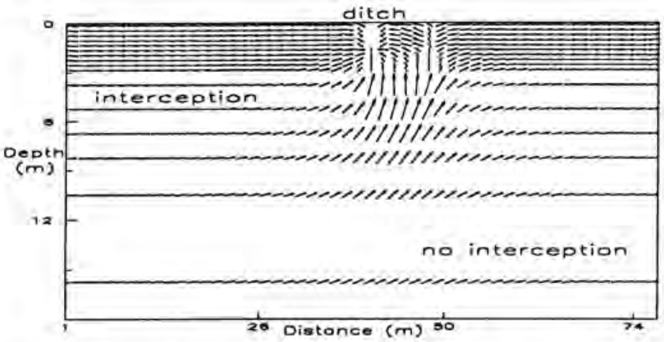


Fig. 6. Groundwater flux distribution. Demonstration of dividing streamline created by the interceptor ditch.

ratio of total removed LNAPL and discharged water, can then be calculated. We studied the ditch effectiveness factors for water-table gradients ranging from 0.0008 to 0.008,surface infiltration rates from 0 to 380 mm/year, and head differences from 0.03 to 0.3 meters. The head difference is defined here as the difference of ditch head and the initial average water table head (Fig. 7). The impact of heterogeneous distribution of hydraulic conductivity and NAPL irreducible saturation were also studied (12).

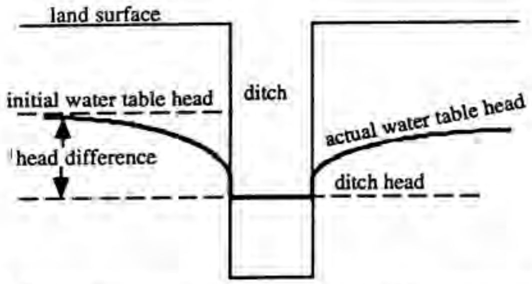


Fig. 7. Definition of head difference of interceptor ditches.

From this study, we found that the optimal placement of the ditch for removing LNAPL is such that the head difference creates a dividing streamline just deep enough to enclose the LNAPL plume. Further increasing the head difference results in substantial increases in groundwater removal but not removal of LNAPL. The total LNAPL removal is controlled by the irreducible LNAPL saturation. These effects can only be studied using multiphase simulators.

CONCLUDING COMMENTS

These studies demonstrate that the ECLIPSE simulator originally developed for petroleum engineering can be successfully applied to multiphase environmental fate and transport modeling. With highly efficient and robust solution techniques and numerous advanced capabilities, the ECLIPSE code can be a valuable and cost-effective tool in assessing the performance of soil and groundwater remedial systems under complex site conditions. To better serve environmental scientists, an environmental version of ECLIPSE is being planned.

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