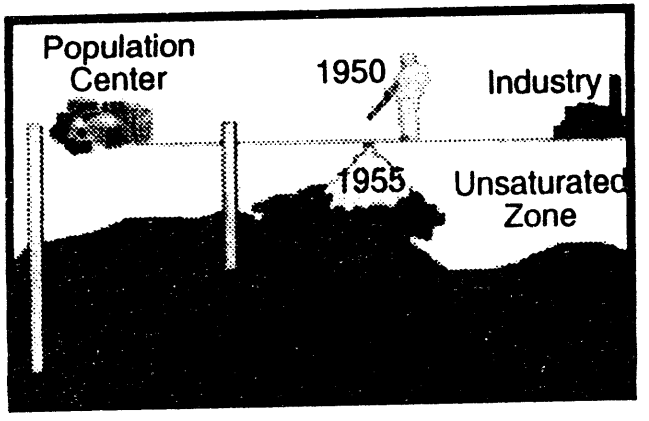
The need to clean up contaminated sites has led to the development of new technologies and capabilities at the national laboratories. Some examples of these are the development of instrumentation and techniques for the rapid characterization of contaminated sites, the use of advanced computers for the modeling of contaminant plumes, testing and validation of in-situ and pumped slurry reactors, new methods for the stripping of organics from aquifers and recovering the organics, and site restoration experience -- returning environmentally distressed lands into productive use.

Advanced Instrumentation is Used for Rapid Site Characterization and Assessment

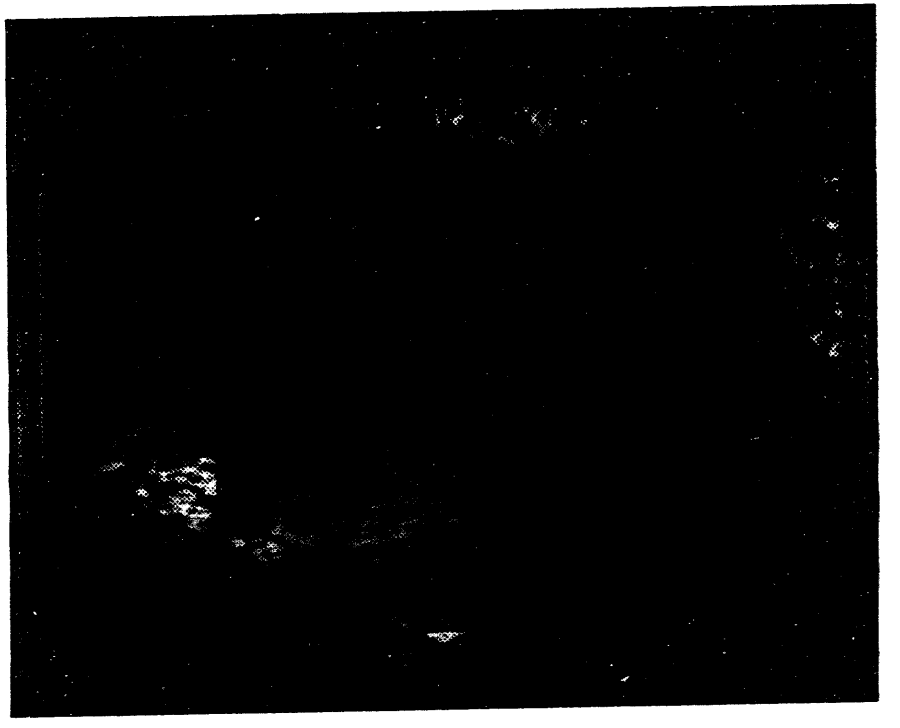
To more rapidly characterize and assess environmentally damaged sites, the laboratories have developed instrumentation and sampling techniques. These include such items as a cone penetrometer, that allows sampling up to 100 feet deep in appropriate soils without drilling and not requiring the use of drilling muds. Other examples include the use of electrical resistance tomography to monitor the rate and location of steam stripping (see slide 13)

An Interdisciplinary Team is Using High Performance Computing Technologies to Model Contaminant Migration



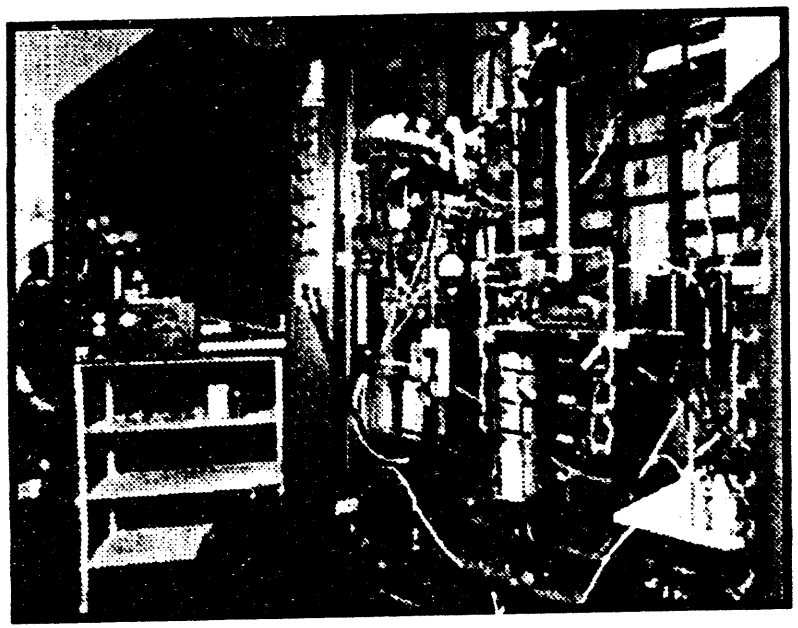
Subsurface heterogeneities give rise to *preferential flow channels* which lead to *fingering* in the contaminant migration.

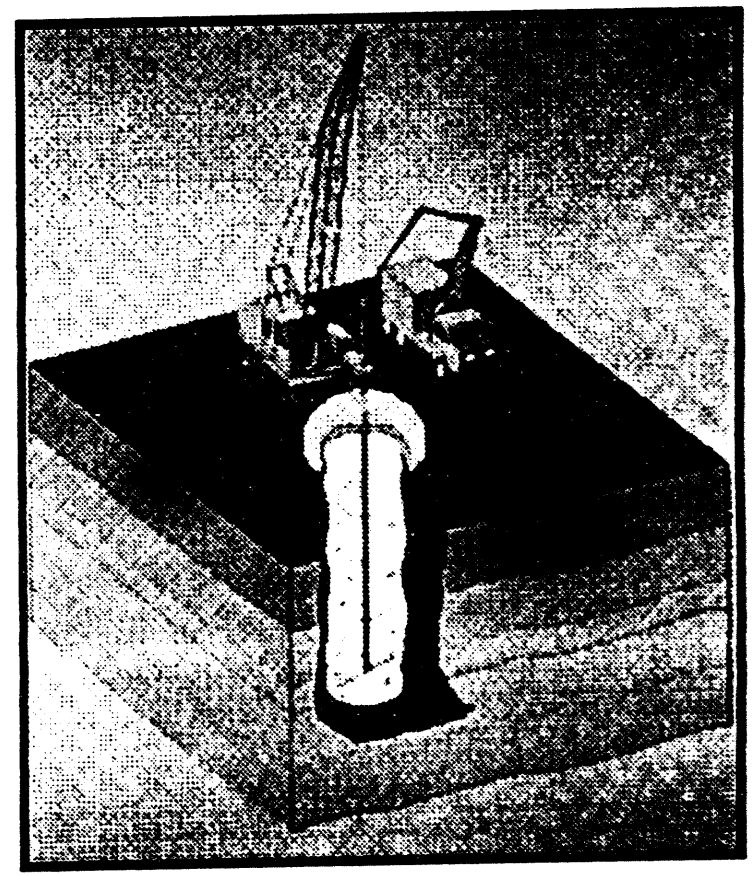
Velocity Magnitude
Computed by ParFlow



When trying to track a spill from several decades ago, through the unsaturated and saturated zones, the use of high performance computing capabilities of the laboratories is being applied to the modeling of contaminant plumes. Subsurface heterogeneity can give rise to preferential flow channels which can lead to *fingering* in the contaminant migration. The right side illustrates the velocity magnitudes, showing a region of dense clay which has blocked the flow of the contaminant, with the different velocities through the uneven porosity being shown in different colors.

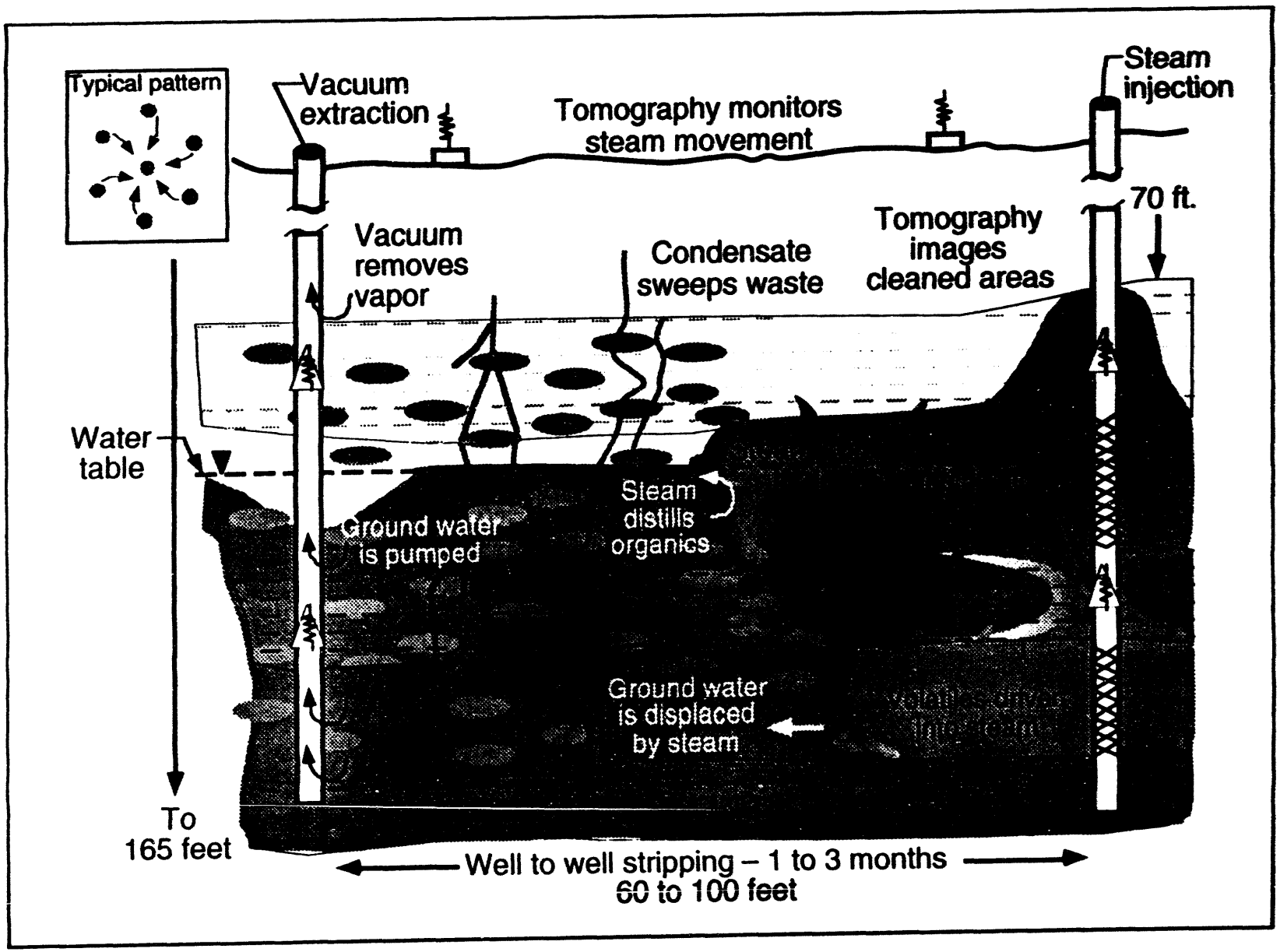
The Laboratories Use Innovative Soil Remediation Technologies for In-Situ Cleanup





The photo on the left shows laboratory apparatus used to develop an innovative stripping technology. The mixer attached to the crane is an artists drawing of an application used to clean up TCE at Portsmouth. A site of one acre 22 feet deep was remediated with 95-98% removal of the organics. This site was a former land farm. Hot air was injected at the trailing edge of the blades of the augur, which is 10 feet in diameter, and the vapors were collected by a shroud at the surface. This technique saved DOE ~$20 million over what had initially been planned for the removal, extraction, and replacement of the soil.

A Dynamic Underground Stripping Process has been Demonstrated to be 50 Times More Effective than Pump-and-Treat

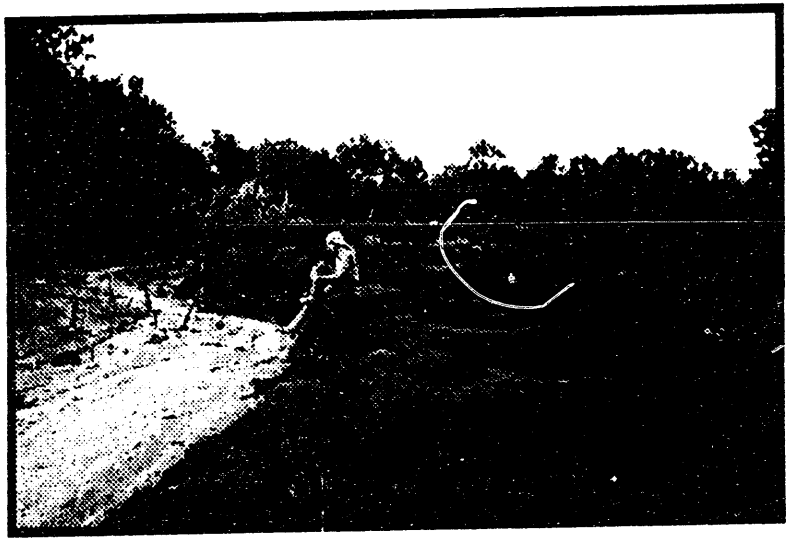


A dynamic underground stripping process has been developed for the removal of organics from underground spills. This process has been shown to be over 50 times as effective as conventional pump and treat, recovering over 7400 gallons of gasoline from an estimated 6200 gallons trapped in soil both above and below the water table.

Steam is injected into the formation, the steam dries the formation, and drives the volatiles into the vapor phase. Vacuum extraction pulls the material out from a central well

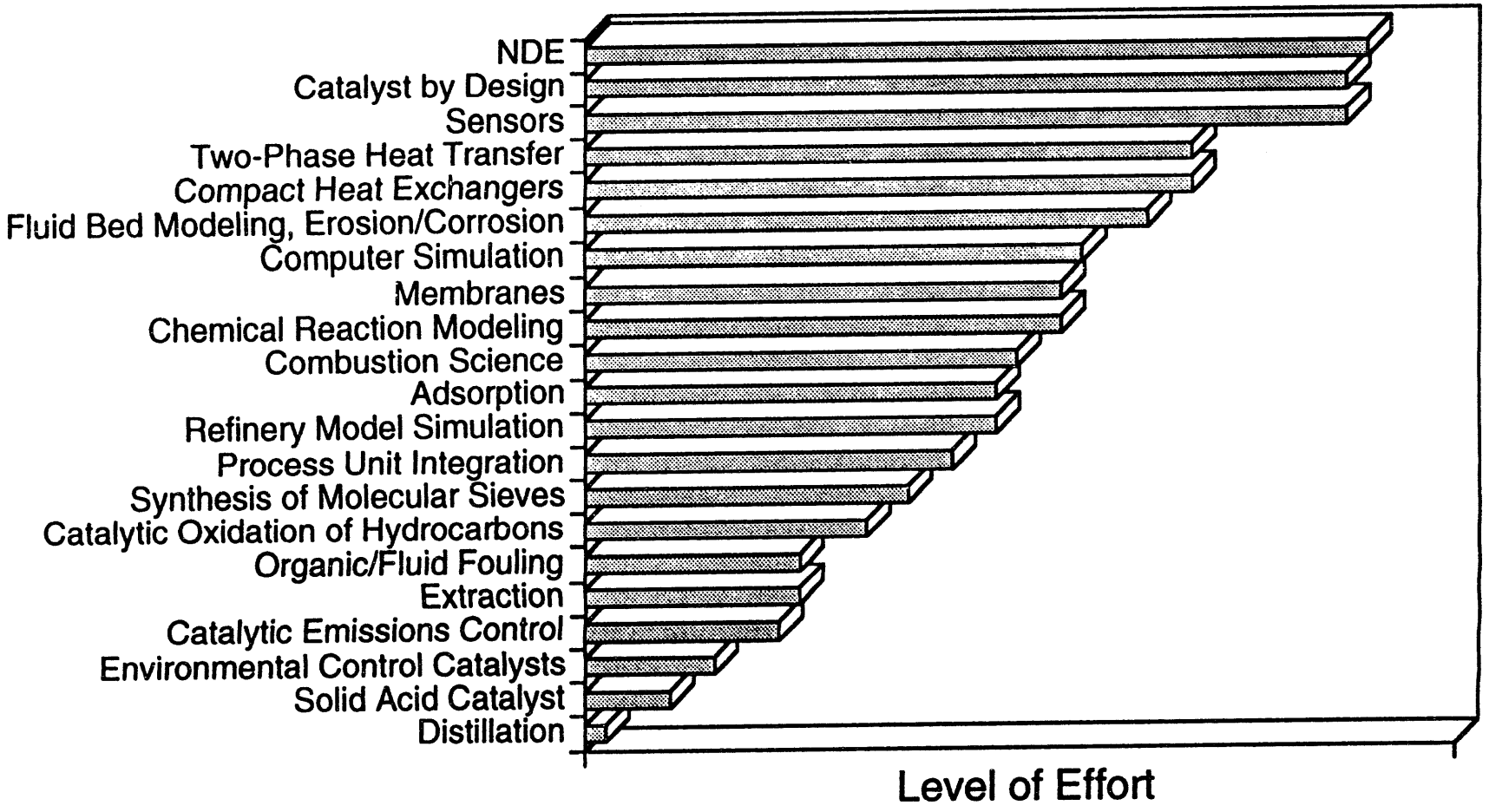
To monitor the dynamic stripping process, imaging methods are used to map the boundary between the contaminated zone and the coo, damp surrounding areas. Electrical resistance tomography has proven to an effective imaging technique for near real-time images of the heated zones.

Environmentally Distressed Sites Have Been Effectively Restored



This slide shows a before and after shot of an environmentally distressed area. This was an abandoned coal mining area, with a polluted stream and eroded soil that could not support vegetation. Restoration of this site resulted in the photo on the right, with a meadow, pond and stream. Similar restorations have been done for the DOD, repairing the damage done from tank training grounds.

The Laboratories Strengths in the Area of Advanced Base Technology Can Complement Refinery Development Needs



The area of Advanced Base Technology is a strength of the laboratory system of DOE. The categories shown in this slide were taken from the draft program plan, and the longest bars on the slide represent over 200 man-years of effort over the past 5 years. Following slides will give examples of some of the technologies in the base technology area.

The Laboratories Have Developed Sophisticated Nondestructive Evaluation Techniques and Specialized Facilities

- Neutron irradiation and Intense Pulsed Neutron Sources
- Synchrotron X-ray radiation sources
- NMR for on-line process control (polymerization)
- Residual and applied stress in components
- Stress corrosion cracking, thermal aging and embrittlement, corrosion fatigue, erosion studies

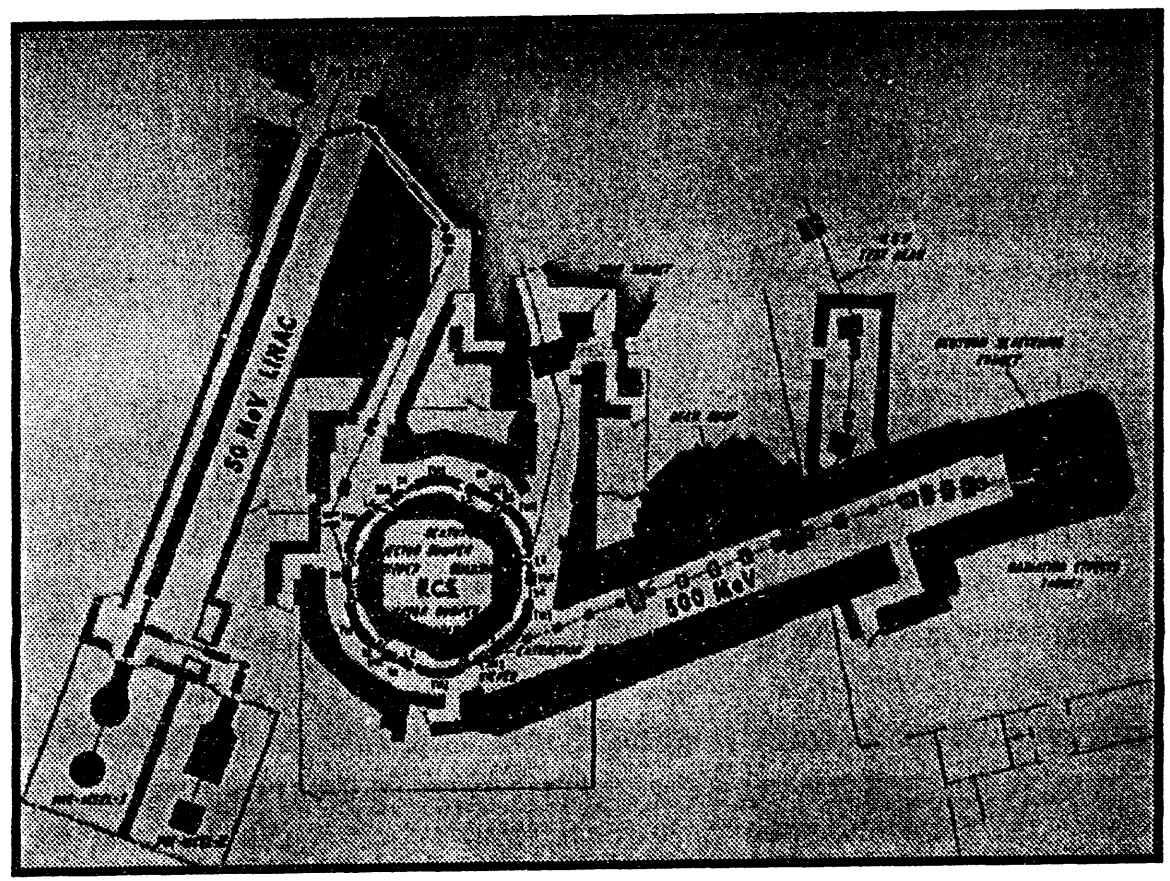
One of the key strengths of the laboratories is the user facilities and specialized equipment that can be applied to industrial problems. These include facilities such as neutron irradiation and Intense Pulsed Neutron Sources that can be used for neutron scattering studies. Neutron scattering allows the measurement of materials properties deep within samples, including residual and applied stress.

The laboratories also operate synchrotron X-ray radiation sources as user facilities. These facilities may be used to study the structure of biocatalysts, and conventional catalysts.

NMR is currently being developed for the on-line control of a polymerization process. The advantage is that quick feedback of operating upsets can prevent the production of lower quality off-spec polymer batchs. This technique may be very applicable for the on-line monitoring of refinery streams, including heavy crudes and asphaltene's.

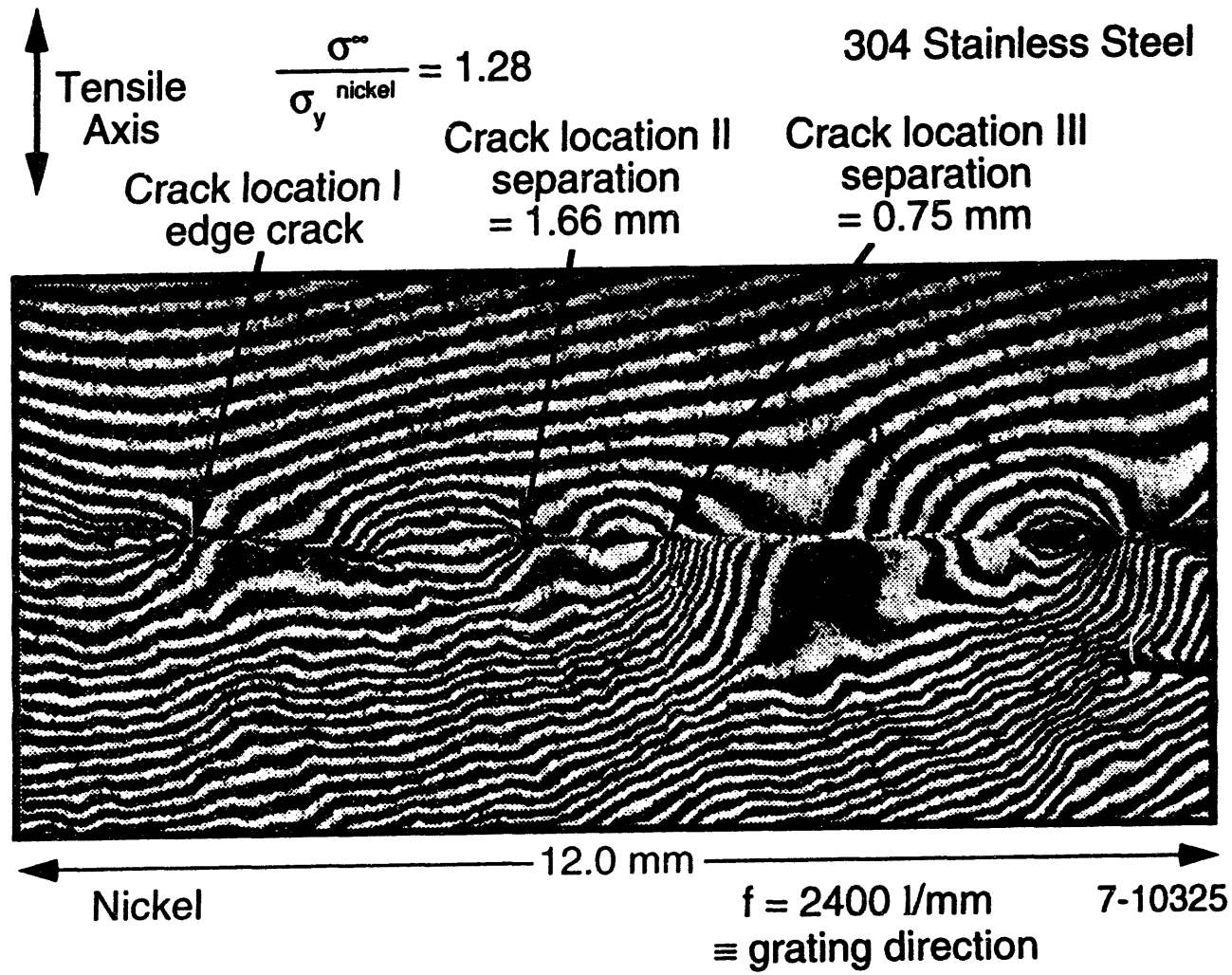
The laboratories have developed considerable expertise in materials related topics, including stress corrosion cracking, thermal aging of materials, embrittlement, corrosion fatigue, and erosion studies. This was developed in support of the nuclear industry, but the expertise and facilities should be applicable to other high temperature, high pressure applications.

The Intense Pulsed Neutron Source (IPNS) is Used for Material Studies and Stress Measurements



An Intense Pulsed Neutron Source (IPNS) may be used for materials studies and stress measurements. Neutrons can penetrate deeply into a sample, and the scattering of the neutrons can be used to measure residual stresses in a composite material. These measurements can also distinguish between the stress born by the fibers and the matrix in fiber reinforced composite materials. Facilities such as these are operated as user facilities by the laboratories, and industrial users can run proprietary experiments with the assistance of the national laboratory staff (if needed).

Moire Interferometry Gives Quantiative Displacement Information at Weld Defects/Crack Growth



Moiré interferometry is used to show the Y or tensile axis displacement fields for a defective 304 stainless steel /pure nickel filler metal weldment. The moiré pattern gives the quantitative displacement field for the weld defect region that forms at the filler/base boundary due to lack of fusion of the nickel filler metal to the 304 SS base metal. The displacement patterns can be used to quickly determine the severity of the defect and to assess the validity of many computer codes predicting failure of a structure. Field portable systems have been developed and used with success.

New Tools and Facilities at the DOE Laboratories Offer Superb Opportunities for the Petroleum Industry in Catalysis

- X-ray synchrotrons for basic catalysis studies
- Computer aided molecular design
- Theoretical analysis of catalytic performance, development of synthetic pillared clays, molecular sieve synthesis
- Scanning Tunneling Microscopy to determine heterogenous catalyst morphology

An example of technologies that exist at the national laboratories that may be of interest to the refinery industry include techniques and facilities that can be applied in support of the refinery development of catalysts. These include:

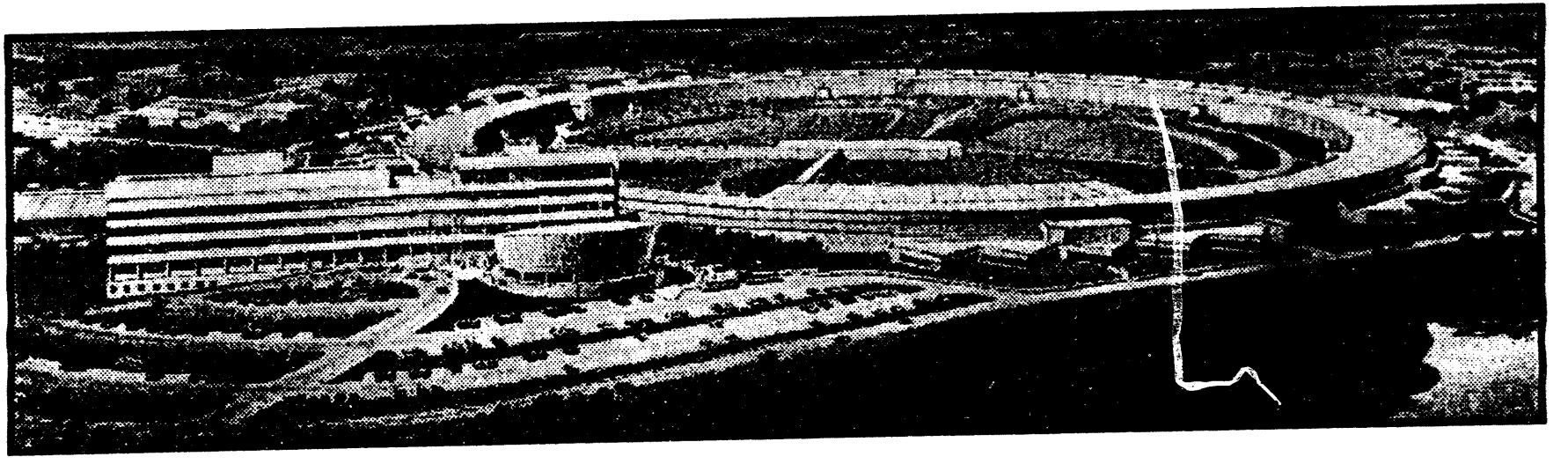
User facilities such as X-ray synchrotrons that can be used for basic catalyst studies. Such devices can allow very fine grained analysis of the catalytic process, including the direct observation of catalytic activity on the surface of the catalyst while the reaction is taking place.

The laboratories are heavily involved in computer aided molecular design that can be used "try out" different molecular configurations in support of catalyst development.

Other activities include the development of synthetic pillared clays that can either have catalytic activity, or can serve as molecular traps, synthesis of molecular sieves, and the theoretical analysis of catalysis performance.

Scanning tunneling microscopy has also been used to study the morphology of heterogeneous catalysts.

Petroleum, Chemical, and Catalyst Companies Have Formed a Collaborative Access Team (CAT) on the Advanced Photon Source



This is an artist's conception of the Advanced Photon Source, which is being constructed by the Department of Energy. This user facility has a diameter greater than the height of the Sear's Tower, and will produce X-ray beams that are 10,000 times brighter than any existing source. These intense X-ray beams may be used for studies of polymerization, catalysis, and other materials studies of interest to the refining industry. A collaborative Access Team (CAT) comprised of petroleum, chemical, and catalyst companies will be setting up a beam line during 1994 for early access to the X-rays when the facility begins operation in 1995.

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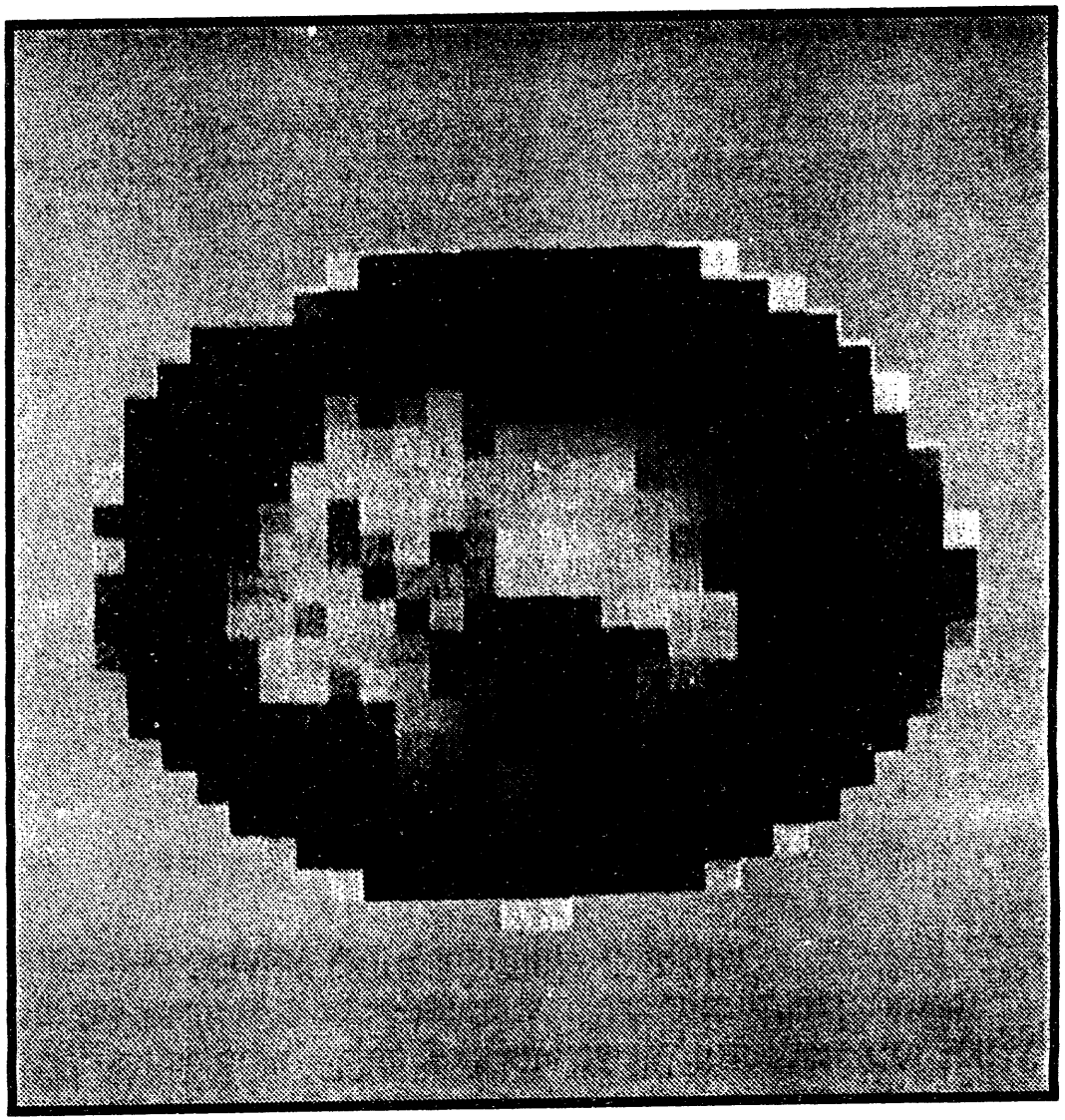
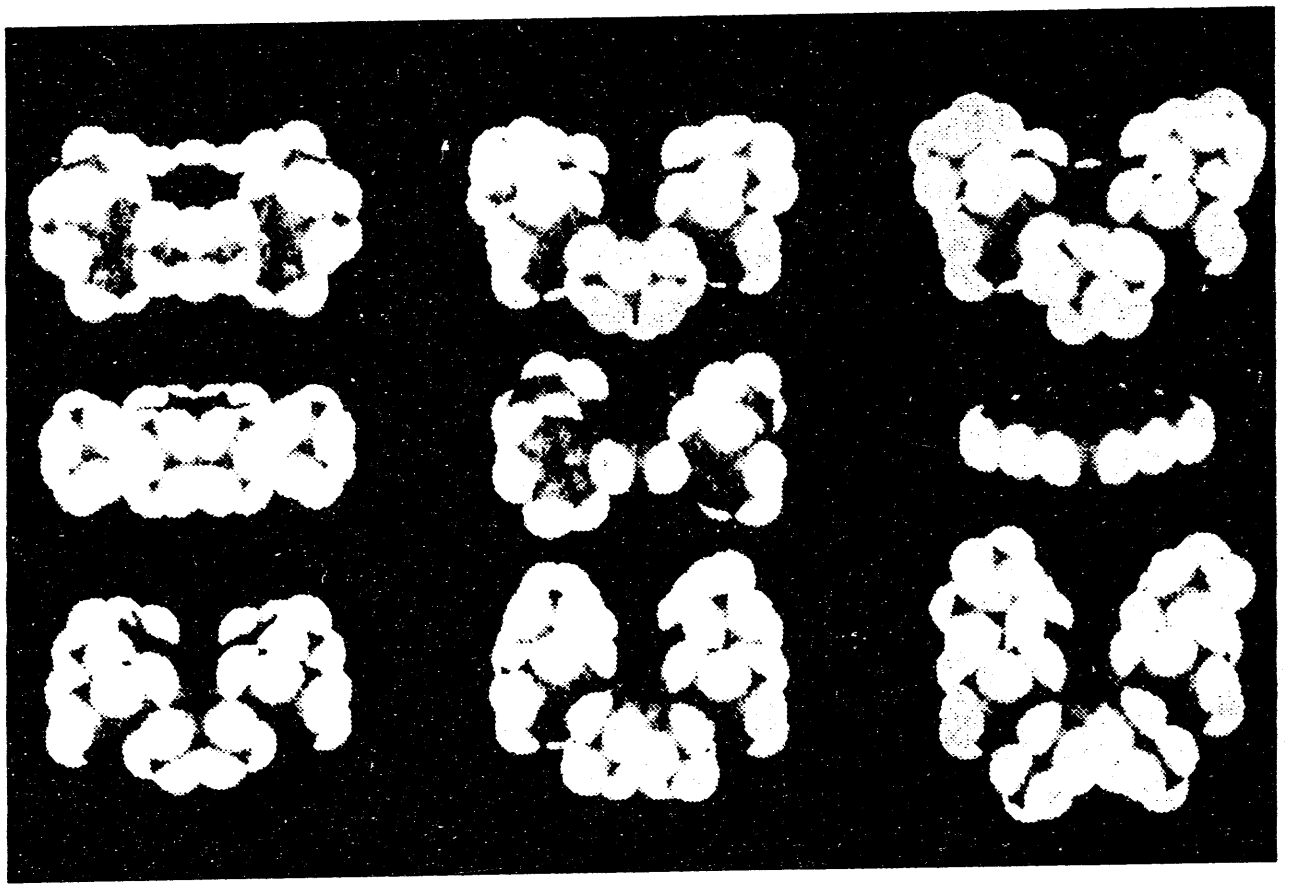
3 of 3

An X-Ray Synchrotron Light-Source Can Be Used to Measure Distribution of Metals in a Catalyst Particle



This is an example of the use of an X-ray synchrotron light-source to study the distribution of metals in a catalyst particle. The particle is 90 micrometers in diameter, and the resolution is at the level of 5 micrometers. The dark (black) areas on the surface represent the presence of Nickel and Vanadium deposits.

Molecular Modeling on the Computer Has Allowed the Design of Molecules Having Specific Properties that Facilitate Catalytic Activity



Molecular modeling on high speed computers can be used to allow the design of specialized molecules. This photo shows different configurations, including some that have been designed to form a "pocket" to help facilitate catalytic activity.

Scanning Tunneling Microscopes are Used to Reveal Heterogeneous Catalyst Morphology

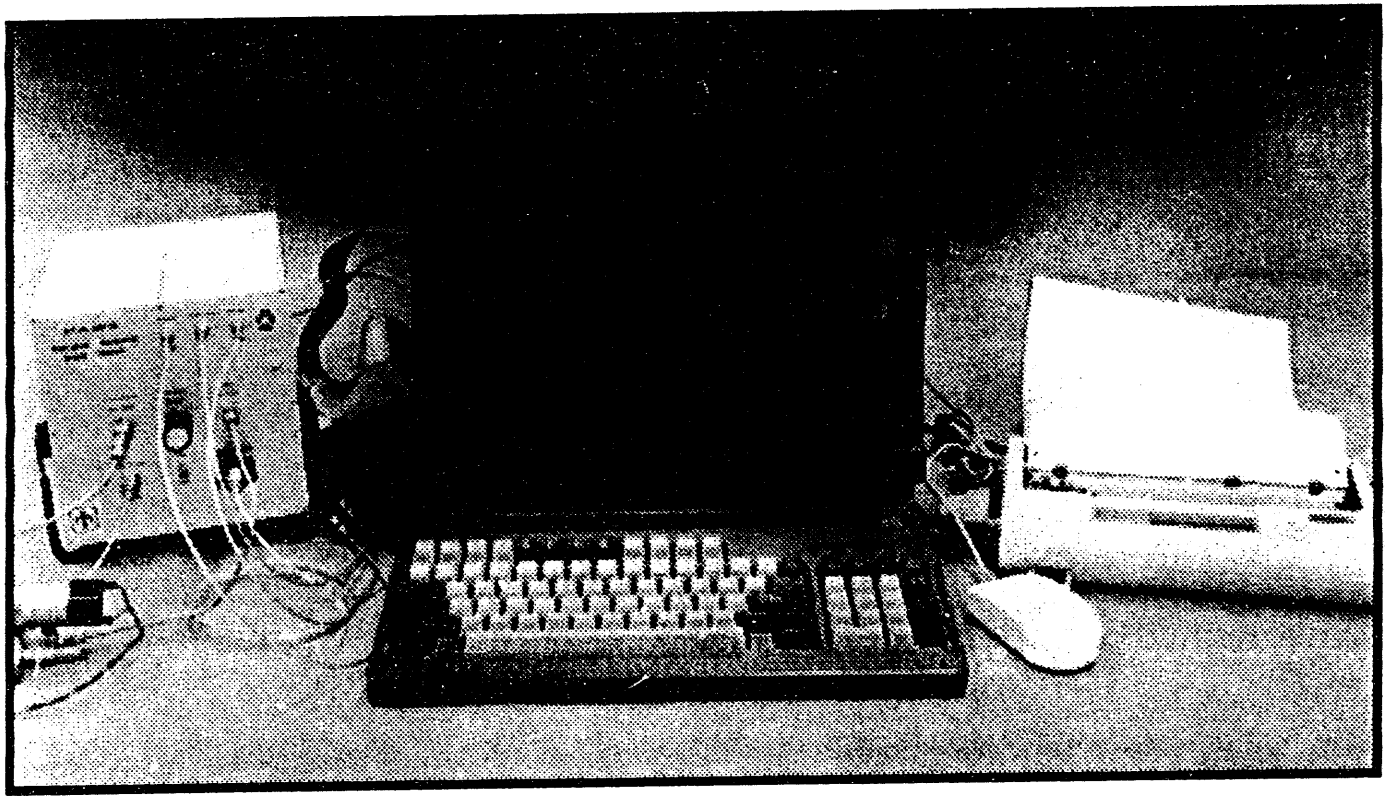
This is a photomicrograph of a catalyst surface, taken using a Scanning Tunneling Microscope to measure the morphology of a heterogeneous catalyst particle. The area scanned measures 300 nanometers on a side.

Advanced Sensor Technologies Being Developed Can Assist in Environmental and Process Control

- Thick-film cermet sensors for gas analysis in hostile environments
- Surface Acoustic Wave Sensors
- Microwave and millimeter wave spectrometry for remote gas sensing
- Mini/micro mass spectrometers for on-line gas sensing
- Ultrasonic velocity and viscosity measurements

The laboratories have considerable work in progress on the development of new sensor and instrumentation technologies. These include thick film cermet sensors that can be used in hostile environments, surface acoustic wave sensors that can selectively detect VOC's, millimeter and microwave spectrometry suitable for remote gas sensing, micro mass spectrometers that can be used for on-line gas sensing (a version is of interest for onboard monitoring of automobile exhaust), and ultrasonic velocity and viscosity measurement devices that are non invasive to the piping system.

A Portable Acoustic Wave Sensor is Being Commericalized for On-line VOC Emissions Measurements

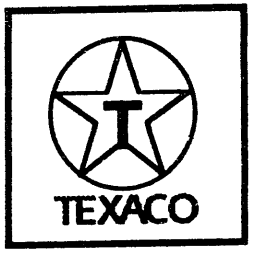


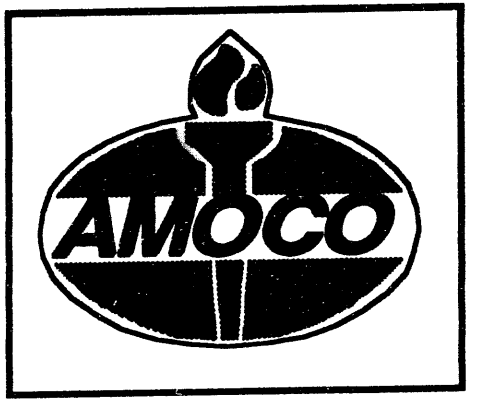
This is a photo of a portable acoustic wave sensor that is being commercialized for on-line measurements of VOC emissions.

Thick Film Cermet Sensors Can Distinguish Multiple Gases in Hostile Environments

This is a photo of a thick film cermet sensor being developed by the laboratories. The sensor is compared in size to a nickel, and contains a heating array, sensing elements, and reference electrodes in a solid state ceramic configuration that allows operation at temperatures of up to 300 °C.

A CRADA to Assess Air Toxic Emissions, Understand Their Origin, Fate, and Mechanisms of Formation and Destruction is Being Negotiated With





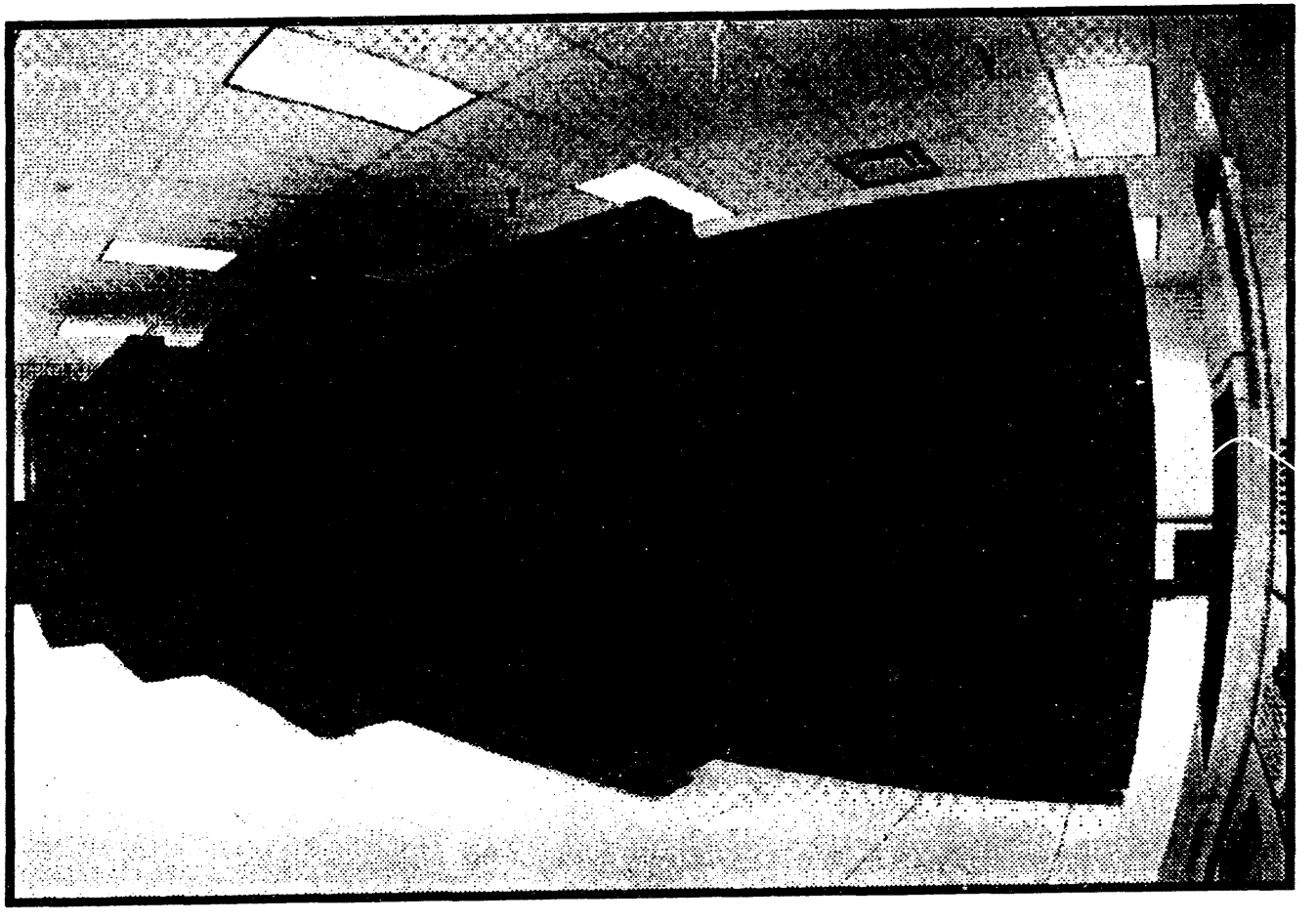
Six oil refinery companies are currently negotiating a CRADA to assess air toxic emissions, understand their origin, fate, and mechanisms of formation and destruction with some DOE national laboratories. This activity stems from a long term ongoing effort to better understand combustion processes at the national laboratories.

DOE Laboratories Have Developed Enormous Computer Modeling Capabilities for Complex Problems Applicable to Refinery Problems

- Reactive flows in engines, burners, etc.
- CVD processes
- Sprays and particulates
- Porous media flow – subsurface contaminants
- Flows over and through catalysts
- Process reactors
- 3D fluidized-bed reactors

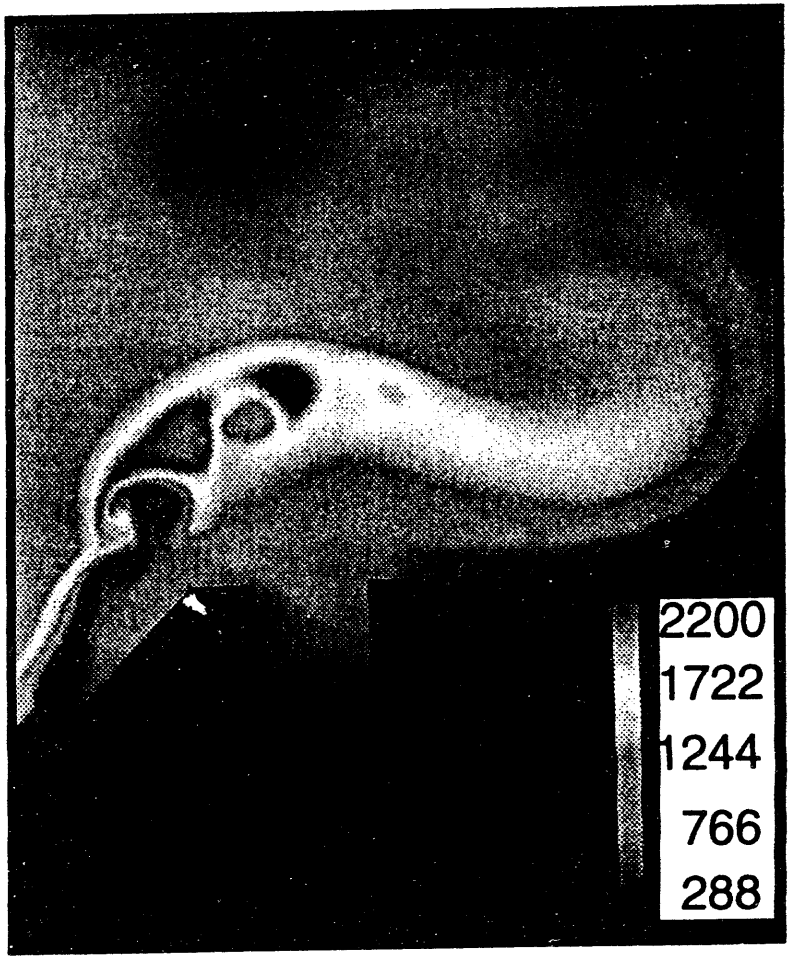
The laboratories have developed considerable computer facilities and expertise for modeling complex problems applicable to refineries. These include reactive flows in engines and burners, CVD processes, the modeling of sprays and particulates, porous media flow -- particularly of subsurface contaminants, the flow over and through catalysts, modeling of process reactors, and the modeling of erosion and corrosion of fluidized bed reactors. The next several slides will provide a few examples.

The DOE Laboratories Have Unparalleled Facilities and Staff for Advanced Computations



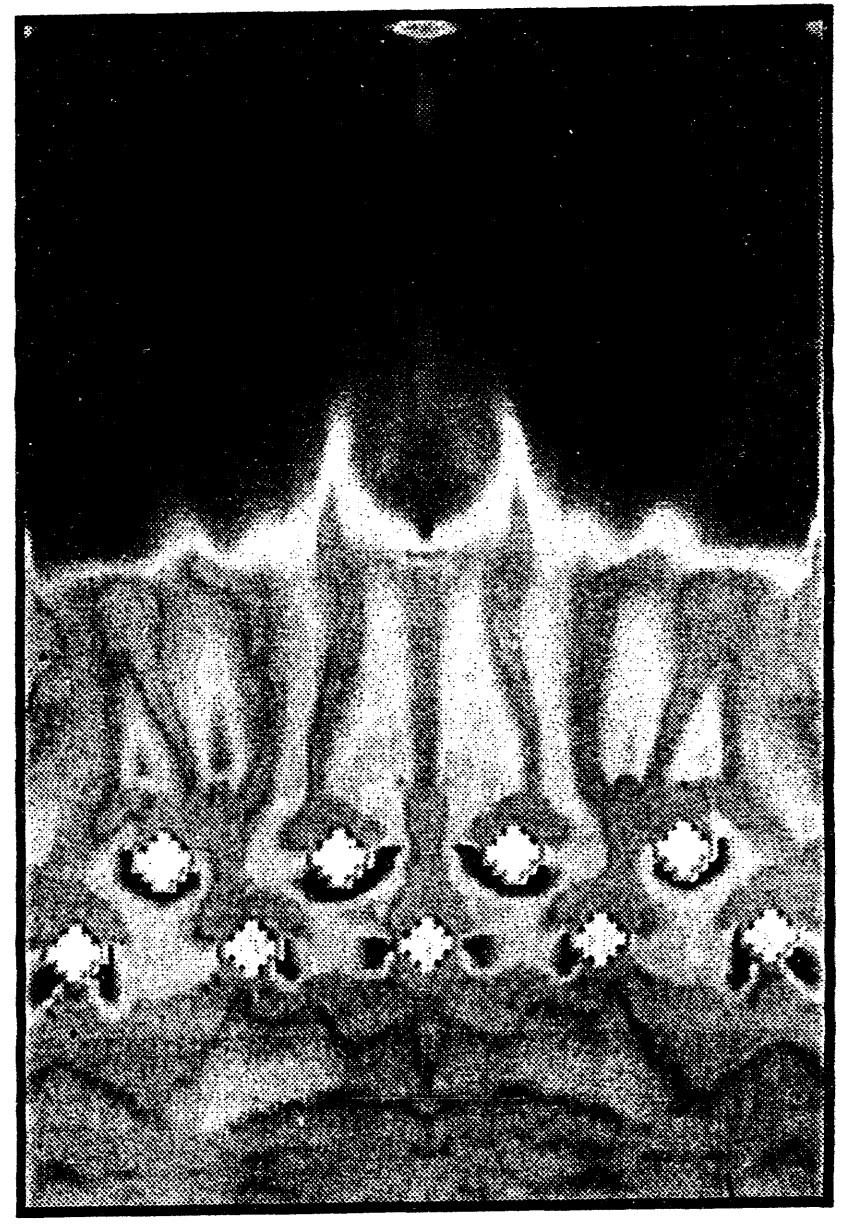
This is a photo of 5 parallel computers that are representative of the facilities that the laboratories can bring to bear on massive computational problems

Computer Models of an Industrial Burner Assists in the Design of an "Ultra Low NO_x" Burner



This is a computer generated model of a flame in a burner. By modeling the flame temperatures, engineers can modify the design of the burner to achieve lower NO_x performance. Similar modeling efforts can help design combustion processes to limit the amount of particulates, etc.

Validated Models of Fluidized Bed Reactors Allow Determination of Erosion, Corrosion, and Efficacy of Fluidized Catalytic Reactors



This is a computer generated flow map of a fluidized bed with heat exchanger tubes in place. The model predicts variations of the density of solids, the velocity and density of gases, and the particles motion. This model was used to study the erosion of heat transfer surfaces in fluidized bed combustors.

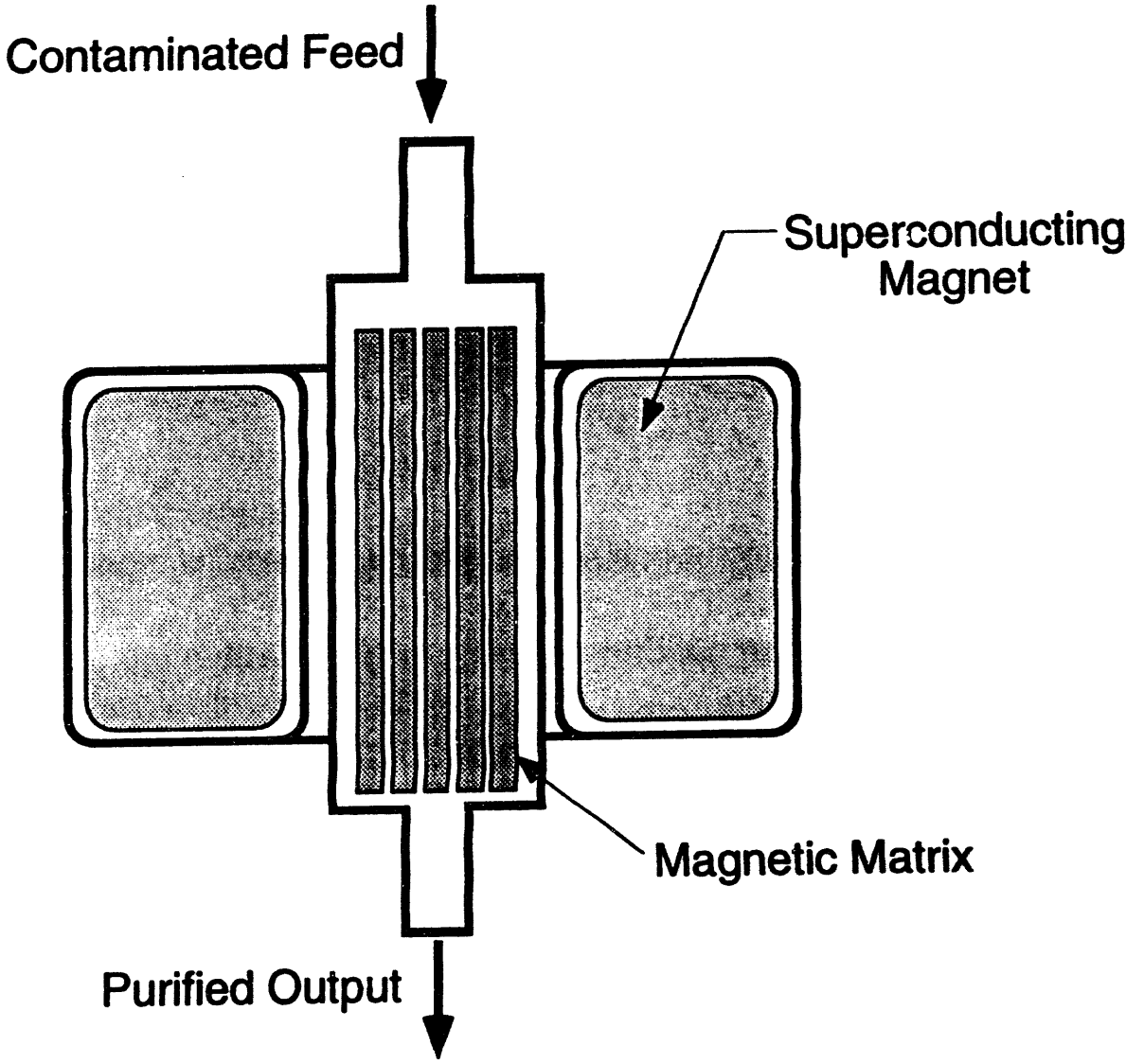
Separation Sciences Developed for DOE Purposes can be Utilized in Refinery Processes

- Advanced organic and inorganic membranes
- High gradient magnetic separation
- Open gradient magnetic separation
- Ion-exchange for metals removal
- Electrochemical recovery of metals from spent catalysts
- Electrodialysis for desalting, purification, and concentration
- Emulsion phase contactors
- Liquid-liquid extraction

The laboratories have developed skills, facilities, and expertise in the area of separations for DOE problems that can be used for refinery processes. These include:

Membranes, both organic and inorganic, magnetic separation facilities (both high gradient and open gradient techniques), ion-exchange for metal removal (discussed earlier), electrochemical recovery of metals from spent catalysts, electrodialysis for desalting, purification and concentration of organics and salts, emulsion phase contactors that utilize electrical charge to disperse and coalesce organics in aqueous media for intimate contact, and liquid-liquid extraction capabilities (discussed earlier).

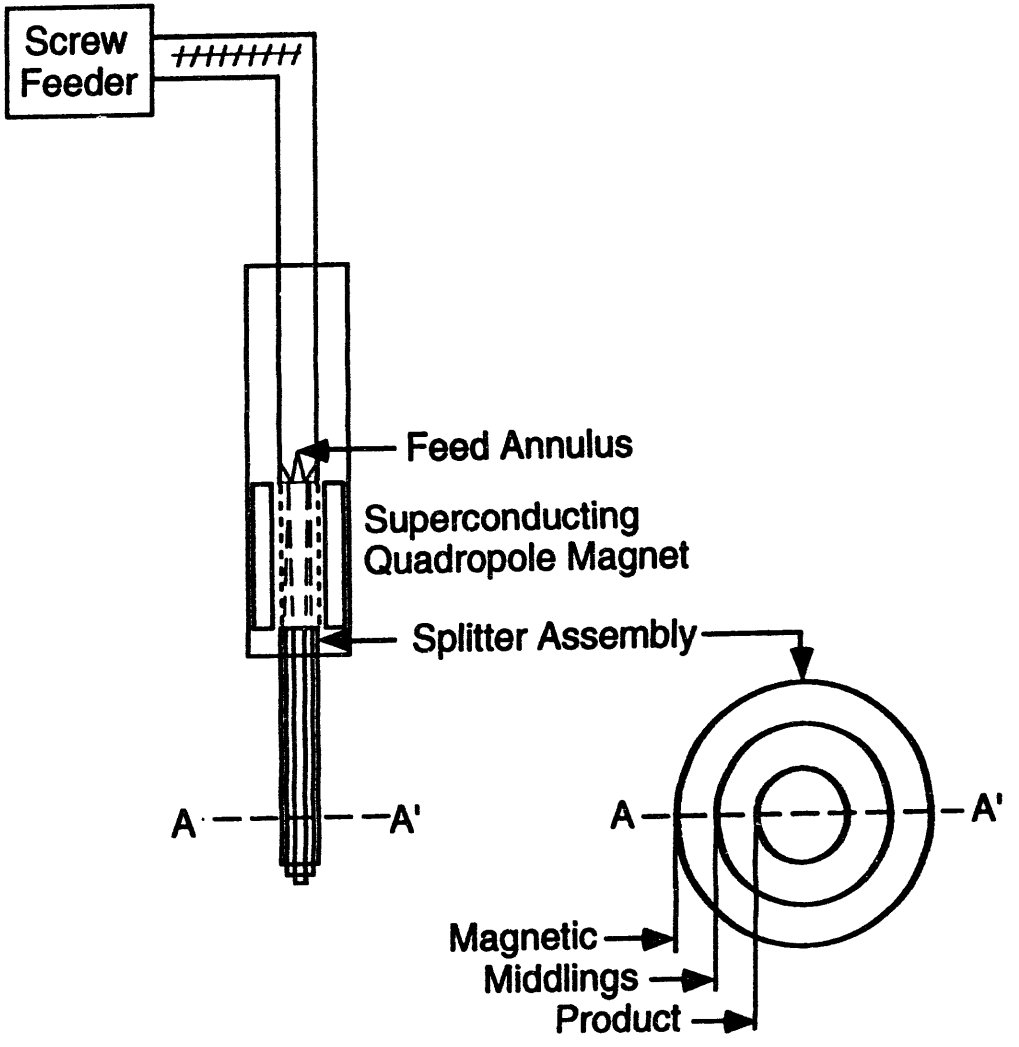
High Gradient Magnetic Separation (HGMS) Removes Paramagnetic Contaminants from a Liquid Slurry



High Gradient Magnetic Separation (HGMS) uses a matrix of magnetic material (such as steel wool) in the flow system, surrounded by a magnetic coil. When the coil is energized, magnetic particles contained in a liquid slurry are attracted to the matrix material, and removed from the slurry. Periodically, the flow is reversed and the magnetic field is turned off to flush the trapped impurities from the matrix.

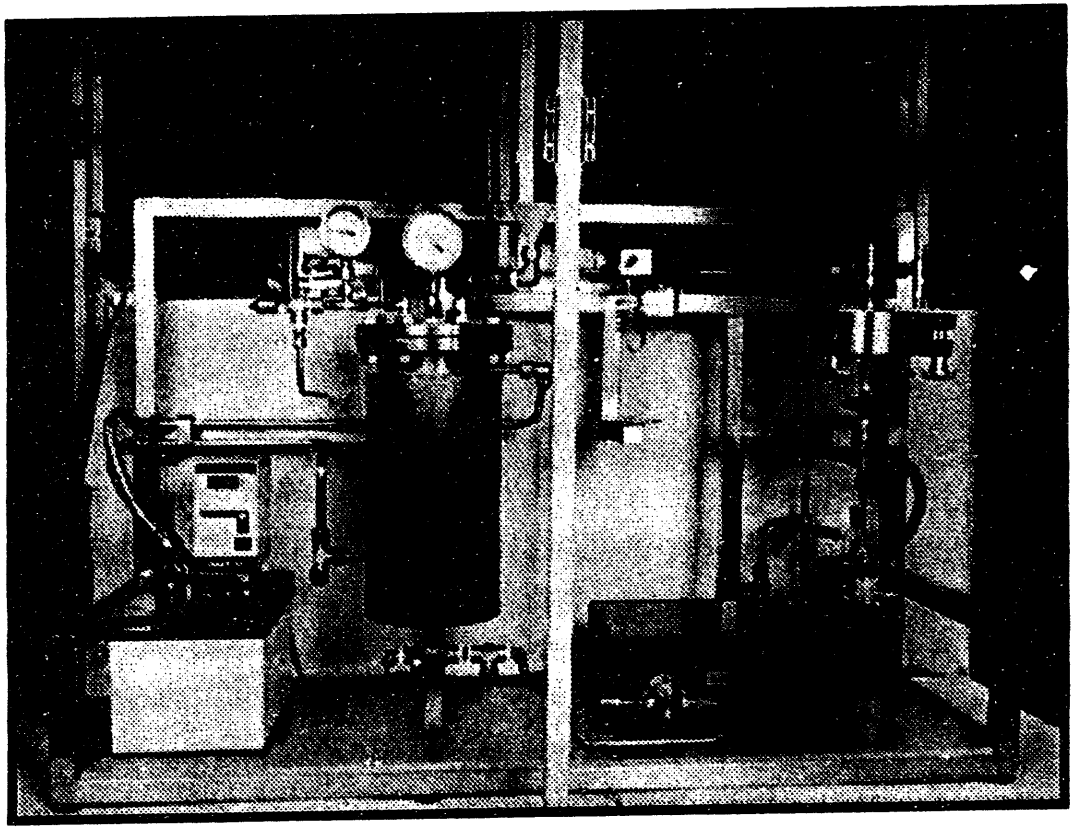
This type of magnetic separation is particularly suited for removing magnetic fines from liquid suspended slurries.

Open Gradient Magnetic Separation (OGMS) Can Separate Active and Inactive Fluid Cat-Cracking Catalysts



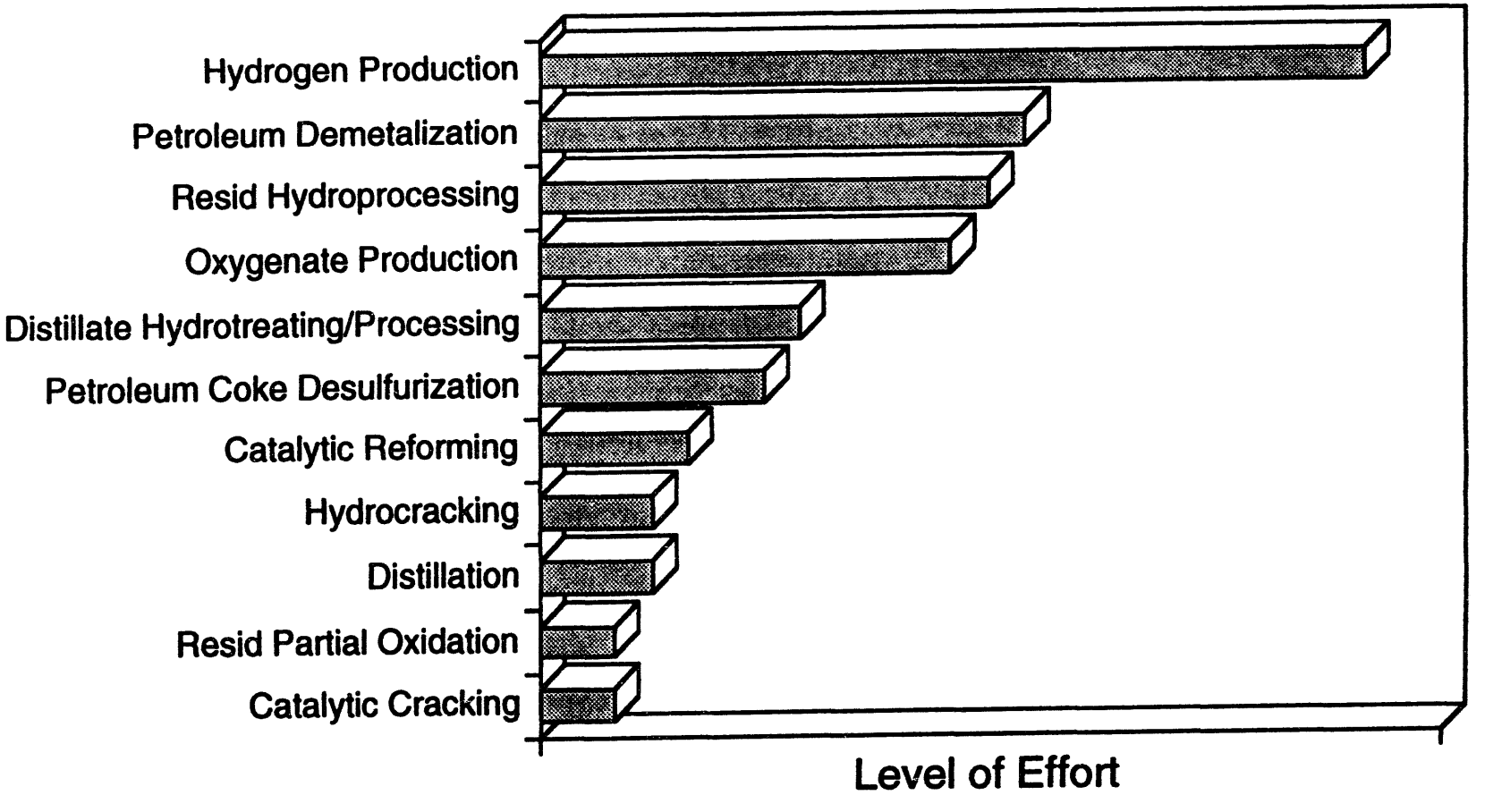
Open Gradient Magnetic Separation (OGMS) utilizes a continuous process, in which a dry powder containing materials of differing magnetic properties are dropped through an open bore. A super conducting quadrapole magnet creates a very steep gradient across the bore, and para-magnetic materials are moved to the outer circumference, and diamagnetic materials move towards the center of the bore. This apparatus lends itself to continuous operation, and the potential for using multiple stages in a separation process.

Inorganic Polymer Membranes Based on Polyphosphazenes Can Function in Harsh Environments



This photograph displays a bench scale membrane separation system that has been used to develop polymer membrane systems designed to operate in harsh environments. Work is in progress under a CRADA to develop bench and commercial scale systems based upon a family of inorganic polymers called polyphosphazenes. An integrated capability is in place for the synthesis, casting, and testing (gases and liquids). These membranes look particularly attractive in the area of halocarbon from water separations and other membranes are available for SO_x and other acid gas separations.

DOE Laboratories Have Process Development Capabilities That Can Augment Refinery Expertise



This chart shows the relative levels of laboratory capabilities for direct support in process technologies that are of interest to the refinery industry. The longest bar (Hydrogen production) represents ~ 110 man-years of effort over the past 5 years.

In this category, the laboratories have only recently begun efforts in such areas as resid hydroprocessing, etc. but have some approaches and techniques that can support the refinery industry in their efforts to improve processes.

DOE Laboratories Have Process Development Capabilities That Can Augment Refinery Expertise

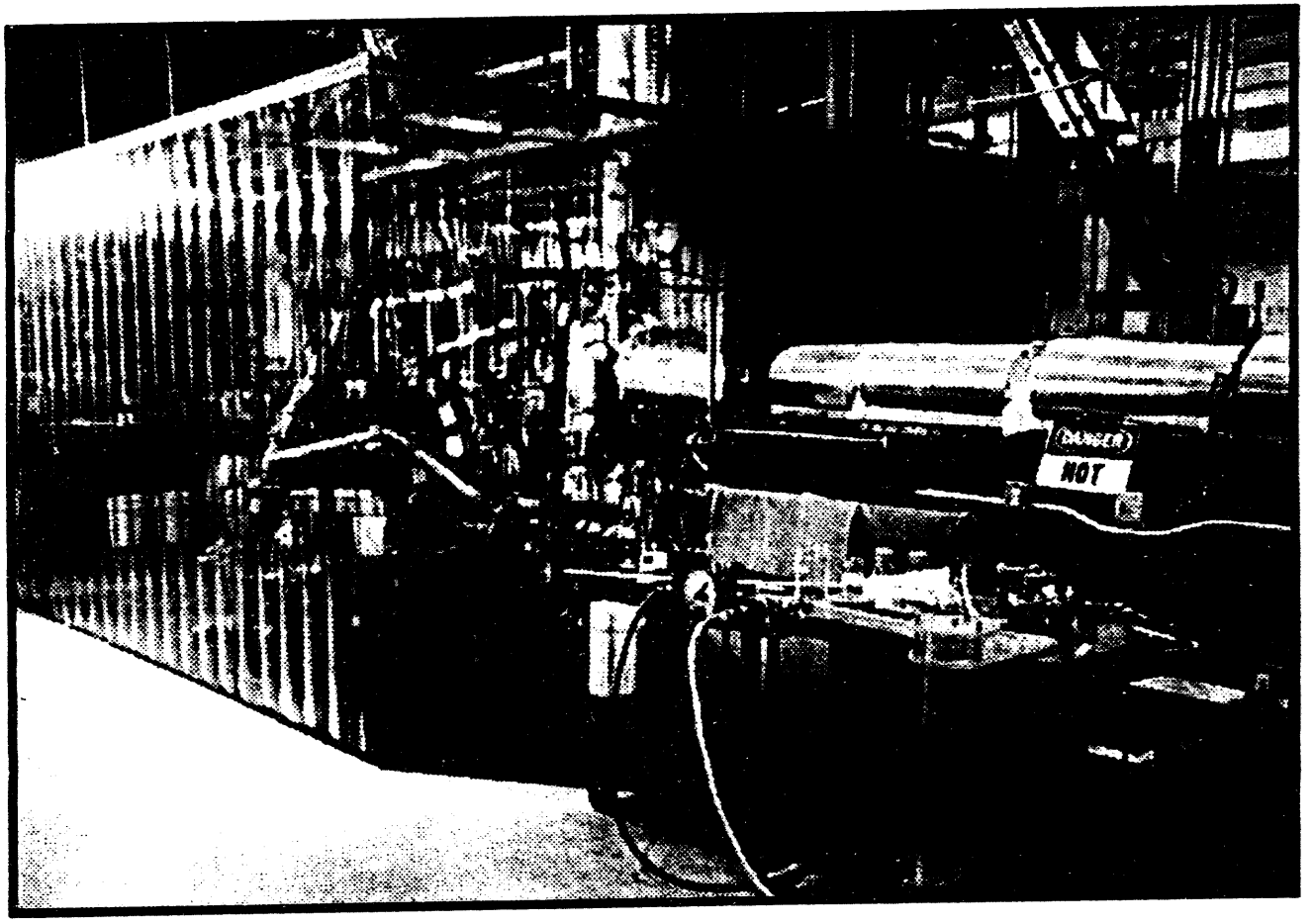
- Hydrogen production and management
- Thermodynamic measurements in support of the oil industry
- Engine and fuel testing facilities
- Oxygenate production

In hydrogen production, one of the processes currently under development with DOE sponsorship is the splitting of H_2S into H_2 and S, so that the hydrogen can be recycled in the plant, and not be discarded as waste water as is current practice with the Claus-SCOTT process.

The laboratories also have extensive capabilities for making very careful and fully supported thermodynamic measurements in support of the oil industry.

Other capabilities include complete engine and fuel testing facilities, and expertise in the production of oxygenate fuels, particularly alcohols.

A Vortex Fast Pyrolysis Reactor Has Been Developed to Convert Materials to Chemical Components for Synthesis



This is a Vortex Fast Pyrolysis Reactor, which was developed specifically to convert bulky, solid particulate material, such as biomass or solid waste, into chemical components for synthesis. This reactor uses external heating (rather than partial combustion), and achieves extremely high heating rates by injecting the solid bearing gas steam at a tangent to the reactor wall. This results in very rapid heat transfer, rapid heating and pyrolysis, and the ability to make fine cuts in the temperature profile seen by the feed material. Although developed for biomass applications, this reactor concept may be useful for other high solids operations in refinery settings.

Thermodynamics Laboratories in the DOE System Provide a Resource to the Petroleum Industry

- Thermochemistry measurements
- Adiabatic calorimetry
- Combustion calorimetry
- Vapor pressure measurements
- Densities
- Spectroscopic measurements

The thermodynamics capabilities in the DOE system can provide a resource for the petroleum industry. Capabilities include adiabatic and combustion calorimeters, vapor pressure and equilibrium measurements, densities, spectroscopic measurements, etc.

Testing Provides Support to the Petroleum Industry on the Performance of Fuels in Engines

- Emissions
- Alternative fuels
- Fuel-engine interactions (auto-oil)
- Engine durability, surface layer activation for on-line engine wear measurements
- Additives (deposit, valve seat sticking and recession)

Testing capabilities at the laboratories includes extensive emissions testing expertise and facilities, the use of alternative fuels (some of the largest alternative fuel fleets are operated by the laboratories for testing purposes), and fuel-engine interactions.

A unique surface layer activation technique for measuring engine durability in hours rather than days of testing has been developed by one of the labs. Other expertise includes the development of additives for inhibiting deposits, valve seat sticking, etc.

The Following Laboratories Contributed to the Information In This Presentation

Argonne National Laboratory
BDM-Oklahoma
Brookhaven National Laboratory
Idaho National Engineering Laboratory
Lawrence Berkeley Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
National Renewable Energy Laboratory
Oak Ridge National Laboratory
Pacific Northwest Laboratory
Sandia National Laboratory

Further information on DOE capabilities may be obtained from:

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