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Final Report

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NONLINEAR PHENOMENA AT GEOLOGICAL REACTION FRONTS WITH ENERGY APPLICATIONS

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I. OVERVIEW

The interaction of aqueous fluids with the rock matrix within which they reside can yield a variety of phenomena due to the coupling of reaction-transport and mechanical processes. In this study, many of these phenomena were found to have potentially important implications for the exploration and exploitation of energy and mineral resources.

In a series of four studies we investigated 1) the effects of nucleation to produce banded precipitation, 2) Darcy-mineral dissolution coupling to produce scalloped, fingered and more complex alteration front morphologies, and 3) diagenetic alteration in chemically complex, multi-mineralic systems. In a separate study, the migration of methane driven by buoyancy effects was shown to lead to cellular and temporally oscillatory flows. Sandstones at depth experiencing pressure solution were shown to display unstable compaction leading to the formation of stylolites and band-like regions of augmented compaction alternating with low porosity bands with augmented overgrowth. Finally, it was shown that transfer of natural gas from shale source rock into neighboring sandstones could occur through a series of discrete pulsatile events through a cycle of fracturing and healing. As all these phenomena involve the genesis of the spatial distribution of porosity and permeability, and of petroleum through diagenesis, they are of potential importance in the development of resource exploration and extraction strategies.

As a result of our DOE supported work we have received significant industrial support. This support is a direct measure of success of this project in enabling us to develop the skills, personnel and techniques needed to solve practical problems for the petroleum industry.

In what follows we briefly describe these studies and refer to the attached papers for the complete presentation. Numbers in parentheses refer to papers listed at the end of this report and attached as appendices.

II. REACTION FRONT MORPHOLOGY (1,2,3,4)

When fluids flow through a rock that is undersaturated with respect to one or more minerals in that rock, one or more reaction fronts may advance downflow. As a given front advances it causes a change of permeability. If the permeability is greatest on the upstream side, a mechanism of flow self-focusing operates whereby the planar front becomes unstable. As a result, reaction fronts can take on scalloped, fingered or more complex morphologies. In a series of studies we demonstrated the possible morphologies of these fronts. Another study focused on fingering phenomena in tar sands wherein the mixed dynamic of the Saffman-Taylor instability and reaction front self-focusing due to viscosity due to tar dissolution upon the injection of active fluids.[3]

These studies have applications to the morphology of natural and engineered fronts. The former may be of interest in determining the distribution of porosity and permeability within a basin or the shape of ore bodies as in uranium roll fronts. Engineering examples include formation damage and oil and the recovery of very viscous oils and tars.

III. MINERAL BANDING THROUGH NUCLEATION PHENOMENA (5,6)

Two mechanisms for the precipitation of banded cements were investigated. In one case nucleation at a reaction front of an authigenic mineral was seen to lead to a hierarchy of transitions of precipitate profile ranging from continuous deposition to complex banding patterns consisting of alternations of precipitate and precipitate-free zones. A second study showed that after nucleation of a pair of interacting minerals, the uniform sol can become unstable and yield a pattern of alternating bands of the two minerals which may be periodic or chaotic in nature.

. Such oscillations occur in nature - including banded iron oxide minerals behind a uranium bearing or other redox (or roll) front. Our study shows that banding is not necessarily the result of changing external conditions but can rather evolve spontaneously - i.e. they can self-organize. In this way, we may gain insights into ore body formation processes.

IV. DIAGENETIC ALTERATION FRONTS AND THE SPATIAL DISTRIBUTION OF POROSITY AND PERMEABILITY (7,8)

A modeling study of diagenetic alteration in an arkose was carried out to test response to the effects of temperature, flow rate, inlet fluid composition and initial mineral modes. It was shown that the response can be to increase or decrease porosity and permeability depending on these factors. Hence the spatial distribution of porosity and permeability in a basin may be dramatically altered during diagenesis. The model is quite successful at predicting reservoir quality for given assumptions about the initial state of the system and the composition of the fluid imposed upon it.

The results of the above numerical simulations were complemented with two analytical studies wherein new approximation techniques were introduced to describe reaction fronts in the limit of a) fast reactions and b) very weakly soluble minerals.

V. MECHANO-CHEMICAL FEEDBACK AND POROSITY PRESERVATION AND DIAGENETIC TRAP FORMATION AT DEPTH (9,10,11)

Below about 0.5 km rocks tend to compact via stress mediated dissolution at grain-grain contacts and precipitation on facets in contact with pore fluid. We have developed a model including these processes, stresses in the porous, fluid pressurized medium and diffusion of solutes into which the grains dissolve. As a result we have been able to describe not only compaction but also the genesis of stylolites and of "diagenetic bedding". The latter consists of bands of enhanced compaction and elevated porosity alternating with bands of overgrowth and low porosity/permeability. These effects are an essential mechanism for the preservation of porosity at depth as well as the generation of pressure seals that can trap deep reservoirs of petroleum.

VI. BUOYANCY DRIVEN NATURAL PETROLEUM MIGRATION (12,13)

The generation of methane from kerogen at depth leads to an unstable fluid mass density profile. Thus buoyancy-driven flows can be set up in association with methanogenesis as well as other petroleum producing processes. The methane mechanism was shown to lead to cellular convection cells. The fluid velocity can be oscillatory in time. The model also shows that there may be a natural length between methane bearing reservoirs because of a pattern selection mechanism. This type of study is central in developing an understanding of the timing of methane genesis and migration.

VII. OSCILLATORY METHANE RELEASE FROM SHALE SOURCE ROCK (14)

Overpressuring within shales containing kerogen may occur because of the breakdown of the latter through thermally induced processes. This overpressuring may cause fracturing of the shale and episodic methane release. Healing of the resulting fractures may then lead to a sequence of episodic methane releases during kerogen breakdown. These studies may have important implications for the development of estimates of the timing of methane released from source rock.

VIII. GEOCHEMICAL SELF-ORGANIZATION (15, 16,17)

A unifying aspect of much of the work carried out under this contract is the notion of geochemical self-organization. What we have shown is that repetitive patterns of mineralization or fluid composition in space or time can arise spontaneously without the need for externally imposed periodicities (such as annual variations in deposition rates to form sedimentary bedding). Understanding these phenomena could then lead to new exploration strategies.

Our studies of such geochemical self-organization phenomena under this contract have led to the completion of the book Geochemical Self-Organization (by P. Ortoleva, published by Oxford University Press) and the editing of the Proceedings of the workshop entitled Self-Organization in Geological Systems (edited by P. Ortoleva, published as a volume of Earth Science Reviews by Elsevier Press, Amsterdam). These notions are being developed in an invited paper for Science (18).

LIST OF PUBLICATIONS

1. A weakly nonlinear stability analysis of the reactive infiltration interface, SIAM J. Appl. Math 48, 1362-1378, with J. Chadam and A. Sen.

2. Reaction front fingering in carbonate cemented sandstones, in Self-Organization in Geological Systems: Proc. of a Workshop held 26-30 June 1988, University of California Santa Barbara, P. Ortoleva, B. Hallet, A. McBirney, I. Meshri, R. Reeder and P. Williams, (eds.) Earth Science Reviews 29, 183-198 (1990) with W. Chen.

3. Stability of reactive flows in porous media: coupled porosity and viscosity changes, SIAM J. Appl. Math. 51, 684-692 (1990) with J. Chadam and A. Pierce.

4. Self-organization in far-from-equilibrium reactive porous media subject to reaction front fingering, in Patterns, Defects and Materials Instabilities, D. Walgraef and N.M. Ghoniem, eds., NATO ASI Series, Vol. 183, 203-220 (1990) with W. Chen.

5. Bifurcation of the Ostwald-Liesegang supersaturation-nucleation-depletion cycle, in Self-Organization in Geological Systems: Proc. of a Workshop held 26-30 June 1988, University of California Santa Barbara, P. Ortoleva, B. Hallet, A. McBirney, I. Meshri, R. Reeder and P. Williams, (eds.) Earth Science Reviews 29, 163-173 (1990) with R. Sultan.

6. Periodic and aperiodic macroscopic patterning in two precipitate post-nucleation systems, Physica D, in press, with R. Sultan.

7. Multiple front analysis of mineral zoning sequences, Geochim. Cosmochim. Acta, accepted (1989) with A. Park.

8. The effect of fluid and rock compositions on diagenesis: a modelling investigation, in Prediction of Reservoir Quality Through Chemical Modeling, I. Meshri and P. Ortoleva (eds.), AAPG Memoir 49, 13?-146 (1990) with C.H. Moore.

9. Differentiated structures arising from mechano-chemical feedback in stressed rocks, in in Self-Organization in Geological Systems: Proc. of a Workshop held 26-30 June 1988, University of California Santa Barbara, P. Ortoleva, B. Hallet, A. McBirney, I. Meshri, R. Reeder and P. Williams, (eds.) Earth Science Reviews 29, 283-298 (1990) with T. Dewers.

10. The interaction of reaction, mass transport, and rock deformation during diagenesis: Mathematical modeling of intergranular pressure solution, stylolites, and differential compaction/cementation, in Prediction of Reservoir Quality Through Chemical Modeling, I. Meshri and P. Ortoleva (eds.), AAPG Memoir 49, 147-160 (1990) with T. Dewers.

11. Development of diagenetic differentiated structure through reaction-transport feedback, in Diagenesis, K.H. Wolf (ed.) (1992) in press.

12. The role of geochemical self-organization in the migration and trapping of hydrocarbons, Applied Geochemistry 3, 287-316 (1988) with T. Dewers.

13. Cellular and oscillatory self-induced methane migration, in Self-Organization in Geological Systems: Proc. of a Workshop held 26-30 June 1988, University of California Santa Barbara, P. Ortoleva, B. Hallet, A. McBirney, I. Meshri, R. Reeder and P. Williams, (eds.) Earth Science Reviews 29, 249-265 (1990) with A. Park and T. Dewers.

14. Oscillatory methane release from shale source rock, in Self-Organization in Geological Systems: Proc. of a Workshop held 26-30 June 1988, University of California Santa Barbara, P. Ortoleva, B. Hallet, A. McBirney, I. Meshri, R. Reeder and P. Williams, (eds.) Earth Science Reviews 29, 241-248 (1990) with A. Ghaith and W. Chen.

15. Self-Organization in Geological Systems: Proc. of a Workshop held 26-30 June 1988, University of California Santa Barbara, P. Ortoleva, B. Hallet, A. McBirney, I. Meshri, R. Reeder and P. Williams, (eds.) Earth Science Reviews 29 (Elsevier, Amsterdam) (1990).

16. Geochemical Self-Organization, Oxford University Press, (1992) in press.

17. Geochemical self-organization, Science (1990) in revision (an invited paper).

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