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ADVANCED CHEMISTRY BASINS MODEL SEMI-ANNUAL TECHNICAL REPORT

- Covering the period from June 2, 2002 – November 10, 2002
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ABSTRACT

The DOE-funded Advanced Chemistry Basin model project is intended to develop a public domain, user-friendly basin modeling software under PC or low end workstation environment that predicts hydrocarbon generation, expulsion, migration and chemistry. The main features of the software are that it will:

- afford users the most flexible way to choose or enter kinetic parameters for different maturity indicators;
- afford users the most flexible way to choose or enter compositional kinetic parameters to predict hydrocarbon composition (e.g., gas/oil ratio (GOR), wax content, API gravity, etc.) at different kerogen maturities,
- calculate the chemistry, fluxes and physical properties of all hydrocarbon phases (gas, liquid and solid) along the primary and secondary migration pathways of the basin and predict the location and intensity of phase fractionation, mixing, gas washing, etc., and,
- predict the location and intensity of de-asphaltene processes.

The project has be operative for 36 months, and is on schedule for a successful completion at the end of FY 2003.

EXECUTIVE SUMMARY

The advanced Chemistry Basin Model project has been operative for 36 months. During this period, about half the project tasks are on projected schedule. On average the project is somewhat behind schedule (85%). Unanticipated issues are causing model integration to take longer then scheduled, delaying final debugging and manual development. It is anticipated that a short extension will be required to fulfill all contract obligations.

MILESTONE SCHEDULE/STATUS

The only milestone listed in the project is to have a prototype model operational on a workstation. That milestone was reached during the 2nd project year. The project is set to end in June, 2003.

TASK 1: MATURITY INDICATORS

Primary Responsibility	*Current Subtasks*	*Investigator*
Caltech	Develop algorithms	Tang

Summary

The first task is to "Develop a database of additional and better maturity indicators for paleo-heat flow calibration". Fundamental to this development is to perform a series of controlled kinetic experiments on maturity indicator evolution. The goals for the third task year were:

R0 suppression
Study the vitrinite reflectance suppression.

Compare thermal indicators
Compare different thermal indicators and test them under geological conditions.

Finish R0 Database
Establish the complete database for worldwide vitrinite reflectance kinetics.

The goal for the fourth task year is:

Integration

Integrate all the thermal maturity indicators into basin modeling database. Continue to test the validity of each indicator under geological conditions. Deploy user graphic interface for the final deployment

Performance

Integration of the thermal maturity indicators into the basin model is nearly complete.

TASK 2: COMPOSITIONAL MATURATION

Primary Responsibility	*Subtask*	*Investigator*
Caltech	Establish a reaction network	Tang

Summary

The second task is to "Develop maturation models capable of predicting the chemical composition of hydrocarbons produced by a specific kerogen as a function of maturity, heating rate, etc.; assemble a compositional kinetic database of representative kerogens." For the third year, the task list is:

Expand Reaction Network
Add additional generation models with kinetic parameters describing the breakdown of a typical range of kerogens. Analyze additional pyrolysis experiments to derive the needed parameters.

Verify the reaction network
Verify the reaction network and kinetic modeling by extrapolating to geologic conditions

Performance

Recently completed extrapolation work has shown that there might be some problems within the reaction network developed previously (see reports from 4th quarter 2001 and 2nd quarter 2002). Specifically, extrapolation of results to geological data shows somewhat unrealistic behavior within the secondary cracking kinetics. This unforeseen difficulty has set the project further behind as a reexamination of the experimental data needs to be undertaken. An additional reaction network for type II kerogen has been completed, and is yielding more accurate results, though it needs to be compared to field data. Additional work is ongoing to improve the Green River shale (type I) kerogen reaction network.

Remaining Work

The remaining reaction networks have to be completed and integrated into the model.

TASK 3: EQUATION OF STATE FLASH CALCULATION

Primary Responsibility	*Subtask*	*Investigator*
Caltech	EOS model	Meulbroek

Summary

The third task of the project is to "Develop a 4 phase equation of state-flash model that can define the physical properties (viscosity, density, etc.) of the products of kerogen maturation, and phase transitions that occur along secondary migration pathways."

The tasks for the fourth year include

Integrate

Integrate final viscosity model and 4-phase thermodynamic model into software

Test

Test system on one or two basins.

Display

Working with others, devise suitable methods to graphically display results.

Progress

An ongoing effort to define appropriate oil component classes has yielded a suitable initial composition and a procedure to take existing fluid measurements and use them within the model. The initial composition is derived from mapping a PVT report composition (available for most oil reservoirs) into the reaction network defined under task 2.

New efforts include the implementation of a PRKS[1] equation of state to more accurately predict multi-phase behavior. Though such models were not developed at the time of the proposal submission, a predictive model allows the user to estimate phase behavior of unique mixtures without empirical tuning parameters. Plans for this model include developing and improving asphaltene predictions, and improving water-oil phase behavior. Though very useful to the project, this unanticipated direction has caused this task to fall somewhat behind schedule. Of the three points above, testing remains, and is anticipated to require 6-9 months.

Remaining Work

- The physical connections between the basin model and the EOS have been completed (see below). However, testing in a real problem is not yet finished.

[1] Predictive Relich-Kwong-Soave model.

- The EOS / Flash model has to incorporate the models produced under Tasks 5 (primary migration). Specifically, asphaltene precipitation models have to be linked.

TASK 4: CONVENTIONAL BASIN MODELING

Primary Responsibility	*Subtask*	*Investigator*
Cornell	2-D model	Cathles
Cornell	add maturity indicators	Cathles

Summary: The fourth task of the project is to "Build a conventional basin model and incorporate new maturity indicators and data bases in a user-friendly way". The fourth year projects include:

- Test code
- Incorporate additional kinetic data bases
- Write Manuals

Performance

Code testing is an on-going process with the model. A final delivery set specification is being developed based on the results of the scientific work of the project, and will be ready early next calendar year. Manuals will be developed based on this specification.

TASK 5: PRIMARY MIGRATION

Primary Responsibility	*Subtask*	*Investigator*
Cornell	2-D model	Cathles
Cornell	Prototype algorithm	Cathles

Summary

The fifth task of the project is to "Develop an algorithm which combines the volume change and viscosities of the compositional maturation model to predict the chemistry of the hydrocarbons that will be expelled from the kerogen to the secondary migration pathways."

Chemical Feedback _ Flow
Establish any necessary feedback from chemical to finite difference flow model.

Performance

A prototype primary migration model was build as "scratchpad" in the PC prototype DOE Basin Model early in the project. Independently, Yuling Zhang has been working on a C++ version that is integrated to maturation models and the EOS code (for properties such as viscosity). Asphaltene precipitation will be incorporated in this code based on a colloid precipitation model.

The primary migration model has yet not been integrated with secondary migration in the PC model. However, incorporation has been included in the code architecture. Plans are to abstract "capacitor-chemical filter" parameters from the scratchpad calculator and modify the timing and chemistry of hydrocarbon delivery to the secondary migration algorithm.

Remaining Work

- Integrate capillary model with EOS physical property models.
- Add asphaltene precipitation.
- Adapt best available rock property model from Revil's work.
- Abstract simple capacitor (hydrocarbon expulsion delay) and chemical filter parameters.
- Build delay-filter model into PC code.

TASK 6: SECONDARY MIGRATION

Primary Responsibility	*Subtask*	*Investigator*
Cornell	Develop prototype	Cathles

Summary

The sixth task of the project is to "Develop an algorithm that predicts the flow of hydrocarbons along secondary migration pathways, accounts for mixing of miscible hydrocarbon components along the pathway, and calculates the phase fractionation that will occur as the hydrocarbons move upward down the geothermal and fluid pressure gradients in the basin."

Test simulations
Carry out test simulations to refine chemical methods and debug.

Performance

A prototype has been completed and tested of secondary migration both on the PC and on our workstations. The PC version has been tested only for vertical flow, but the workstation version has been tested for 2D and 2D flow (into faults, through holes in salt, etc.). The model implements a two-pass algorithm: it first matures the solid hydrocarbon phases, and then migrates and matures the mobile hydrocarbon phases. Solid precipitation from the mobile phases is allowed and accounted for

in mass balance calculations. Mass balance on all hydrocarbon phases in 100% accurate. Application has been made in offshore Louisiana, and interesting publishable results obtained.

Hydrocarbon phase separation (flashing) to oil and gas has not yet been tested, however we have successfully integrated EOS code and flash capabilities into the PC prototype. Flash calculations and gas washing will be modeled as a third pass. Volume changes associated with phase separation will propel gas at greater velocities than oil, and the relative motion will "wash" the oil chemically.

A critical need for testing and evaluation is to incorporate the kinetic databases for the various kerogen classes as soon as possible.

Remaining Work

- Implement non-vertical flow on PC prototype.
- Add flash calculations and gas washing.
- Incorporate database for kerogen maturation (5 kerogens from each of 3 kerogen classes).
- Write manual.

TASK 7: INTEGRATION ON PC

Primary Responsibility	*Subtask*	*Investigator*
Geogroup	Connect external code	Manhardt

Summary

The final task for the project is to "Integrate the above components into a functional model implemented on a PC or low cost workstation."

- Complete transfer from workstation to PC environment
- Establish umbrella shell.

Performance

Prototype is completed, but not all parts are present.

Remaining Work

- Simplify the models and the interface.

- Spin off installable code that can be delivered to the public domain.
- Write manuals of software operation.

This task is somewhat behind schedule. We are aiming at delivering a compiled code, with source code available upon request. Because of the DLL integration, only compiled code can be made available over the net. Given the tight schedules for the other tasks, and the limited personnel funded for this project, this task should be considered very tight.

CONCLUSION

The overall project is producing good results, but is slightly falling behind in finishing scheduled tasks. In particular, final integration tasks are taking longer than scheduled, cutting into time budgeted for final debugging, case analysis, and manual development. It is probable that a short extension will be required to fulfill all contractual obligations.