THE ROLE OF COMPUTER SIMULATION IN OIL SHALE BLASTING

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ABSTRACT

Sophisticated computer codes have been developed to simulate the processes that occur in blasting in oil shale. We describe the three ways these codes are used in conjunction with field results. First, there is a code verification stage, where the code is improved through detailed comparisons. Next, there is a stage where critical phenomena in the blasting process are identified by studying areas where there are significant differences between calculations and field results. Finally, as the code is verified and the critical phenomena are explored, the code is used as a design tool. These stages are illustrated with experience from use of the new Los Alamos SHALE code and other codes. Current understanding of blasting in oil shale is reviewed, with an emphasis on areas where simulations and experimental approaches are pushed to their limits. We conclude with a recommendation that computer simulation be done in close coordination with an active experimental program.

INTRODUCTION

Considerable progress has been made in the development of advanced computer codes to simulate rock breakage with explosives. We address here the proper role such codes should play in the design of practical blast patterns to fracture oil shale for in situ processing. They should not be confused with economic modeling programs; these codes follow the physical processes that occur during blasting. They run on the world's most powerful computers, so will generally be used at large research facilities, rather than by engineers in the field. The codes serve primarily as tools to obtain more information about the dynamics of the blasting process. This information can then be used to improve blast designs in the field.

COMPUTER CODES THAT SIMULATE BLASTING

The computer codes follow the physical processes that occur during blasting from the detonation of the explosive through to the fracturing of the rock and movement of the rubble. They do this by integrating in time the differential equations that describe the conservation of mass, momentum, and energy. In recent years, several codes have been applied to blasting in oil shale. These include TOODY (Boade and others, 1981), STEALTH (Trent and others, 1981), 2DL (Johnson, 1979), and the new Los Alamos SHALE code (Adams and others, 1984). In this paper, we refer primarily to the SHALE code, although we present some results obtained with other codes.

Computer simulations require input to specify the blasting pattern and material properties of the explosives and rock. The calculation produces a history of the motion and physical state of the material throughout the region of the blast. This information comes out in the form of tables of numbers and plots at selected times during the calculation. SHALE makes plots of the computational mesh and velocity field and contour plots that show the distribution of density, internal energy, mean stress, and fracture. SHALE also writes data files during a calculation so that movies or predicted gauge records can be made at a later time.

Computer simulations provide a wealth of information, but the user must interpret the results to answer practical questions. Sometimes several computer runs must be compared to see trends. Limitations of the code, such as possible dependence of the results on the size of the computational cells, also become apparent as the code is exercised. The user may have to do more than examine the output to answer some questions. For example, SHALE will show where fracture is predicted, but does not tell whether the broken rock has been loosened and tumbled (see discussion below). These questions may require application of empirical results or further calculations, perhaps with another code.

CODE CALCULATIONS AND FIELD RESULTS

A complex code like SHALE must have built into it the best available physical models and numerical techniques. The code is related to field results in three ways. First, the code is verified by comparing calculations with laboratory and field experiments, and with established empirical results. Second, comparison of experiments and calculations allow the identification of important phenomena that control the end results of blasting in the field. The identification of these phenomena is one of the first products that comes from the use of the code. Which phenomena are important usually becomes clear only when calculations and field data are compared. This starts in the verification stage, but continues through the second stage and even into the final applications stage.

In the third stage, the code is used as a design tool. This stage is reached as verification proceeds and the important phenomena become better understood. The three stages are only loosely a time sequence, since some jumping back and forth is inevitable as our understanding is broadened.

Our experience with the SHALE code illustrates these stages. SHALE is an explicit finite-difference "ALE" (arbitrary Lagrangian-Eulerian) code for solid mechanics calculations. The two-dimensional version is operational and a three-dimensional version is under development. SHALE uses the Bedded Crack Model (BCM) constitutive relation. BCM is a microphysical model for treating the dynamic behavior of quasi-brittle materials like rock.

Code Verification

Code verification began with a series of laboratory-scale blasting experiments conducted by Fugelso (1978). He took flash x-ray radiographs of the cavity produced when a spherical charge, 12.7 mm in radius, of high explosive is detonated in a block of oil shale. He found that the cavity became significantly nonspherical within the first 30 microseconds. Dienes and Margolin (1978) showed that this behavior could not be reproduced in calculations with a tensile failure model for the rock. This difference between observation and theory led to the development of the microphysical fracture model (Margolin, 1983).

Code verification continued with the execution of a number of cratering tests in the Colony and Anvil Points Mines in western Colorado (Harper and Ray, 1981; Ray and others, 1982; Dick, 1984). Comparisons between SHALE simulations and the results of the experiments were encouraging (Adams and others, 1984). Satisfactory agreement was obtained between calculated and observed crater radii. However, this agreement must be treated with some caution. Edwards and others (1983) have shown that joints and other site-specific geologic characteristics can have a major effect on crater shapes and sizes.

Acceleration gauges were deployed in some of the experiments, and calculated peak surface velocities agreed reasonably well with those obtained by integrating the measured accelerations. Comparison of peak accelerations revealed a problem, which was resolved by adjusting the amount of "artificial viscosity" used in the calculations. Thus, the verification stage led to changes in the code to improve its ability to match measured ground motions. This is a necessary step in the development of the code as a predictive tool.

Identification of Dominant Phenomena

Further comparisons between the calculations and field results rapidly led to the second stage as significant differences became apparent. For example, the code predicted fractured rock extending much deeper than cratering was observed in the single-borehole events. This led us to look carefully at the crater produced by a four-borehole test. Unlike the single-borehole craters, this crater was flat-bottomed and looked much like a superposition of four of the predicted single-borehole fracture patterns.

The role of the code is much different here than in the verification stage. Rather than simply checking the code, the comparison points toward a physical phenomenon that may dominate parts of the blasting process. In this case, the evidence points toward the high pressure gases produced by the explosive and their ability to loosen and tumble the broken rock. The comparison led us to distinguish between fracture, the growth of cracks, and complete fragmentation, where the cracks intersect to form fragments that are observed as loose rubble. At present, the code predicts fracture, while the excavated craters in the field are the regions where complete fragmentation has occurred.

As gas effects were identified as an important phenomenon, a theoretical picture was developed in an attempt to understand the observations. Plans were made for new experiments to focus on gas effects. The identification of dominant phenomena is most effective when the codes are used in conjunction with an active experimental program.

The new picture of fracture followed by fragmentation has important implications concerning timing and spacing of charges in complex blasting patterns. According to this picture, the shock wave generated by the explosive causes fracture, but does not make loose rubble, except perhaps in the spall layer near the free surface. The gas then completes the fragmentation and tumbles the rubble in those regions where it is able to penetrate into the shock-induced fracture network. In single-borehole craters, the gas is apparently confined to the vicinity of the borehole by a "stress cage" until it escapes through the stemming or along cracks that extend to the surface above the charge. Such a stress cage is known to confine the high pressure gases produced in underground nuclear tests (Terhune, 1977).

Given the data at the time, this picture explained how the rock under the crater near the charge could be fractured, but not tumbled. We postulated that in the multiple-borehole test, the shock waves from nearby charges disrupt the stress cage and allow the gas to enter the fracture network. This would cause deeper rock that was fractured to be tumbled, resulting in an excavated crater that was deeper and flatter along the bottom.

Specific field experiments were planned, in cooperation with colleagues at Sandia National Laboratories, to focus on gas versus shock effects. The first of these were stemming tests. They were done to make sure that the gas would not leak out prematurely through the stemming. These tests showed that the stemming was generally satisfactory. Venting of gas through a joint that passed near the charge was observed in one of the tests.

The next tests were matched stemmed and unstemmed single-borehole tests. Two pairs of tests were done, one in lean shale, and one in medium-grade shale. These tests, prompted by the the code comparisons that led to the two-step picture of fracture and fragmentation, were intended to study gas effects. The matched tests did not resolve the issue of gas versus shock effects, but did expose a second important phenomenon, the resistance of medium and rich shale to shock-induced fracturing. This could perhaps have been anticipated from problems that occurred in the large multiple-charge, multi-level tests that were carried out at Anvil Points in 1982 (Dick, 1984), but it is clearer in these smaller controlled tests. A brittle-ductile transition is known from laboratory tests to occur at lower confining stress in rich shale than in leaner shale (Johnson, 1979).

In summary, this stage in the interaction between the code and field data led to the identification of two dominant phenomena, gas effects and the influence of shale grade. These phenomena are critical because an understanding of them could result in fundamental changes in large-scale blast designs for improved breakage, rubble movement, and mitigation of effects caused by the presence of rich layers.

Further development of the code is needed to address these issues. For example, the brittle-ductile transition should be incorporated into the microphysical model using the new fracture criterion developed by Margolin and Smith (1984). Including gas effects in the calculations may be done by modifying the code (see Trent and others, 1981) or coupling the code with a separate code that follows gas flow in porous and fractured media. New controlled experiments are also needed. The code-field interaction may revert to the code verification stage for a while before returning to this stage or moving on to the next.

The Code as a Design Tool

The code will be ready to be used as a tool for designing blasts after it has been verified and the dominant phenomena have been identified and treated satisfactorily. Even before these steps are completed, though, the code can be used to give useful design information. For example, SHALE was used for "pre-shot" calculations for the recent stemmed and unstemmed tests. The calculations were used to estimate how big the craters would be, and to predict acceleration and velocity amplitudes to aid in the deployment of the gauges.

Perhaps the most ambitious application of a code as a design tool was that of Boade and others (1981), who used TOODY to design a large-scale blast pattern for a modified in situ oil shale retort. They superposed two-dimensional calculations of single-borehole craters to approximate a large blast pattern with several decks and many charges per deck.

By moving quickly through the earlier stages of code-field interaction, Boade and others were able to produce a baseline retort design. This is important for engineering purposes, and also for code development, since it forces attention to issues that may only become apparent at large scale. One problem that appears at this scale is "dead-pressing" (shock desensitization) of the explosive. When several separate charges (decks) are emplaced in a single long borehole, as in this retort design, the delayed charges are shocked and compressed by the first one to fire. Tests at Anvil Points (Dick, 1984) indicate that the delayed charges do not detonate properly.

A major drawback to moving directly to the design stage with a code is that some of the assumptions may later be found to be seriously in error. In addition, direct tests of large-scale designs are very costly, so very few can be done, even in a major research program (Romig, 1981). Further, without a basic understanding of the dominant phenomena, "failures" or unexpected events in large-scale tests may be very difficult to interpret.

The assumptions in the calculations of Boade and others (1981) begin with the use of the continuum damage model of Grady and Kipp (1980) to describe fracture. Grady and Kipp do compare calculations with the results of a small cratering test. Even so, the damage model may give erroneous results when applied at a scale much larger than where it was calibrated. Microphysical models, such as BCM in the SHALE code, should scale naturally because of their basis in fracture mechanics.

Other assumptions of Boade and others involve ignoring gas effects and using a two-dimensional code to simulate a truly three-dimensional situation. The continuing work on gas effects described above should show which parts of their work are valid. Similarly, the three-dimensional version of SHALE, under development, should be useful for exploring multiple-borehole interactions and other three-dimensional effects.

We will be using SHALE to develop new blast designs as the tests proceed and code verification and the examination of important phenomena continue. Our working hypothesis is that penetration of the gases into the fracture network is the key to good fragmentation and permeability enhancement. In multiple-borehole tests, shock waves from adjacent charges disrupt the stress cage that confines the gas to the borehole. If this picture is correct, then the spacing of the charges in practical blast designs will have to be close enough for the shock waves to be effective, and the delays will have to be short enough to avoid having the gases vent prematurely. The two-dimensional version of SHALE is being used at present to explore further the processes that occur in single-borehole tests, including the development of the stress cage. The three-dimensional version will be used to study how strong a shock wave is needed to disrupt the stress cage.

CURRENT UNDERSTANDING OF BLASTING IN OIL SHALE

The areas where code verification has been successful generally overlap with those areas where blasting is well understood. This is not a coincidence, since the role of the code is not to replace human thought, but rather to serve as an aid to thinking. The code does well at predicting the extent of the craters and the velocity peaks as stress waves propagate away from the explosive. This success is a reflection of the fact that the physical processes involved, rock fracture in tension and stress wave propagation, are adequately understood (see Duvall and Atchison, 1959). These remarks should not be taken to minimize the effort required to make the codes do what they do.

The areas where problems remain will be solved through a combination of experimental work and computer simulations. They involve the role of gas and

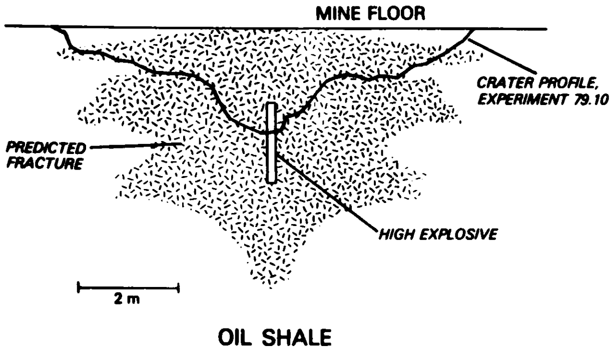

Figure 1. Predicted fracture distribution and observed crater profile for Colony Mine experiment 79.10. The charge was 25 kg of ANFO in a 0.15 m diameter borehole, with the bottom of the charge 3.3 m below the mine floor. Note the extensive region of predicted fracture below the observed crater.

the conditions under which fracture occurs. Figure 1 shows the predicted fracture and observed crater profile for a single-borehole cratering tests. As we have discussed, the predicted fracture extends much deeper than the observed region of loose rubble (the crater). We suspect that the fracture is there, but that the gas could not enter the cracks. Field and Ladegaard-Pederson (1971) reached similar conclusions about the relative importance of gas and stress waves from their laboratory work with plastics.

The role of gas in oil shale blasting is not yet understood. A different perspective on this issue can be gotten by considering another simulation. Figure 2 shows the predicted fracture calculated by L. G. Margolin with SHALE for a different single-borehole cratering test. The regions of fracture are distinguished here according to whether fracture first occurred because of tensile or shear stresses. The region of deep fracture we have been discussing is where failure first occurs in <u>shear</u>.

The choices seem clear. If gas plays a critical role, then it is possible that shear-induced fractures are so tight that gas cannot penetrate into them. Butkovich and others (1977) suggested that rock that fails in shear has little enhanced permeability. Whether or not gas is important, the other possibility is that no significant fracture occurs in the region in Figure 2 marked "shear failure."

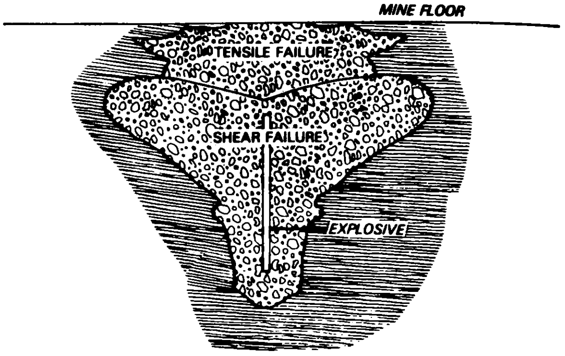

Figure 2. Regions of fracture predicted by code, labelled to show whether fracture first occurred in tension or shear. The charge was 91 kg of ANFO in a 0.15 m diameter borehole, with the bottom of the charge 5.5 m below the mine floor. Note that the deep fracture all lies in the shear failure region.

The recent matched pairs of tests seem to point toward the second possibility, since the stemmed and unstemmed pair in medium-grade shale both showed shallow craters like the region marked "tensile failure" in Figure 2. We cannot resolve the problem now, but we can reach a conclusion about the role of simulations. Both experiment and theory are at their limits, and the computer simulations provide a language and arena for addressing the issues. The state of the art will be advanced by clever experiments guided by clever simulations.

Improving our current understanding of blasting in oil shale is not an academic exercise. If gas effects dominate, the gas may be used in very unconventional ways to improve fragmentation in an <u>in situ</u> retort. We might even fire some deeper charges first to distribute the gas before firing the shallower ones. If shock waves are needed to liberate gas trapped in by stress cages around the boreholes, nonuniform spacing in the blast pattern might enhance the effects of nearby charges without increasing the "powder factor." Finally, if gas is unimportant, then extreme precision in detonation times may be critical to getting shock wave interactions for improved breakage.

IMPLICATIONS FOR THE OIL SHALE INDUSTRY

We have illustrated how the SHALE code is being used to explore blasting phenomenology and to improve blast designs. The effective use of the code clearly requires close interaction between calculations and results from the field. In general, this means that modelers must work directly with the people who carry out the experiments or do the production blasting. Effective use of codes also requires experienced modelers who work intensively on computer simulations. These codes are research tools.

Some companies and research organizations will have the resources and scale of activities to do both field experiments and computer simulations. Universities, as educational and research institutions, may also pursue both activities. To these organizations, we at Los Alamos can offer our codes and experience. We are now completing a SHALE users manual, and the code will soon be available for distribution to interested parties.

Other organizations with research and development or production activities in the field may sensibly choose not to do modeling themselves. Close interaction with a laboratory like Los Alamos doing computer simulations may supply the sort of insight and stimulation we have been discussing. In return, access to field data is essential to keep the modeling effort on track. The codes are not as far along as we would like toward being reliable predictive tools. A cooperative effort, where the code is developed and more data are obtained, is a productive way for both organizations to use their limited resources.

A final possibility is that an organization may choose to ignore computer simulations entirely. This may be safe in established blasting applications where there are proven empirical methods. In oil shale blasting, especially for in situ recovery, to ignore simulations creates a potentially serious and expensive blind spot. A research program that emphasizes only empirical approaches will miss the fresh outlook that comes from trying to apply basic physical principles to complex processes.

Our use of SHALE in conjunction with a continuing field program has been productive. It has led us to focus on critical issues. They are being addressed with specific field experiments and new code development. As this work continues, the code will be an increasingly valuable design tool.

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