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A Comprehensive Simulation Model of Kerogen Pyrolysis for the In-situ Upgrading of Oil Shales

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Summary

Oil shale, which is composed of abundant organic matter called kerogen, is a vast energy source. Pyrolysis of kerogen in oil shales releases recoverable hydrocarbons. Here, we describe the pyrolysis of kerogen with an in-situ upgrading process, which is applicable to the majority of oil shales. The pyrolysis is represented by six kinetic reactions resulting in 10 components and four phases. Expanding the Texas A&M Flow and Transport Simulator (FTSim), which is a variant of the TOUGH+simulator (Moridis 2014), we develop a fully functional capability that describes kerogen pyrolysis and accompanying system changes.

The simulator describes the coupled process of mass transport and heat flow through porous and fractured media and includes physical and chemical phenomena of reservoir systems. The simulator involves a total of 15 thermophysical states and all transitions between them and computes a simultaneous solution of 11 mass- and energy-balance equations per element. The simulator solves the equations in a fully implicit manner by solving Jacobian matrix equations with the Newton-Raphson iteration method. To conduct a realistic simulation, we account for geological structure of oil-shale reservoirs and physical properties of bulk-oil shale rocks by considering phases and components in the pores. In addition, we involve interaction between fluids and porous media, diverse equations of state (EOSs) for computation of fluid properties, and numerical modeling of fractured media.

We intensively reproduce the field-production data of Shell In-situ Conversion Process (ICP) implemented in the Green River

formation by conducting sensitivity analyses for the diverse reservoir parameters, such as initial effective porosity of the matrix, oil-shale grade, and the spacing of the natural-fracture network. We analyze the effect of each reservoir parameter on the hydrocarbon productivity and product selectivity. The simulator provides a powerful tool to quantitatively evaluate production behavior and dynamic-system changes during in-situ upgrading of oil shales and subsequent fluid production by thoroughly describing a reservoir model, phases and components, phase behavior, phase properties, and evolution of porosity and permeability.

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References

- Baughman, G. L. 1978. *Synthetic Fuels Data Handbook*, second edition. Cameron Engineers, Inc.
- Bauman, J. H. and Deo, M. D. 2011. Parameter Space Reduction and Sensitivity Analysis in Complex Thermal Subsurface Production Processes. *Energy & Fuels* **25** (1): 251-259. <http://dx.doi.org/10.1021/ef101225g>.
- Bear, J. 1972. *Dynamics of Fluids in Porous Media*. Elsevier Science.
- Bejan, A. 1984. *Convection Heat Transfer*. New York: John Wiley & Sons.
- Biglarbigi, K., Dammer, A., Cusimano, J. et al. 2007. Potential for Oil Shale Development in the United States. Presented at the SPE Annual Technical Conference and Exhibition, Anaheim, California, USA, 11-14 November. SPE-110590-MS. <http://dx.doi.org/10.2118/110590-MS>.
- Biglarbigi, K., Crawford, P., Carolus, M. et al. 2010. Rethinking World Oil-Shale Resource Estimates. Presented at the SPE Annual Technical Conference and Exhibition, Florence, Italy, 19-22 September. SPE-135453-MS. <http://dx.doi.org/10.2118/135453-MS>.
- Brandt, A. R. 2008. Converting Oil Shale to Liquid Fuels: Energy Inputs and Greenhouse Gas Emissions of the Shell in Situ Conversion Process. *Environ. Sci. Technol.* **42** (19): 7489-7495. <http://dx.doi.org/10.1021/es800531f>.
- Braun, R. L. and Burnham, A. K. 1990. Mathematical Model of Oil Generation, Degradation, and Expulsion. *Energy & Fuels* **4** (2): 132-146. <http://dx.doi.org/10.1021/ef00020a002>.
- Brooks, R. H. and Corey, A. T. 1964. Hydraulic Properties of Porous Media, Hydrology Papers, No. 3, Colorado State University, Fort Collins, Colorado.

Camp, D. W. 1987. Oil Shale Heat-Capacity Relations and Heats of Pyrolysis and Dehydration. In *Proc.*, 20th Oil Shale Symposium, Golden, Colorado, USA, 21–22 April.

Chang, C.-H. and Zhao, X. 1990. A New Generalized Equation for Predicting Volumes of Compressed Liquids. *Fluid Phase Equilibria* **58** (3): 231–238. [http://dx.doi.org/10.1016/0378-3812\(90\)85134-V](http://dx.doi.org/10.1016/0378-3812(90)85134-V).

Chung, T. H., Lee, L. L., and Starling, K. E. 1984. Applications of Kinetic Gas Theories and Multiparameter Correlation for Prediction of Dilute Gas Viscosity and Thermal Conductivity. *Industrial & Engineering Chemistry Fundamentals* **23** (1): 8–13. <http://dx.doi.org/10.1021/i100013a002>.

Chung, T. H., Ajlan, M., Lee, L. L. et al. 1988. Generalized Multiparameter Correlation for Nonpolar and Polar Fluid Transport Properties. *Industrial & Engineering Chemistry Research* **27** (4): 671–679. <http://dx.doi.org/10.1021/ie00076a024>.

Corey, A. T. 1954. The Interrelation Between Gas and Oil Relative Permeabilities. *Producers Monthly* **19** (1): 38–41.

Dyni, J. R. 2006. *Geology and Resources of Some World Oil-Shale Deposits*, original edition. US Department of the Interior, US Geological Survey.

Fan, Y., Durlofsky, L., and Tchelepi, H. 2010. Numerical Simulation of the in-Situ Upgrading of Oil Shale. *SPE J.* **15** (2): 368–381. SPE-118958-PA. <http://dx.doi.org/10.2118/118958-PA>.

Fowler, T. and Vinegar, H. 2009. Oil Shale ICP-Colorado Field Pilots. Presented at the SPE Western Regional Meeting, San Jose, California, USA, 24–26 March. SPE-121164-MS. <http://dx.doi.org/10.2118/121164-MS>.

Ghosh, A., Chapman, W. G., and French, R. N. 2003. Gas Solubility in Hydrocarbons—A SAFT-Based Approach. *Fluid Phase Equilibria* **209** (2): 229–243. [http://dx.doi.org/10.1016/S0378-3812\(03\)00147-X](http://dx.doi.org/10.1016/S0378-3812(03)00147-X).

Gilliam, T. M. and Morgan, I. L. 1987. Shale: Measurement of Thermal Properties (No. ORNL/TM-10499). Oak Ridge National Laboratory, Tennessee, USA.

Hazra, K., Lee, K., Ehlig-Economides, C. et al. 2013. Comparison of Heating Methods for In-Situ Oil Shale Extraction. Presented at the IOR 2013—17th European Symposium on Improved Oil Recovery, From Fundamental

Science to Deployment. <http://dx.doi.org/10.3997/2214-4609.20142631>.

Jupp, T. and Woods, A. 2003. Thermally Driven Reaction Fronts in Porous Media. *J. Fluid Mechanics* **484**:329-346. <http://dx.doi.org/10.1017/S0022112003004348>.

Kahl, W. R. 1999. *Numerical Simulation of Primary Petroleum Migration*, MS thesis, Massachusetts Institute of Technology, Cambridge, Massachusetts (September 1999).

Kaviany, M. 2012. *Principles of Heat Transfer in Porous Media*. Springer Science & Business Media.

Kay, W. 1936. Gases and Vapors at High Temperature and Pressure—Density of Hydrocarbon. *Ind. Eng. Chem.* **28** (9): 1014-1019. <http://dx.doi.org/10.1021/ie50321a008>.

Kibodeaux, K. R. 2014. Evolution of Porosity, Permeability, and Fluid Saturations During Thermal Conversion of Oil Shale. Paper presented at the SPE Annual Technical Conference and Exhibition, Amsterdam, 27-29 October. SPE-170733-MS. <http://dx.doi.org/10.2118/170733-MS>.

Kuo, K. K. 1986. *Principles of Combustion*, second edition. New York: Wiley.

Kyle, B. 1999. Chemical and Process Thermodynamics. In Prentice Hall PTR (Upper Saddle River, New Jersey). 0130812447.

Lee, S., Speight, J. G., and Loyalka, S. K. 2007. *Handbook of Alternative Fuel Technologies*, original edition. CRC Press.

Lee, K., Moridis, G. J., and Ehlig-Economides, C. A. 2014. Oil Shale In- Situ Upgrading by Steam Flowing in Vertical Hydraulic Fractures. Presented at the Unconventional Resources Conference, The Woodlands, Texas, USA, 1-3 April. SPE-169017-MS. <http://dx.doi.org/10.2118/169017-MS>.

Lee, K. 2014. *Rigorous Simulation Model of Kerogen Pyrolysis for the In-situ Upgrading of Oil Shales*, PhD dissertation, Texas A&M University, College Station, Texas (December 2014).

Logvinyuk, V., Makarenkov, V., Malyshev, V. et al. 1970. Solubility of Gases in Petroleum Products. *Chemistry and Technology of Fuels and Oils* **6** (5): 353-355. <http://dx.doi.org/10.1007/BF01171678>.

Lucas, K. 1981. Die Druckabhängigkeit Der Viskosität Von Flüssigkeiten--Eine Einfache Abschätzung. *Chemie Ingenieur Technik* **53** (12): 959-960.

Meyer, C. A., McClintock, R., and Silvestri, G. 1993. ASME Steam Tables: Thermodynamic and Transport Properties of Steam: Comprising Tables and Charts for Steam and Water, Calculated Using the 1967 IFC Formulation for Industrial Use, in Conformity with the 1963 International Skeleton Tables, as Adopted by the Sixth International Conference on the Properties of Steam, original edition. American Society of Mechanical Engineers.

Moridis, G. 2008. Tough+Hydrate V1.0 User's Manual: A Code for the Simulation of System Behavior in Hydrate-Bearing Geologic Media, original edition. Berkeley: Lawrence Berkeley National Laboratory.

Moridis, G. 2014. Tough+Hydrate V1.2 User's Manual: A Code for the Simulation of System Behavior in Hydrate-Bearing Geologic Media, original edition. Berkeley: Lawrence Berkeley National Laboratory.

Mualem, Y. 1976. A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media. *Water Resources Research* **12** (3): 513-522. <http://dx.doi.org/10.1029/WR012i003p00513>.

Nimblett, J. and Ruppel, C. 2003. Permeability Evolution During the Formation of Gas Hydrates in Marine Sediments. *J. Geophysical Research* **108** (B9): 2420. <http://dx.doi.org/10.1029/2001JB001650>.

Nottenburg, R., Rajeshwar, K., Rosenvold, R. et al. 1978. Measurement of Thermal Conductivity of Green River Oil Shales by a Thermal Comparator Technique. *Fuel* **57** (12): 789-795. [http://dx.doi.org/10.1016/0016-2361\(78\)90141-2](http://dx.doi.org/10.1016/0016-2361(78)90141-2).

Parker, J., Lenhard, R., and Kuppusamy, T. 1987. A Parametric Model for Constitutive Properties Governing Multiphase Flow in Porous Media. *Water Resources Research* **23** (4): 618-624. <http://dx.doi.org/10.1029/WR023i004p00618>.

Peng, D.-Y. and Robinson, D. B. 1976. A New Two-Constant Equation of State. *Industrial & Engineering Chemistry Fundamentals* **15** (1): 59-64. <http://dx.doi.org/10.1021/i160057a011>.

Poling, B. E., Prausnitz, J. M., O'Connell, J. P. et al. 2001. *The Properties of Gases and Liquids*, original edition. New York: McGraw-Hill.

Pruess, K. 1985. A Practical Method for Modeling Fluid and Heat Flow in Fractured Porous Media. *SPE J.* **25**(1): 14-26. SPE-10509-PA. <http://dx.doi.org/10.2118/10509-PA>.

Pruess, K., Moridis, G., and Oldenburg, C. 1999. Tough2 User's Guide, Version 2.0, original edition. Berkeley: Lawrence Berkeley National Laboratory.

Ragland, K., Aerts, D., and Baker, A. 1991. Properties of Wood for Combustion Analysis. *Bioresource Technology* **37** (2): 161-168. [http://dx.doi.org/10.1016/0960-8524\(91\)90205-X](http://dx.doi.org/10.1016/0960-8524(91)90205-X).

Riazi, M. and Roomi, Y. 2007. A Method to Predict Solubility of Hydrogen in Hydrocarbons and Their Mixtures. *Chemical Engineering Science* **62** (23): 6649-6658. <http://dx.doi.org/10.1016/j.ces.2007.08.005>.

Riedel, L. 1954. Liquid Density in the Saturated State. Extension of the Theorem of Corresponding States. *Chem. Ing.-Tech* **26**: 259-264.

Shen, C. 2009. Reservoir Simulation Study of an In-Situ Conversion Pilot of Green-River Oil Shale. Presented at the SPE Rocky Mountain Petroleum Technology Conference, Denver, 14-16 April. SPE-123142-MS. <http://dx.doi.org/10.2118/123142-MS>.

Smith, J. W. 1976. Relationship Between Rock Density and Volume of Organic Matter in Oil Shales. [Linear equation specific for Green River Formation oil shales] (No. LERC/RI-76/6). Energy Research and Development Administration, Laramie, Wyoming, USA. Laramie Energy Research Center.

Stone, H. 1970. Probability Model for Estimating Three-Phase Relative Permeability. *J Pet Technol* **22** (2): 214-218. SPE-2116-PA. <http://dx.doi.org/10.2118/2116-PA>.

Teja, A. and Rice, P. 1981. Generalized Corresponding States Method for the Viscosities of Liquid Mixtures. *Industrial & Engineering Chemistry Fundamentals* **20** (1): 77-81. <http://dx.doi.org/10.1021/i100001a015>.

Thomas, G. W. 1966. Some Effects of Overburden Pressure on Oil Shale During Underground Retorting. *SPE J.* **6** (1): 1-8. SPE-1272-PA. <http://dx.doi.org/10.2118/1272-PA>.

Van der Waals, J. 1890. Arch. Neerlandaises 24 (1891) 1, *Trans. Z. Phys. Chem* **5**: 133.

Van Genuchten, M. T. 1980. A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. *Soil Science Society of America J.* **44** (5): 892-898.

Vinegar, H. 2006. Shell's In-situ Conversion Process. Presented at the Colorado Energy Research Institute 26th Oil Shale Symposium, Golden, Colorado, USA, 16-18 October

(Downloaded 31 October 2008 from <http://www.ceri-mines.org/document/R05a-HaroldVinegar.pdf>).

Wellington, S. L., Berchenko, I. E., De Rouffignac, E. P. et al. 2005. In Situ Thermal Processing of an Oil Shale Formation to Produce a Desired Product. US Patent Grant No. US6880633 B2.

White, M., Chick, L., and McVay, G. 2010. Impact of Geothermic Well Temperatures and Residence Time on the In Situ Production of Hydrocarbon Gases From Green River Formation Oil Shale. Presented at the 30th Oil Shale Symposium, Golden, Colorado, USA.

Xu, L., Liu, C., Xian, X. et al. 1999. Compressibility of Coal Matter and Coal Pore. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **157** (1): 219-222. [http://dx.doi.org/10.1016/S0927-7757\(99\)00112-0](http://dx.doi.org/10.1016/S0927-7757(99)00112-0).

Yaws, C. 2003. Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds, Knovel (Online version available at: <http://www.knovel.com/knovel2/Toc.jsp>).

Youtsos, M., Mastorakos, E., and Cant, R. 2013. Numerical Simulation of Thermal and Reaction Fronts for Oil Shale Upgrading. *Chemical Engineering Science* **94**: 200-213. <http://dx.doi.org/10.1016.j.ces.2013.02.040>.