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Model Capabilities for In-Situ Oil Shale Recovery

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ABSTRACT

The extensive oil shale reserves of the United States are now under development as an energy source. One of the approaches for extracting oil from shale is the so called modified in-situ retort. The operation of such retorts for maximum yield requires an understanding of oil loss mechanisms so that operating strategies that minimize these losses can be developed. The present modeling capabilities for describing the behavior and yield from a modified in-situ retort are discussed. It is shown how the advances made in describing retort chemistry have greatly increased the predictive capabilities of these models. Two models that have been subject to comparison with laboratory retorts are described. The first is a one-dimensional model that treats the retort as a packed bed reactor, the second is a quasi-two-dimensional examination of block retorting. Both models are capable of predicting retorting rates, off gas composition and oil yield losses to coking and combustion. The block model, for example, describes conditions where local oil yield losses can be as high as 50%. Areas for further model improvement include additional work on describing retort chemistry, such as the steam/char and gas phase combustion reactions. The major need for modeling now is expansion to multi-dimensional simulation. This is necessary if a predictive capability is to be developed for field situations where sweep efficiency losses and gravitational effects become important.

INTRODUCTION

The oil shale reserves in the contiguous United States are very extensive. The resource has been estimated to be between three and seven trillion barrels of oil equivalent.¹ While much of this resource may not be recoverable, merely recovering 10 percent of the high grade resource (> 50 $\frac{\text{lb}}{\text{tonne}}$) in the Green River Formation of the western U. S. would support a two million barrel per day industry for 300 years. Obviously, a resource of this magnitude must and is being considered for development as an energy source for the late 1980's and beyond.

Basically oil shale is a marlstone rock containing a solid organic constituent known as kerogen. The amount of kerogen in the rock determines the shale grade: for example, in a shale with a grade of $100 \frac{\text{lb}}{\text{tonne}}$ (24 gal/ton) the kerogen will comprise about 14 percent by weight of the shale. Upon heating to temperatures on the order of 400°C the kerogen decomposes, yielding a synthetic crude oil and gaseous products and leaving behind a carbonaceous residue on the rock. This phenomena forms the essential element necessary for all oil shale processing schemes, i.e., heating the rock to sufficient temperatures to induce kerogen decomposition. In addition, many schemes, although not all, attempt to utilize the carbonaceous residue as a fuel.

The present methods being developed for extracting oil from shale can be roughly divided into the two areas of surface retorting and in-situ retorting. Surface processing schemes involve retorting the shale in a continuously moving packed bed reactor mode utilizing either direct or indirect combustion. Treatment of the shale in this manner involves significant efforts in mining, crushing and disposal of the spent shale. These operations have associated economic and environmental concerns. The in-situ schemes for processing shale are attempts to mitigate partially the environmental and economic problems of surface retorting by reducing the mining and disposal operations. True in-situ retorting is a concept with no mining, while modified in-situ (MIS) is an approach that involves partial mining or a near surface operation. The potential advantages of in-situ techniques may be offset by higher oil yield losses compared to surface retorting. The thrust of this paper is to describe current modeling capabilities for quantifying these loss mechanisms and for predicting in-situ retort operations. There is obviously an important role here for modeling because, if yield is to be increased, the loss mechanisms and the effect of potential control schemes on these mechanisms must be understood.

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HIGH YIELD SYSTEMS

The majority of present schemes for in-situ retorting, particularly MIS, attempt to replicate, in-situ, the conditions that give high yields in a surface retort. Thus in order to understand the modified in-situ problems one must start with an understanding of the features of a surface retort that lead to high yield. Figure 1 examines an idealized vertical,

Figure 1. Schematic of a High Yield Direct Combustion Retort Including Approximate Temperature and Concentration Profiles.

direct combustion surface retort. The figure points out a number of features that are necessary to obtain high yields from a retort. First, the flow through the system is uniform so that the full shale charge is swept, leaving no shale unretorted. This is the result of a uniform high porosity and results necessarily in a system that is one dimensional. Next, it is seen that there is no overlap in the oxygen and oil vapor concentration profiles, in other words, complete separation of the retorting and combustion fronts. Thus there is no loss of product oil by combustion. This requires efficient oxidation of the carbonaceous residue left on the shale by kerogen decomposition. This will occur when the shale particle sizes are small (< 0.10 m) with porosity sufficient to permit active flow over a large percentage of the particle surface area. Both conditions lead to the efficient gas-solid heat and mass transfer necessary for carbon utilization. The final condition necessary for efficient retorting is not depicted in Figure 1. This is the need to process the shale at sufficient heating rates to minimize oil losses to coking; as will be shown, this requires rates of $2^{\circ}\text{C}/\text{min}$ or greater.

These then, qualitatively, are the criteria necessary for obtaining high

yields from an oil shale direct combustion retort. The challenge for oil shale modeling is to quantify the retorting process so that the physical parameters in an in-situ operation necessary to best approach these efficient operating conditions can be determined.

RETORT CHEMISTRY

The first step in oil shale modeling, regardless of whether the application is surface or in-situ retorting, is an accurate description of the retort chemistry. Obviously, this is essential if product yields and heat and mass transfer within the retort are to be predicted. It is almost certainly the significant advances that have been made in the understanding of retort chemistry in the past five years that have resulted in the much improved modeling capability that now exists. Much of this work has been done at the Lawrence Livermore National Laboratory and has been reviewed by Campbell and Burnham.² For the purposes of this paper a detailed review of retort chemistry is not appropriate; however, to appreciate fully the numerical retort models a brief description of the important chemical kinetics and stoichiometry upon which the models are based is useful.

The first set of important reactions that occur when shale is processed are those associated with kerogen decomposition. Figures 2, 3, and 4 give examples of how the production from kerogen decomposition of oil, hydrogen, and methane can be described using present kinetic and stoichio-

Figure 2. Calculated Oil Production During Kerogen Decomposition for Three Heating Rates.

Figure 3. Calculated Hydrogen Production During Kerogen Decomposition for Three Heating Rates.

Figure 4. Calculated Methane Production During Kerogen Decomposition for Three Heating Rates.

metric models.^{2,3} As can be seen, the models are sufficiently detailed to account for differences in local heating rate and secondary decompositions that occur at higher temperatures. The higher production of hydrogen and methane seen at the lower heating rates is the result of increased oil degradation due to coking that occurs at lower heating rates. This points out that models are now sufficiently developed to describe quantitatively the important oil loss mechanism of coking. Using the kinetics and stoichiometry presented by LLNL, a relationship between oil loss to coking and heating rate during retorting can be calculated. Figure 5 shows the coking

loss-heating rate correlation as calculated from the LLNL kinetics.

In addition to the decomposition of organic material, another important group of decomposition reactions occurring during retorting are those relating to mineral matter. The two principle minerals of interest are dolomite ($\text{MgCa}(\text{CO}_3)_2$) and calcite (CaCO_3). The reaction of these minerals is important because they are significant sources of CO_2 and their decomposition is highly endothermic. Just as with organic decomposition, models have been developed to describe the behavior of dolomite and calcite in shale.^{2,3} Figure 6 summarizes the mineral decomposition models by showing the calculated CO_2 evolution rate as a function of temperature. The initial peak is the result of dolomite decomposition followed by the reactions of free calcite and calcite formed from dolomite with silica and finally by the decomposition of calcite itself.

In addition to the decomposition reactions, three additional important reactions involving the solid phase occur during retorting. Specifically, these are the heterogenous reaction of char (essentially carbon on the rock matrix) with the gases O_2 , CO_2 , and H_2O . The first of these, char oxidation, is important because it is exothermic and thus an important source of energy to drive the retort. The reaction is typically characterized by using a so-called shrinking core model. This model assumes that the reaction is essentially controlled by the diffusion of oxygen into the shale to the location of a discrete char boundary. There is considerable experimental evidence to support this formulation. A comparison of predictions using a shrinking core model with the results of an actual block retorting experiment will be discussed later in this paper.

The gasification of char with steam and carbon dioxide is important because these reactions generate the gases CO and H_2 which can increase the heating value of the produced gas or be burned within the retort instead of oil. There are kinetic expressions available to describe the char/ CO_2 reaction.^{2,4} This reaction is essentially only kinetically limited since CO_2 is present throughout the matrix whenever carbonate decomposition is occurring. The steam/char reaction is more complex being neither totally diffusion-controlled like oxidation or kinetically-controlled like the carbon dioxide reaction. There are, based on experiments with small particles, expres-

Figure 5. Calculated Oil Loss to Coking as a Function of Heating Rate.

Figure 6. Calculated CO_2 Production from Mineral Decomposition.

sions for the kinetics of this reaction, and some modeling work that combines the kinetic and diffusional limitations of this reaction has been done. This reaction in shale, however, has not been studied as thoroughly as, for example, the char oxidation reaction, and there is a need for additional work so that the extent of this important reaction can be confidently predicted when dealing with large shale particles, particularly when steam is used in the inlet gas stream.

The important reactions occurring within the gas stream in an oil shale

retort include the water-gas shift reaction and the combustion of CO , CH_4 , CH_x , H_2 , and oil.

The water-gas shift reaction, while not significant from an overall energy standpoint, to a large extent determines the final off-gas composition. The reaction is believed to be strongly catalyzed by the presence of oil shale. However, little is known about the actual kinetics in the presence of shale. The reaction is typically handled in the models by assuming a temperature below which the reaction does not occur, but above which compositions are set to the equilibrium compositions. Figure 7 shows the effect, for typical in-situ retort conditions,* that the assumed equilibrium temperature for the shift reaction has upon the final CO_2 , H_2 , and CO compositions. Improved knowledge of the kinetics of this reaction will allow models to predict more accurately the final gas composition but will probably not affect major conclusions reached as to resource recovery.

The gas phase combustion reactions mentioned above are an area where there is very little kinetic information directly applicable to shale retorting. There is, of course, extensive information about these combustion reactions in simpler mixtures. However, for the complex mixtures present in retorting, little is known about important parameters such as flammability limits and ignition temperatures. Present models typically

*For a retort operated with air only.

Figure 7. Effect of the Assumed Water/Gas Shift Reaction Temperature on the Final Gas Composition.

treat these reactions as occurring extremely rapidly once certain temperature levels are reached. This may be an appropriate treatment, but work is needed to verify this approach for describing actual retort conditions. It should be mentioned that one of these reactions, the combustion of oil, is the dominate product loss mechanism in in-situ retorting; thus, the obvious need to describe it accurately.

ONE-DIMENSIONAL RUBBLE MODELS

With a description of the retort chemistry available, numerical and to a limited degree analytical models describing the retort process can be constructed. The majority of models to date have examined the geometry of a vertical column of packed oil shale particles. This geometry simulates vertical surface retorts and to a certain extent vertical modified in-situ retorts. There have been a number of models which address this geometry including ones by Dockter,⁶ Nuttall,⁷ Braun,⁵ and George.⁸ Of these efforts the work by Braun at LLNL has been the most thoroughly documented and utilized for examining a variety of retorting questions. A discussion of this model fairly well summarizes the present one-dimensional model capabilities. This model includes the following physical phenomena: axial convection of heat and mass in the gas stream; axial heat conduction in the solid phase; and heat trans-

fer at the gas-solid interface. It relies upon a quasi-steady state approximation for the gas stream energy equation. This is appropriate in most oil shale modeling situations where the temperature is dominated by interaction with the solid (where the majority of the system energy is stored). The gas flow is assumed to be simple plug flow. In order to simulate more appropriately actual retorts (particularly in-situ) the model includes the capability for up to five different particle sizes. The individual particles are treated as spherical. The chemical reactions considered in the model are basically those discussed in the previous section.

The primary outputs from the model are gas and solid temperatures as a function of time and location, and the local gas stream composition of the species N_2 , O_2 , CO , CO_2 , H_2 , CH_4 , CH_x , H_2O , and oil. The rather complete treatment of the chemistry contained in this model allows it to address a variety of retort phenomena that relate to the effects of retort chemistry on yield. This model has been compared with numerous laboratory retort runs. The results have been quite good with typical agreement better than 10 percent for such quantities as the retorting rate, oil yield, off-gas composition, carbonate decomposition and char combustion. Figure 8 (from Braun) shows typical agreement between calculated and measured temperature distributions within a retort. It should be mentioned that the laboratory runs used to verify the model typically operated with conditions that resulted in recoveries greater than 85 percent of Fischer Assay. Thus while the model can and is being used to address situations

Figure 8. Comparison of Measured and Calculated Gas Phase Temperatures for Laboratory Retort (from Braun Ref. 5).

where the yield is expected to be less than 80 percent,⁹ there is as of yet no good laboratory data for comparison at low yield conditions. Low yield conditions typically imply an increase in oil combustion. Under conditions where a significant amount of oil combustion is beginning to occur, the model tends to give poorer agreement with the measured oil yield and gas compositions (particularly CO and H₂). This points out one area of weakness, alluded to earlier, in the present understanding of retort chemistry, i.e., in the treatment of gas phase oxidation reactions and the water-gas shift reaction. While in homogeneous systems without catalysts these reactions can be handled individually, in a real system where all the species are present at once the lack of any real kinetic information makes the calculation semi-quantitative at best. These uncertainties are aggravated in low yield situations where there is an increase in gas phase combustion. This situation is not likely to change until there is more fundamental information about these reactions in complex systems.

As mentioned, the strength of the Braun model is its detailed treatment of the retort chemistry. An example of this is shown in Figure 9 (from Braun) which plots oil yield versus the percent of steam in the injected gas. This particular calculation utilized a shale bed designed to simulate a modified in-situ retort. In particular, the bed porosity was 20% with the shale particles distributed as 60 wt

Figure 9. Effect of Air-Steam Inlet Gas Composition (Total Inlet Flow Rate of 0.64 mol/m²·s) on Oil Yield (From Braun, Ref. 5).

percent 14.6 cm diameter, 24 wt percent 57.4 cm and 16 wt percent 124.4 cm. The increased yield obtained with increasing steam is the result of the combustion of CO and H₂ (produced by the steam/char reaction) instead of oil, and a reduction in the amount of endothermic mineral decomposition. This type of effect could only be predicted by a model containing a detailed description of the retort chemistry.

Figure 9 points out that the one-dimensional modeling is sufficiently accurate to quantify oil loss mechanisms. For example, using the same bed distribution as above, 100 l/tonne (24 gpt) shale and air injection at 0.64 mol/m²·s (3 SCFM/ft²) Braun has calculated the oil loss to coking and combustion as a function of depth. This is shown in Figure 10. Also shown in the figure is the relative consumption of oxygen by the fuels available. If these same conditions are run on a bed with smaller particles, very little oil combustion is predicted, and the front separation shown in Figure 1 occurs. By contrast, these particular results indicate that as the larger particles typical of a modified in-situ retort are encountered, oil loss to combustion becomes significant. This is the case because the time needed to heat the larger particles results in overlap of the retorting and combustion

Figure 10. a) Oil Loss to Coking and Combustion and b) Oxygen Consumption by Oil, Carbon, CO, and H₂ as a Function of Depth in the Retort (Inlet Flow Rate same as Figure 9.) (From Braun Ref. 5.).

fronts. Also, diffusional limitations make it difficult to utilize char in the interior of the particles, making carbon less effective as a fuel source.

To summarize, the one-dimensional rubble models are well developed and can be very useful in investigating the effect of various operating conditions and initial bed characteristics on resource recovery.

QUASI-TWO-DIMENSIONAL BLOCK MODEL

The one-dimensional rubble models are appropriate for addressing retort schemes involving relatively large void fractions (>20%) that would be encountered in surface processing and the current large scale vertical MIS retort concepts. There is also an interest and need to develop models that address retorting under low void conditions. Any scheme for combustion retorting in low void situations will necessarily involve the treatment of large regions of competent shale. The term "large" here implies either blocks (or regions without active flow) of sufficient size that (1) typical heating rates will produce significant internal temperature gradients leading to an expanded retorting zone, and (2) surface area/diffusion-rate limitations will result in limited char oxidation.

A two-dimensional block model has been developed by Tyner and Hommert¹⁰ to address low void retorting. The model can simulate a number of geometries, three of which are shown in Figure 11. The shale bed is composed of seams of competent shale of finite thickness separated at intervals by discrete regions of active flow. The model can also simulate retorting down a central borehole in a cylindrical region of competent shale.

The physical processes included in the model are listed in Table I.

TABLE I

- *Two-Dimensional Heat Conduction and Composition Variation in Solid
- *One-Dimensional Heat and Mass Transport by Gas Flow
- *Gas-Solid Heat Transfer by Convection and Radiation
- *Mass Transport Between Solid and Gas

The consideration of heat conduction in two dimensions is extremely important in describing the retorting process in

Figure 11. Example of Simulation Geometries Available for Block Retorting Model.

large blocks, and it is primarily that feature which distinguishes this from other work. The chemical processes considered in this model are essentially the same as those of Braun's model with the exception that steam/char gasification is not presently included. The model calculates, as a function of time and position in the bed, the temperature of the solid and gas phases and the concentration of all species.

Laboratory experiments are being conducted in an attempt to verify model predictions of block retorting. The sample geometry used for the experiments is shown in Figure 12. Beds with voids in the range of 5 to 20% can be conveniently prepared in this configuration. Rubble has been used in the fractures because of previous problems caused by shale expansion in laboratory block retorting experiments.¹¹ Model-laboratory comparisons must then necessarily assume that the rubble does not seriously affect retorting and combustion in the block. (Ultimately, the effects of rubble in the fractures will be considered in the model.)

Figure 12. Schematic of Geometry for Laboratory Runs Examining Block Retorting.

Retort run 027 (for which comparisons are made here) consisted of 1.27 cm thick blocks of 110 kg/Mg (26.6 gpt) shale separated by 0.63 cm thick 169 kg/Mg (40.5 gpt) rubble zones. The insulated sample was ignited with electric heaters and burned with air at a flux of $0.027 \text{ kg}_{\text{air}}/\text{m}_{\text{sh}}^2 \cdot \text{s}$.

Figure 13 shows typical temperature profiles (of block surface temperatures) versus time at several locations in the retort bed (6, 12, and 18 cm from the top). The result of model calculations at these locations are shown as solid lines for comparison.

As mentioned in the discussion of retort chemistry, char oxidation is handled in the numerical models through the use of a shrinking core approximation. These block retort experiments provide a chance to check the accuracy of this approach. Figure 14 shows the position of the calculated and observed char boundaries, i.e., the boundary between the shrinking core of retorted but unburned shale and the burned shale. It is seen that the model predicts nearly the same amount of char burned as was observed,

Figure 13. Comparison of Measured and Calculated Temperatures at Block Surface for Laboratory Run (dashed line measured data).

Figure 14. Comparison of Measured Char Boundary and That Calculated by Shrinking Core Model for Laboratory Run.

although there is a difference in the final slopes of the boundaries.

These results and comparisons from similar experiments tend to verify (although not rigorously as yet) the block model results. Further experiments to investigate the effects of block size

and grade, void fraction, and gas flux and composition are in progress.

One interesting effect that can be examined with the block model is the effect of seam thickness on yield and loss mechanisms. The results discussed below are for a true in-situ retort with model geometry shown in Figure 11a where the seam thickness has been varied from 0.1 to 4 m. A constant void fraction of 2% was maintained by varying the crack size with the seam thickness.

Calculations made using thin (less than 0.1 m) shale coams (where internal temperature gradients are generally negligible) yield results similar to those of rubble-bed models with small particles, i.e., complete retorting of the kerogen, effective char utilization as fuel, uniform advance of a thermal wave through the bed, and oil yields as high as 90% of Fischer Assay.

The results of retorting thick (greater than 1 m) seams are considerably different, however. Figure 15 is a

Figure 15. Typical Retort Conditions for Thick Seams Indicating Temperature Distribution and Regions of Unretorted Shale.

"snapshot" of a 2 m thick seam retort after 600 hours. Bed and operating conditions for this case are listed in Table II. Shown are the regions of raw, retorted, and burned shale and the gas and solid temperature profiles at that time. Peak gas temperatures (1700 K) are located about 8 m down the seam.

Peak solid temperatures (over 1600 K) occur on the shale surface in this same region.

The heavy dashed line marks the limit of char combustion within the block. Because of oxygen diffusion limitations, only the "skin" of the block has been burned. As a result of this ineffective char utilization, and because product oil and gas are being generated over a broad

TABLE II

Retorting Conditions Used for Block Calculations

Bed Length	10 m
Seam Thickness	2 m
Crack Thickness	0.0408 m
Void	2%
Shale Grade	100 t/tonne
Gas Flux	.004 kg _g /m ² ·s
Steam Dilution	40 volume %

front which overlaps the gas phase combustion zone, product combustion provides a significant fraction of the process heat (98% in this case).

As indicated by the heavy solid line on Figure 15, a significant amount of raw (unretorted) shale has been left behind in the center of the first 5 m of the retort, although retorting has extended to the center of the block beyond this zone. This expansion of the retorted shale zone toward the block center in the latter stages of the retort is due to increased shale preheating as the retort progresses.

There are a number of sources of oil loss affecting yield. These include incomplete retorting (18% FA for this case), oil combustion (17% FA, 21% of that retorted), and oil coking due to the low heating rates (16% of FA, 19% of that retorted). These factors combine to decrease the overall yield to 49% of Fischer Assay. The term "yield" here refers to the free oil escaping combustion that is available for recovery. It does not include losses due to incomplete recovery.

Figure 16 summarizes the effect of seam thickness on the extent of retorting, oil coking and combustion, and overall

Figure 16. Effect of Seam Thickness on Yield and Loss Mechanisms.

yield. All conditions, except crack size (varied to maintain a 2% void) and seam thickness, are the same as in Table 5. For thin seams (< 0.25 m thick) yields are quite high (nearly 90%) and the only significant loss is to coking. Char consumption is significant since oxygen diffusion into thin seams is not a major limitation. As seam thickness is increased, char combustion becomes less effective and the combustion and retorting fronts begin to overlap, resulting in losses to oil combustion. Finally, at seam thicknesses of about 1 m, unretorted regions begin to appear; for seam thicknesses greater than 2 m, this incomplete retorting is the dominant loss mechanism at these conditions.

These results clearly indicate that seam thickness (or block size in other retort configurations) has an extremely strong effect on yield, and they stress the importance of adequate bed preparation to control maximum particle size. (Note, however, that because the effects of shale expansion are not included in the model, these results do not necessarily indicate that 2% void is adequate for in situ retorting.) While it might seem that a block model is not appropriate for describing the current modified in-situ schemes, it is interesting that the low local yields (~50%) predicted by this model have been observed in modified in-situ retorts¹², indicating that these retorts contain either very large particles or, more likely, extensive regions where the breakage has not been sufficient to create active flow paths.

TWO-DIMENSIONAL MODELING

The previous discussion has shown that the presently available one-dimensional and quasi-two-dimensional models can be very useful in describing basic retort phenomena. There are, however, important questions concerning in-situ retorting that can only be addressed by multi-dimensional modeling. Figure 17a schematically attempts to highlight some of these problems in a hypothetical vertical modified retort. As illustrated on the figure, one of the features almost certain to be found in all field retorts is rubble porosity distribution non-uniformity. This will certainly have subsequent effects on the retort front location.

This leads to the realization that in addition to the local oil loss mechanisms of combustion and coking, as Figure 17a indicates, there can be a loss of yield due to sweep inefficiencies. The first

Figure 17. Schematic Indicating Multi-Dimensional Considerations in Modeling: a) Vertical and b) Horizontal Modified In-Situ Retorts.

step of two-dimensional modeling, then, is to quantify the effects of porosity variations on the subsequent retort process. Figure 17a also indicates a natural follow-on question to the effect of rubble bed variations, namely, given those variations what can be done to control them. Modeling is needed to address the effectiveness of varying from point to point either injection rate or injected gas composition. Figure 17b indicates also that there are similar questions that need answering with respect to horizontal modified retorting. In this configuration, though, there are additional considerations introduced by the gravitational field such as oil flow and buoyancy effects. As Figure 17b indicates in horizontal retorting the two-dimensional structure of the retorting front can have a significant effect on product yield depending on whether oil flows into a region where there is oxygen (dashed line on figure) or into a region that is oxygen depleted (solid line on figure). Obviously, then, there is considerable need to expand present modeling capabilities to two or three dimensions.

The primary difficulty in expanding the modeling to a second dimension is that this necessitates a more complete treatment of the fluid mechanics. In the one-dimensional models the fluid mechanics problems are essentially eliminated by the assumption of plug flow. Fluid flow within an actual retort is quite complex, being a mix of Darcy-law porous media flow and extensive channel flow regimes.

Work in characterizing flow in oil shale beds is now on-going.^{13,14}

To date, while there have been no models developed that rigorously combine a solution to the two-dimensional flow and energy equations with the retort chemistry, there have been some initial attempts at two-dimensional modeling. For example, the sweep efficiencies modeling of Gregg and Campbell¹² provides an interesting first look at some of the important two-dimensional questions. Their approach was essentially to decouple the flow problem from the retort chemistry. This is done by first obtaining a solution to the cold flow velocity field given a certain porosity/permeability distribution. This solution is obtained using Darcy law flow. Locally then, the retorting front motion is tracked by moving it proportional to the local velocity. In such a manner the retorting front shape can be reconstructed as a function of time. Gregg obtained qualitative agreement between a calculated retorting front distribution and that believed to have occurred on Occidental Oil Shale's modified in-situ retort 5. In order to make their calculations they reconstructed the bed porosity/permeability structure from pretest tracer data. These results are encouraging in that they indicate that a simple model using Darcy law flow and decoupled chemistry can qualitatively interpret the effects of flow non-uniformities on large scale retorts.

There has been some initial modeling undertaken by George and Harris¹⁵ to examine horizontal in-situ retorting. Their work essentially involves simultaneously solving a set of four parallel one-dimensional solutions with the only interconnection between the levels being oil flow. An empirical approach is used to move oil downward between levels. This model does show effects (on retort front structure and eventual yield) of the oil migration, but is not rigorous in its treatment of multi-dimensional flow or gravitation effects.

The next step in the two-dimensional modeling is to combine the retort chemistry now contained in the one-dimensional models with a numerical code that solves the appropriate flow and energy equations in two dimensions. Some of the capabilities that such a model should possess are listed in Table III.

Codes that presently have all the capabilities needed except the retort chemistry will probably be used as the basis for such a model. One such code is the WAFE¹⁶ code developed at Los Alamos National Scientific Laboratories. Figure 18 gives

TABLE III

Capabilities Needed for a Two-Dimensional Model

- *Separate Energy Equations for Gas and Solid,
- *Non-uniformities in shale composition and bed structure,
- *Non-Darcy flow,
- *Gravitational effects,
- *Flow of condensable fluids (oil, water),
- *Internal heat conduction in low flow regions,
- *Concentration variations of multiple gas and solid species (those presently in one-dimensional models).

Figure 18. Porosity Distributions used for Sample Two-Dimensional Calculation (a) and Predicted Isotherms (b).

an example of this code's present capability. Figure 18a shows the three rubble bed porosity distributions used for this example simulation. In each case the upper 0.75 m of the bed was treated as a high void plenum region. As Figure 18b indicates, gas injection was made from a point within the rubble. The standard Ergun equation was used to estimate relative permeabilities from the

porosity (a permeability of 600 Darcies was used for the 25% porosity region). Figure 18b shows the position of the 430 C isotherm after 100 hours of injecting 1100 K air at rate of 1 sm³/s into a bed of 15 cm diameter shale particles. As expected the code predicts more rapid advancement of the temperature front in regions of high porosity. This indicates the code's capability to handle rubble bed non-uniformities. Presently, work is on-going to adapt this model to include heat conduction within the particles and retort chemistry.

SUMMARY

Significant advances have been made in the mathematical modeling of oil shale retorting in the past five years. This has been accomplished by the combination of a detailed description of retort chemistry with models that incorporate a sufficiently complete treatment of the mass and energy transport within the retort. For systems where the flow, as a first approximation, can be considered one-dimensional, present models can reliably predict as a function of injected gas composition and rate such things as retorting rate, oil yield, oil loss mechanisms, temperature distributions and off-gas composition. This makes the present models already powerful predictive tools for laboratory or larger surface retorts where the one-dimensional approximation is valid.

In order for models to have a comparable predictive capability for in-situ retorts they will have to contain a more complete description of the multi-dimensional fluid flow within the retort. This is necessary if the important questions of sweep efficiency and operational control for an MIS retort are to be addressed. Thus the challenge for oil shale modeling in the next few years is to incorporate retort chemistry into models that contain an accurate description of the necessarily two-dimensional retort fluid flow and heat transfer. The encouraging results obtained so far with relatively simplistic two-dimensional flow models allows one to be optimistic that oil shale models will reach the same level of predictive capability in the next few years for multi-dimensional systems as they now possess for one dimension.

References

1. Synthetic Fuels Data Handbook, 2nd Edition, Cameron Engineers, Inc., 1978.

2. Campbell, J. H. and Burnham, A. K., "Reaction Kinetics for Modeling Oil Shale Retorting," In-Situ, 4, 1, pp 1-39.
3. Gregg, M. L., Campbell, J. H., and Taylor, J. R., Laboratory and Modeling Investigation of Oil-Shale Block Retorting to 900°C," Lawrence Livermore Laboratory, Preprint UCRL-83265, Sept. 1979.
4. Thomson, W. J., "The Oxidation/Gasification of Retorted Oil Shale," Final Report DOE/ET/12099-1, October 1979.
5. Braun, R. L., "Results of Computer Simulation of In-Situ Oil Shale Retorting," presented at the AIChE Meeting, Houston, TX, April 1979, also submitted to In-Situ.
6. Dockter, L. and Harris, H. G., "A Mathematical Model of Forward Combustion Retorting of Oil Shale," Laramie Energy Technology Center, Technical Progress Report (July 1978).
7. Nuttall, H. E., "Mathematical Modeling and Experimental Investigation of Oil Shale Retorting," Proc. 51st Annual Meeting SPE-AIME, New Orleans, LA, (1976).
8. George, J. H. and Harris, H. G., "Mathematical Modeling of In-Situ Oil Shale Retorting," SIAM J. Numer. Anal., 14, 137 (1977).
9. Rothman, A. J., Ed., Lawrence Livermore Laboratory Oil Shale Project Quarterly Report, Jan.-March 1980, UCID-16986-80-1, June 1980.
10. Tyner, C. E. and Hommert, P. J., "Numerical Modeling of a True In-Situ Oil Shale Retort," Sandia National Laboratories Report, SAND78-1307, Jan. 1979.
11. Duval, J. J. and Tyner, C. E., "Laboratory and Modeling Studies of the Combustion Retorting of Large Blocks of Oil Shale," 86th AIChE National Meeting, Houston, TX, April 1979.
12. Gregg, M. L. and Campbell, J. H., "Sweep Efficiency Modeling of Modified In-Situ Retorts," Proceedings of the 13th Oil Shale Symposium, Golden, CO, April 1980.

13. Carbonell, R. G., "Flow Nonuniformities in Packed Beds: Effect on Dispersion," Lawrence Livermore Laboratory Report UCID 17974, Livermore, CA, Nov. 1978.
14. Minster, R. A. and Fausett, D. W., "Fluid Flow through Packed Columns of Crushed Oil Shale," Laramie Energy Technology Center, Report of Investigation, LETC/RI-80/5, April 1980.
15. George, J. H. and Harris, H. G., "Mathematical Modeling of Oil Shale Retorting," Laramie Energy Technology Center Report, LETC 1761-15/1, Dec. 1979.
16. Travis, B. J. and Davis, A., "Model of Two Phase Mass and Heat Transport in Porous Media," Los Alamos Scientific Laboratories, Report No. LA-UR-80-611, May 1980.