ADVANCED CHEMISTRY BASINS MODEL TECHNICAL REPORT

- Covering the period from December 1, 2002 – June 1, 2003
- Compiled by Peter Meulbroek
- Sections written by Mario Blanco, Lawrence Cathles, Paul Manhardt, Peter Meulbroek, and Yongchun Tang.
- Issued May, 20004

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

EXECUTIVE SUMMARY

The advanced Chemistry Basin Model project has been operative for 48 months. During this period, about half the project tasks are on projected schedule. On average the project is somewhat behind schedule (90%). Unanticipated issues are causing model integration to take longer than 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

<i>Primary Responsibility</i>	<i>Current Subtasks</i>	<i>Investigator</i>
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 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

<i>Primary Responsibility</i>	<i>Subtask</i>	<i>Investigator</i>
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 fourth year, the task list is:

Add all maturation model parameters to data base and fully integrate into basin modeling software

Performance

Most of the problems reported in the last summary report have been reconciled, and integration into the basin model is nearly complete.

Remaining Work

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

TASK 3: EQUATION OF STATE FLASH CALCULATION

<i>Primary Responsibility</i>	<i>Subtask</i>	<i>Investigator</i>
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

A completed EOS model has been delivered both in stand-alone form (see <http://ruby.wag.caltech.edu>), and as an integral part of the basin model. Testing of the connection has been 90% completed.

Remaining Work

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

TASK 4: CONVENTIONAL BASIN MODELING

<i>Primary Responsibility</i>	<i>Subtask</i>	<i>Investigator</i>
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 by mid-summer. Manuals will be developed based on this specification.

TASK 5: PRIMARY MIGRATION

<i>Primary Responsibility</i>	<i>Subtask</i>	<i>Investigator</i>
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. In a major disappointment, the proposed delivery scheme for Asphaltene precipitation has been delayed due to the departure of a supported student.

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

<i>Primary Responsibility</i>	<i>Subtask</i>	<i>Investigator</i>
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 is 100% accurate. Application has been made in offshore Louisiana, and interesting publishable results obtained.

Hydrocarbon phase separation (flashing) to oil and gas has now been tested, with encouraging results. 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

- Incorporate database for kerogen maturation (5 kerogens from each of 3 kerogen classes).
- Write manual.

TASK 7: INTEGRATION ON PC

<i>Primary Responsibility</i>	<i>Subtask</i>	<i>Investigator</i>
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. A major effort towards moving the model to an distributable state continues to be made, with an expected conclusion at the end of the summer.

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 now certain that a short extension will be required to fulfill all contractual obligations.