Mathematical Modeling of Oil Shale Pyrolysis

28th Oil Shale Symposium, Colorado, USA

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HATCH LTD.

overview

Who Are We? Hatch Overview

- Employee-owned
- Projects in more than 125 countries
- More than 10,400 professionals worldwide
- More than CAD$50 billion of projects now under management, including oil sands projects
- Full-service EPCM company
- Consulting – process and technology
- In-house engineering services for operations support
- Hatch Procurement in China
- Serving mining & metals, energy and infrastructure for 50 years
- World class systems

About Hatch

about us

- Employee owned
  - >10,400 professionals worldwide
- More than US$50 billion of CAPEX projects under management
- EPCM, integrated teams, project and construction management
- Serving energy, mining & metals and infrastructure for more than 55 years

Global Operations

10,400 staff – June 2008

Canada

- Calgary, Alberta
- Montreal, Quebec
- Niagara Falls, Ontario
- St. John's, Newfoundland
- Sorel-Tracy, Quebec
- Sudbury, Ontario
- Toronto, Ontario
- Hamilton, Ontario
- Vancouver, British Columbia
- Winnipeg, Manitoba

3950

USA

- Boston, Massachusetts
- Buffalo, New York
- New York, New York
- Millburn, New Jersey
- Pittsburgh, Pennsylvania
- San Francisco, California
- Seattle, Washington

South America

- Antofagasta, Chile
- Santiago, Chile
- Lima, Peru
- São Paulo, Brazil
- Belo Horizonte, Brazil
- São Luís, Brazil

1550

Europe

- London, England
- Moscow, Russia

50

China

- Shanghai
- Beijing

150

- Abu Dhabi

India

- New Delhi

Malaysia

- Kuala Lumpur

South Africa

- Johannesburg

1550

Australia

- Perth
- Sydney
- Townsville
- Whyalla
- Wollongong
- Brisbane
- Gladstone
- Mackay
- Melbourne
- Newcastle

2900

(Yellow indicates regional hub)

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Kerogen Composition

Kerogen

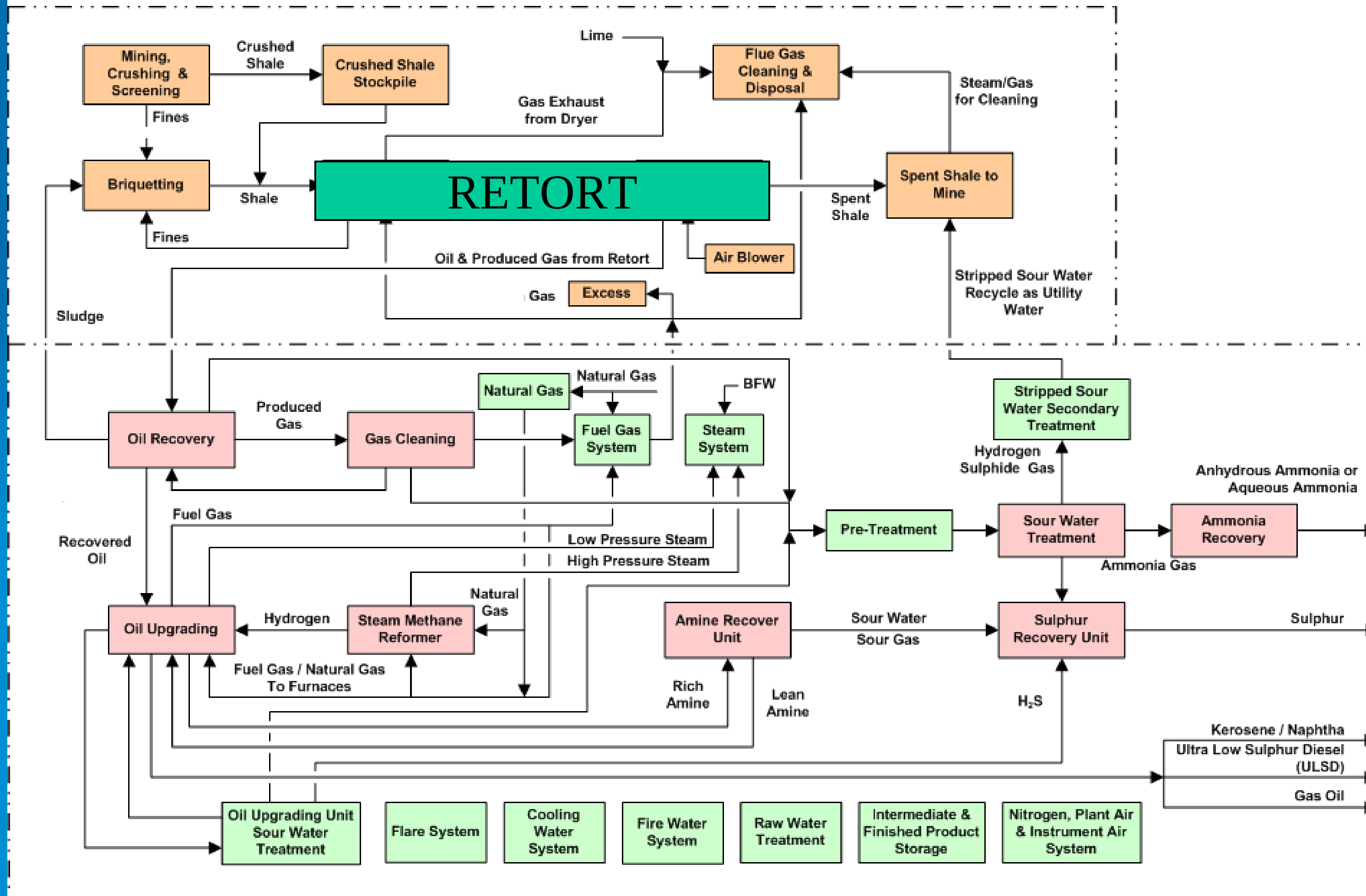
- **Kerogen is a mixture of organic chemical compounds that makes up a portion of organic matter in sedimentary rocks. It is insoluble in normal organic solvents because of its large molecular weight**
- **Kerogen is converted to different kinds of hydrocarbon by pyrolysis. A range of different light and heavy hydrocarbons is produced during kerogen decomposition**
- **Kerogen is initially converted to bitumen by heating, the bitumen is in turn decomposed to different kinds of hydrocarbons.**

Kerogen Composition

Table1 Kerogen Composition at different locations

Deposit	C	H	O	S
Leningradskoye (Russia)	77.7	9.8	11.3	1.2
Timahdit (Morocco)	70.5	9.3	12.4	7.8
El-Lajjun (Jordan)	74.5	8.5	4.5	12.5
Green-River (USA)	80.9	11.4	6.9	0.8
Irati (Brazil)	68.1	10.3	17.9	3.7
Render (Australia)	63.1	7.9	28.3	0.7
Rotem (Israel)	66.9	7	15.4	10.7
Nerke (Sweden)	69.5	7.7	16.8	6

Complex Technology Chain



Issues

- Technical feasibility
  - Driven by choice of retorting process
- Commercial Viability
  - Driven by overall process integration

Integration becomes increasingly important in order to drive advantage out of Economics of Scale

Challenges

- Do we understand enough about retorting process to develop integration strategy?
  - CO_2 footprint
  - Water consumption /bbl
  - Power Consumption/bbl
- Can we model integrated operations to depict start-up shutdown and other non-steady conditions?

Oil Shale Processing

- **Oil Shale Extraction**
  - Oil shale extraction refers to the process in which kerogen is converted into synthetic crude oil through the chemical process of pyrolysis.
- **Oil Shale Processors**
  - PARAHO
  - Alberta Taciuk Processor (ATP)
  - Petrosix
  - UTT-3000
  - Ecoshale In-Capsule process

Oil Shale Pyrolysis

Geometry

- **Geometry**

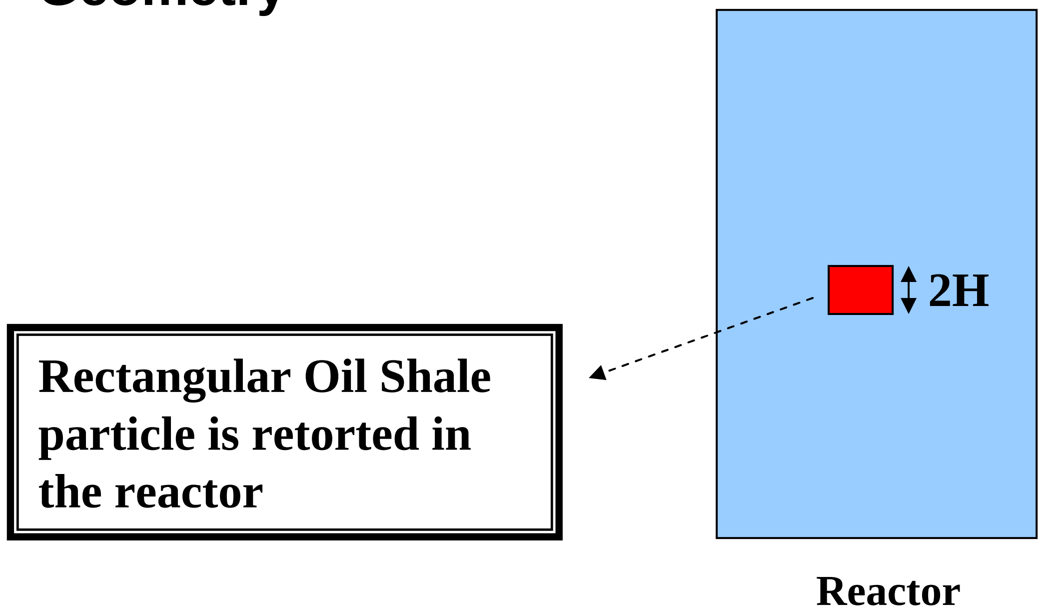


Figure 2 Oil shale particle and reactor geometries

Oil Shale Pyrolysis

Reactions

- **Reactions:**

Kerogen Decomposition

$$n_1HHC + n_2CO_2 + n_3CH_4 + n_4H_2O + n_5CO$$

$$\text{ker}\,ogen \rightarrow LHC + Bitumen$$

$$Char$$

Carbonate Decomposition

$$MCO_3(Carbonates) \rightarrow MCO + CO_2$$

Pyrite Decomposition

$$Pyrite \rightarrow m_1CO + m_2CO_2 + m_3SO_2 + m_4Sulphide + m_5Sulphite$$

WorkingTogether SAFELY

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Oil Shale Pyrolysis

Governing Equations

- **Mass Conservation Equations**
  - **Kerogen**

$$\frac{\partial c_{kr}}{\partial t} = -k_1 c_{kr}$$

  - **Light HC**

$$\frac{\partial c_{LHC}}{\partial t} = k_1 c_{kr} + k_{HHC} c_{HHC} + D\nabla^2 c_{LHC}$$

  - **Carbon Dioxide**

$$\frac{\partial c_{CO_2}}{\partial t} = k_{CO_2} c_B + k_5 c_{caco_3} + k_6 c_p + D\nabla^2 c_{CO_2}$$

Oil Shale Pyrolysis

Mathematical Modeling

- **Equations are made dimensionless**
- **Equations are solved using integration, integrating factor and integral methods**
- **Mathematical Equations Predicting Oil Vapor is:**

$$c_{LHC} = \left[\frac{k_1 \left(e^{-k_1\tau} - e^{-\frac{k_{HHC}\left(1-x^2\right)+2D\tau}{1-x^2}} \right)}{2D-\left(k_1-k_{HHC}\right)\left(1-x^2\right)} - \frac{k_1 k_3 k_{HHC}}{1+k_3-k_1} \frac{e^{-k_1\tau} - \left((-t+1) e^{-\frac{k_{HHC}\left(1-x^2\right)+2D\tau}{1-x^2}} \right)}{2D-\left(k_1-k_{HHC}\right)\left(1-x^2\right)} - \frac{k_1 k_3 k_{HHC}}{1+k_3-k_1} \frac{e^{-\left(k_{HHC}+k_3\right)\tau} - \left((-t+1) e^{-\frac{k_{HHC}\left(1-x^2\right)+2D\tau}{1-x^2}} \right)}{2D-k_3\left(1-x^2\right)} \right] \left(1-x^2\right)$$

Oil Shale Pyrolysis

Mathematical Modeling Results

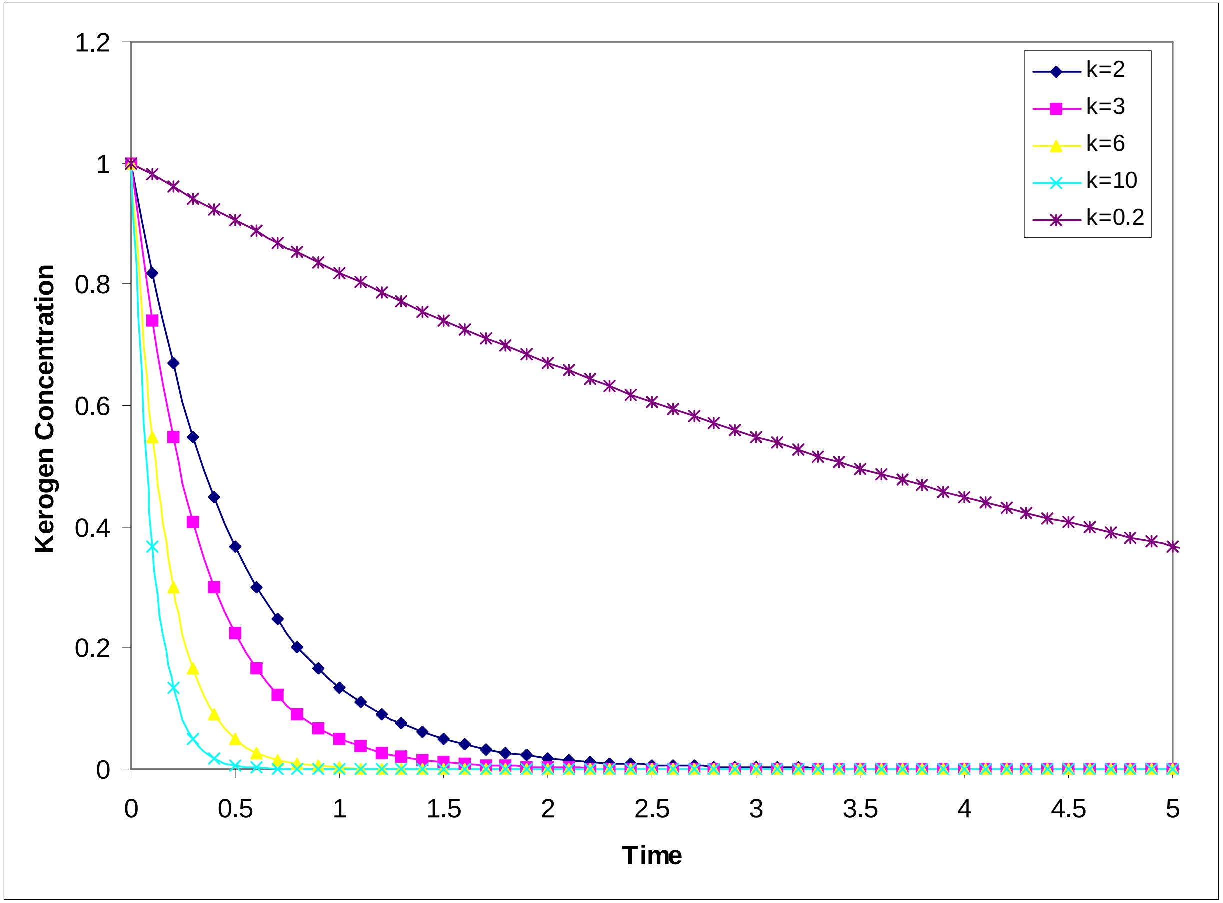

Figure 3 Variation of kerogen concentration with time for different kinetic constants

Oil Shale Pyrolysis

Mathematical Modeling Results

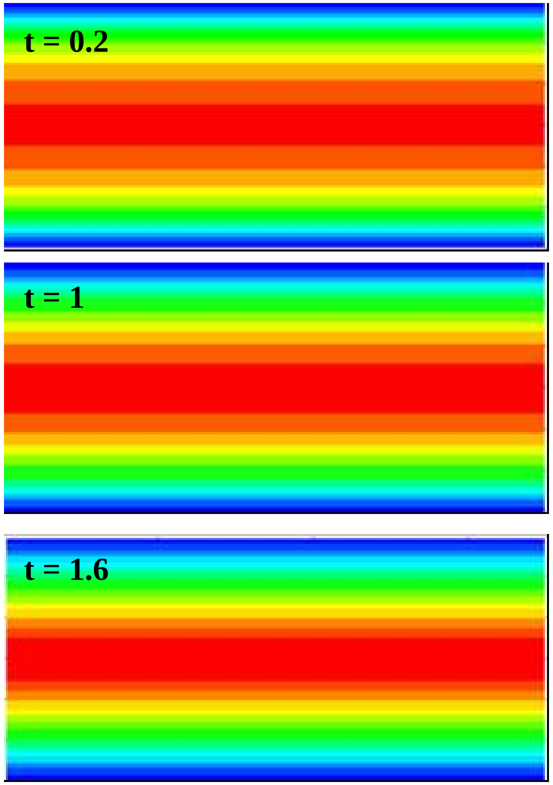

Figure 4 Concentration contours of CO_2 inside the particle

Oil Shale Pyrolysis

Mathematical Modeling Results

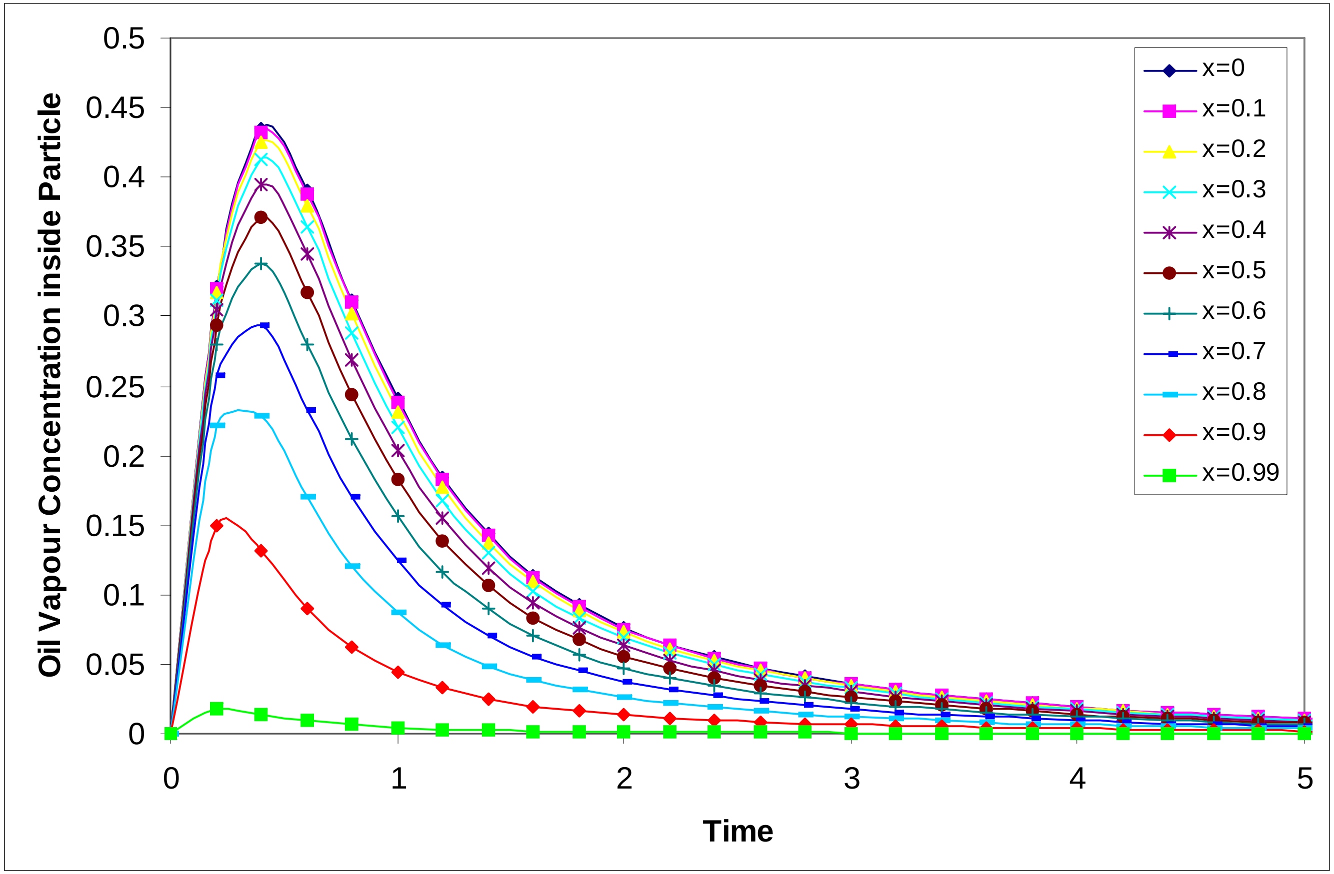

Figure 5 Oil vapour production rate versus time at different particle locations

Oil Shale Pyrolysis

Mathematical Modeling Results

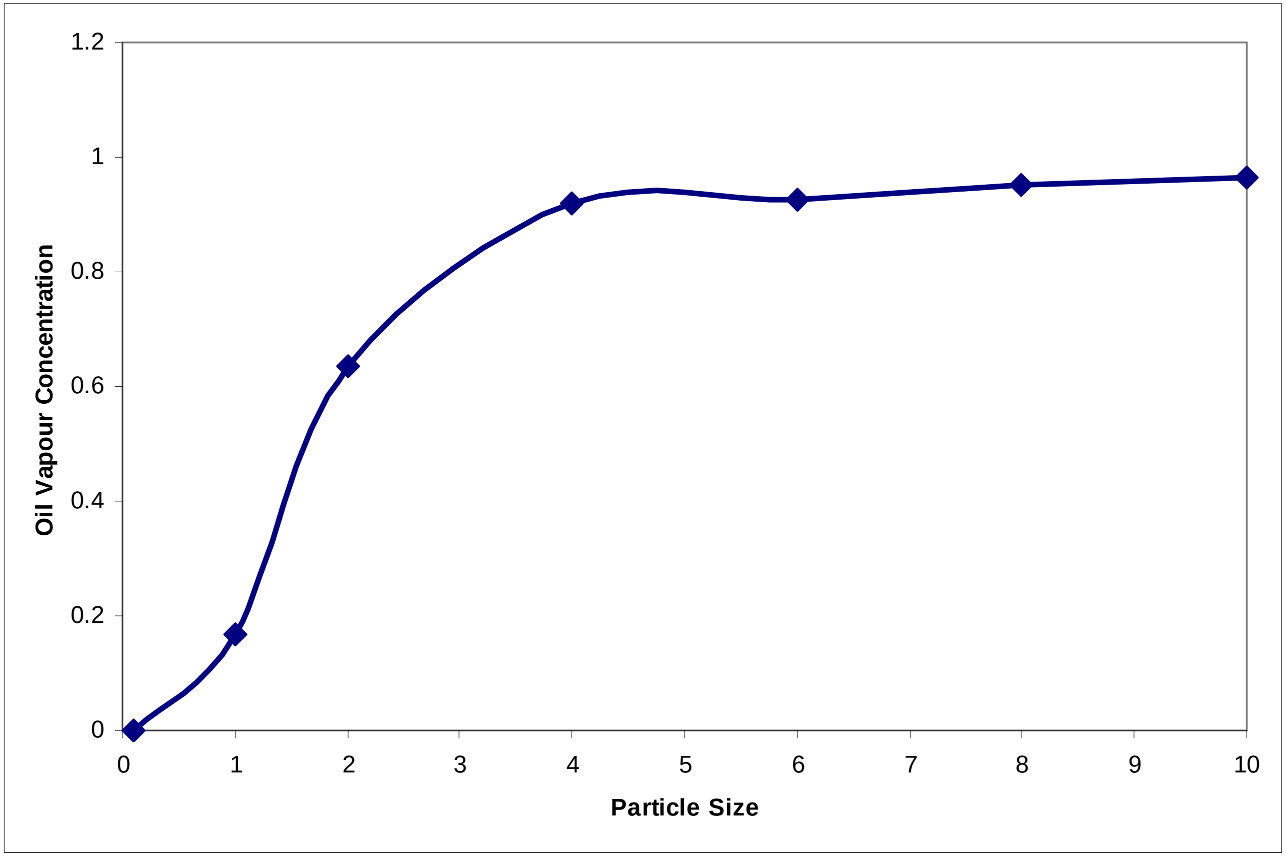

Figure 6 Effect of Particle Size on oil concentration inside particle

Oil Shale Pyrolysis

Conclusions

- Diffusion of produced oil vapors and other components inside the particle was found to influence highly the rate of oil production.
- Particle size would also play a significant role in oil production such that the smaller size, the more and faster production of oil.
- Carbonates found to be an important source of carbon dioxide production in oil shale particles.

Thank You

Global Operations

8700 staff – June 2008

(Yellow indicates regional hub)

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