APPENDIX E

DEVELOPMENT OF RESEARCH RECOMMENDATION DATABASE

E.1 GENERATION OF COAL LIQUEFACTION RESEARCH NEEDS

A preliminary list of research needs for each technology area was generated by the panel during the first panel meeting. Additional research recommendations were developed through the following sources:

- o Technology overview reports and papers
- o DOE coal liquefaction contractors' reports
- o IEA/International trip reports
- o Personal communications between panel members and other experts
- Technical presentations during site visits.

An updated list of research recommendations was prepared by SAIC staff, disseminated, and passed to panel members during site visits. Panel members reviewed the research needs list and provided additional suggestions and ideas during the course of site visit discussions.

E.2 CATEGORIZATION AND DATABASE DEVELOPMENT

A comprehensive detailed list of research recommendations was generated during this research needs assessment as a result of the site visits and presentations made to the panel and the other activities described above. This list contained recommendations which were both general needs as well as specific projects. A number of the specific projects overlapped one another or were redundant, etc. To make this list of recommendations manageable, it was revised and categorized. and six specific technology areas were defined so that smaller areas would not be overlooked and lost compared to the more dominant technologies. The six technology areas so defined direct are liquefaction, coprocessing, bioliquefaction, pyrolysis, indirect liquefaction, and The recommendations for each area are direct conversion of methane. shown in a separate list.

The research recommendations for each technology were categorized and put into a research breakdown structure and database. This breakdown structure starts with the basic research types of Fundamental and Applied. Each research type has a number of appropriate research categories or general research needs. Specific research recommendations are then listed within each general category as examples of specific projects which can be carried out to fulfill the general research need. The utility of this approach for DOE is that the general research needs or categories can be used to define parts of an overall program while specific recommendations embody specific ideas of work to be carried out. Each general category is given a two-digit number for easy reference within the database, and each specific recommendation has a three-digit number.

As the result of this effort, a total 178 research recommendations in 57 general categories were prepared in this manner to comprise the database, which is shown in Table E-1.

TECHNOLOGY AREA -- DIRECT LIQUEFACTION

Type						
,,	Category					
	No.	Description of Research Need				
1.0 FUI	1.0 FUNDAMENTAL					
	1.1	Characterize coal structure, properties, and reactivity as applied to direct liquefaction.				
	1.1.1	Study ways of separating coal macerals, and their chemical properties.				
D5±	1.1.2	Develop a coal structure-reactivity model based on analytical and behavioral phenomena.				
	1.1.3	Investigate the role of coal porosity in liquefaction.				
D9	1.1.4	Determine role of mineral matter in initial reactions of coal.				
	1.1.5	Talder of the second of the se				
	1.1.6	liquefaction performance with coal structure, properties, and reactivity and develop liquefaction database.				
01	1.1.7	Identify the structures that are responsible for retrograde reactions and study their reactivity and their kinetics.				
	1.2	Study preconversion chemistry of coal feedstock including pretreatment.				
	1.2.1	Study free-radical formation during heating of coal with or without a solvent.				
	1.2.2	Study the interaction of mineral matter and coal macerals as it pertains to coal beneficiation.				
D3	1.2.3	Test pretreatments, such as low-temperature catalytic pretreatment, to enhance coal reactivity and otherwise improve the overall process.				
	1.2.4	Study effects of handling procedures on chemical and physical properties , and reactivity of coal feedstocks.				
	1.2.5	Study application of coal cleaning the feedstock for liquefaction. Study the chemistry and the mechanisms of coal dissolution.				
	1.3.1	Study the multicomponent catalytic dissolution of coal.				
	1.3.2	Conduct model polymer studies of liquefaction chemistry.				
	1.3.3	Investigate effect of solvent mediation in thermal and catalytic processes.				
D7	1.3.4	Develop kinetic models of liquefaction based on coal structure.				
D10	1.3.5	Develop intrinsic quantitative rate expressions for conversions of				
		individual components and ensembles of components as a basis for under- standing initial reaction paths during coal dissolution.				
	1.3.6	Explore the role of electron transfer and oxygen functional groups in coal liquefaction.				
	1.4	Investigate the chemistry involved in the conversion of resid and distillate.				
	1.4.1	Study relationship between chemical composition and reactivity of resids, including reaction kinetics.				
	1.4.2	Conduct a quantitative investigation of the reactivities of various coal liquids in catalytic hydroprocessing with emphasis on competitive reactions and inhibition effects (high-pressure, high-temperature reaction networks, kinetics, modeling).				
	1.4.3	Conduct a quantitative investigation of the reactivities of asphaltenes and compounds representative of asphaltene functional groups in catalytic hydroprocessing.				
	1.4.4	Study product quality as a function of conversion and reaction conditions.				

RESEARCH BREAKDOWN STRUCTURE

TECHNOLOGY AREA -- DIRECT LIQUEFACTION

Type			
41	Category		
		No.	Description of Research Need
	1.5		Explore the use of novel conditions for coal dissolution.
		1.5.1	Study the potential use of chemically directed selective reactions
		11011	(non-thermal) for direct liquefaction.
	1.6		Study the fundamentals of hydrogen-transfer chemistry.
		1.6.1	Study in detail the hydrogen transfer mechanism.
		1.5.2	Investigate new classes of hydrogen-donor solvents.
		1.6.3	Extract the process implications of competing H-transfer reactions in
			bond scission and formation.
	1.7		Study the chemistry and the catalysis involved in upgrading coal liquids.
		1.7.1	Develop new catalysts/processes for upgrading coal liquids.
		1.7.2	Evaluate methods of refining coal liquids.
	1.8		Investigate new and novel catalysts for direct liquefaction.
D11#		1.8.1	Develop new catalysts for liquefaction (conventional metal on solids).
D6		1.8.2	Investigate potential homogeneous catalysts for liquefaction.
		1.8.3	Develop methods for the recovery/recycle of catalysts (emphasis on
			dispersed).
		1.8.4	Study soluble bifunctional (hydrogenation/acid cracking) liquefaction
			catalysts.
	1.9		Study the fundamentals of catalysis in direct liquefaction.
		1.9.1	Determine the effects of catalytic deactivation on the reactivities of
D12		1.9.2	various coal liquids and mixtures in catalytic hydroprocessing. Study the mechanism of catalytic hydrogenation and cracking functions to
DIZ		1.3.2	establish their interaction and to determine the effects of thermal
			reactions on these functions.
		1.9.3	Determine why iron is catalytic for low-rank coals.
		1.9.4	Study catalyst deactivation with the objective of learning how to
		11317	reduce it or to maintain catalyst activity.
		1.9.5	Study the effect of H2S, added or generated in situ, on coal
			liquefaction reactions.
		1.9.6	Develop in-situ instrumental methods to study catalyst-substrate
			interactions.
	1.10		Analyze coal liquids and determine their physical and chemical
			characteristics.
		1.10.1	Develop analytical procedures for characterizing and analyzing resid.
		1.10.2	Characterize liquefaction products in a chemically significant way.
		1.10.3	Conduct a detailed analytical comparison of products from diverse
			liquefaction processes and contact times, including characterization of
			liquid products and well-defined fractions in terms of compound classes
			(functional groups)(NMR, MS, GC-MS).
			Develop new instrumental techniques for conversion analysis.
		1.10.5	Develop empirical methods necessary for process monitoring that are
			simple, fast, and cheap and can work in a plant environment.
			Develop standardized method of reporting product quality and yields.
		1.10./	Develop methods for meaningful characterization of coal resids related to resid reactivity.
		1 10 0	Develop methods to identify species and quantify 0 and S functional
		1.10.0	groups in coal and coal resids.
		1.10.9	Develop methods to analyze for trace elements in liquefaction streams
		111417	and another

and products.

Type			
-	Sategory		
		No.	Description of Research Need
		1.10.10	Develop chemmometric IR analysis for process monitoring and performance prediction.
	i.11	1.11.1	Study the fundamentals of liquid/solid separation. Study the fundamentals of solids agglomeration as it pertains to liquid/solids separation.
2.0 APPL	IED		
	2.1		Conduct process research studies for further development of direct liquefaction processes.
		2.1.1	Investigate ways of separating aromatic/aliphatic mixtures.
:08±		2.1.2	Develop new approaches to solubilize coal, building on new information on coal chemistry.
		2.1.3	Develop low-severity first-stage reactor for multi-stage process.
		2.1.4	Investigate novel ways of removing heteroatoms, particularly nitrogen.
		2.1.5	Expand the study of using lower-rank coals as liquefaction feedstocks.
		2.1.6	Study the use of coal mixtures as liquefaction feedstocks.
	2.2	2.1.7	Study the effects of using lower-ash coals as liquefaction feedstocks. Conduct economic studies of direct liquefaction processes and products.
		2.2.1	Assess values of coal liquids as finished products and evaluate their upgradability.
		2.2.2	Conduct periodic economics studies both for well-developed processes and emerging concepts.
		2.2.3	Develop an economic-impact guidance tool.
	2.3	2.2.4	Investigate ways of making higher-value products via coal liquefaction. Develop materials, components, and instrumentation for direct
			liquefaction processes.
		2.3.1	Develop new on-line instrumentation for direct liquefaction processes.
		2.3.2	Develop more reliable high-pressure coal slurry feed pumps.
		2.3.3	Study the metallurgy of process equipment under liquefaction conditions.
	2.4	2.4.1	Assess the environmental considerations of direct liquefaction processes. Investigate environmental problems such as toxicity of products and disposal of mineral matter.
		2.4.2	Prepare a comprehensive updated report on the carcinogenic properties of coal liquids.
	2.5		Conduct pilot-plant and scale-up studies for further development of direct liquefaction processes.
		2.5.1	Design, construct, and test a small-scale continuous-flow unit.
D2		2.5.2	Operate large-scale pilot plant to test engineering concepts, including PDU-scale studies of effects of reaction parameters (temperature, H2 pressure, solvent quality, etc.), and to supply samples for other research.
			Investigate alternative deashing methods, bottoms processing schemes, and process configurations for possible development.
	2.6		Formulate new catalysts for process studies.
			Develop improved physical characteristics for ebullation catalyst at Wilsonville.
	2.7	2.7.1	Find new applications for coal liquids. Conduct research to build engines capable of combusting low-H/C liquids.

PESEARCH BREAKDOWN STRUCTURE

TECHNOLOGY AREA -- DIRECT LIQUEFACTION

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Category

- No. Description of Research Need
- 1944 0.8 Investigate new methods and processes for producing and recovering hydrogen.
 - 2.8.1 Find new catalysts for low-temperature steam gasification of carbonaceous materials.
 - 2.8.2 Find catalysts for steam gasification of residual materials for producing H2 and CO2.
 - 2.8.3 Investigate the mechanism of steam gasification catalysis.
 - 2.8.4 Study the interaction of ash components and catalysts in catalytic gasification.

RESEARCH BREAKDOWN STRUCTURE TECHNOLOGY AREA -- ENDIRECT LIQUEFACTION

Type

Category

No. Description of Research Need

A. NON-SYNTHESIS-SPECIFIC FUNDAMENTAL CATALYSIS RESEARCH

- I2# 1.1 Analyze structure, reactivity, function, role of supported organometallic complexes to elucidate the mechanisms of heterogeneous (as well as homogeneous) catalysts.
- Il 1.2 Develop novel catalyst supports, co-precipitated catalyst precursors, novel ways of surface doping, chemical vapor deposition, plasma doping, and analyze catalyst structures.

B. SYNGAS TO HYDROCARBONS

1.0 FUNDAMENTAL

- 1.1 Perform basic studies of F-T syntheses, including catalysis, and reaction chemistry and mechanisms.
 - 1.1.1 Characterize in-situ the surface of F-T catalyst.
 - 1.1.2 Study the liquid-phase F-T synthesis using ultra-fine iron particles as catalyst.
- 18 1.1.3 Investigate the carbon form leading to deactivation of F-T catalyst.
 19 1.1.4 In F-T and related syntheses use probe molecules to understand and
 - 1.1.4 In F-T and related syntheses use probe molecules to understand and modify product composition. Analyze role of poisons and promoters in determining product composition. Analyze the possibility of homogeneous reactions occurring in F-T.
 - 1.1.5 Study the reaction kinetics and mechanisms of F-T reactions including carbon chain growth, chain branching, and the formation of paraffins, olefins, aldehydes, or alcohols.
 - 1.1.6 Measure the rate-determining step in F-T synthesis under commercial conditions.
 - 1.2 Study the fundamentals of chemical reactor engineering as applied to F-T syntheses.
 - 1.2.1 Investigate the fundamentals of hydrodynamics in 3-phase reactors.

2.0 APPLIED

- 2.1 Develop improved catalysts for F-T syntheses.
 - 2.1.1 Improve the stability of iron F-T catalysts.
 - 2.1.2 Improve the specific activity of ruthenium catalyst for F-T.
 - 2.1.3 Study the production of light olefins from synthesis gas catalyzed by ruthenium on rare earth oxides.
- 2.2 Conduct process development studies for F-T processes.
 - 2.2.1 Develop the fixed fluidized-bed and the slurry-phase reactor systems.
 - 2.2.2 Conduct research leading to improved reactor design for 3-phase reactors and scale-up.
 - 2.2.3 Study the oligomerization of lower olefins to octane enhancers and distillate-range olefins by nickel-based homogeneous and supported catalysts.
 - 2.2.4 Investigate ways to get lower light-ends production with Co catalyst in F-T.
- 15 2.2.5 Investigate maximizing middle distillate yield from syngas.
 - 2.2.6 Study combining sequential slurry-phase F-T and ZSM-S catalysis to maximize aromatics, isoparaffins, and olefins and to minimize methane yield.

RESEARCH BREAKDOWN STRUCTURE TECHNOLOGY AREA -- INDIRECT LIQUEFACTION

Type	O-1		
	Categor	ry No.	Description of Research Need
	2.3		Characterize F-T products and develop applications.
		2.3.1	
	2.4		Conduct economic studies and assessments.
		2.4.1	Perform computer simulation studies of indirect liquefaction processes.
		2.4.2	Determine relative importance of catalyst life, activity, and product selectivity on F-T economics.
		2.4.3	Investigate coproduction of energy, fuels, and chemicals.
	SAS TO O		ES
110 145	DAMENTAL	•	Perform havis studies of alcohol sunthness includion actalusis
	1.1		Perform basic studies of alcohol syntheses, including catalysis, and reaction chemistry and mechanisms.
I7 ±		1.1.1	Study the reaction kinetics and alternative catalysts for methanol syntheses.
		1.1.2	Conduct isotopic and mechanistic studies of methanol conversion.
			Determine chemical reaction mechanisms in methanol conversion to gasoline and distillates.
		1.1.4	Study the process of converting methanol to olefins.
	1.2	••••	Study the fundamentals of chemical reactor engineering as applied to alcohol syntheses.
		1.2.1	Investigate the fundamentals of hydrodynamics in 3-phase reactors.
	1.3		Find new paths to produce octane-enhancing ethers from syngas and its oxygenated products.
14		1.3.1	Find catalyzed paths to produce octane-enhancing ethers from alcohols.
		1.3.2	Find high-temperature (>200 C) catalysts for producing octane-enhancing ethers from alcohols.
	1.4		Find new low-temperature catalysts for the water gas shift reaction which are more sulfur tolerant.
16		1.4.1	Develop sulfur-tolerant low-temperature water gas shift catalysts.
		1.4.2	Improve the activity of existing Cu-based shift catalysts by means of chemical promoters.
2.0 APP	I TEN		
200	2.1		Conduct process development studies for alcohol syntheses.
		2.1.1	Develop the fixed fluidized-bed and the slurry-phase reactor systems.
		2.1.2	Conduct research leading to improved reactor design for 3-phase reactor and scale-up.
13		2.1.3	For the conversion of synthesis gas to C1-C5 alcohols, develop synthese with high ethanol selectivity, minimizing the hydrocarbons made.
		2.1.4	Improve the slurry-phase production of methanol from syndas.
		2.1.5	Study plant simplification and integration of the MTG process (TIGAS).
		2.1.5	Develop the fluidized-bed process for producing olefins and aromatic hydrocarbons from methanol.

- 2.2 Conduct economic studies and assessments of alcohol syntheses.
 2.2.1 Perform computer simulation studies of alcohol synthesis processes.
 - 2.2.2 Investigate coproduction of energy, fuels, and chemicals.

RESEARCH BREAKDOWN STRUCTURE

TECHNOLOGY AREA -- PYROLYSIS

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Туре				
	Categor	ry No.	Description of Research Need	
		NO.	pescription of kesemich ween	
1.0 FUN	IDAMENTAL	Ĺ		
	1.1		Characterize coal structure and reactivity as applied to pyrolysis.	
92≢		1.1.1	Characterize coal functional groups and their relationship to pyrolysis	
			reactivity.	
			Study the mechanisms of oxidative weathering of coal. Study the effects of oxidized components on pyrolysis reactions.	
		1.1.4	Correlate product properties with coal feedstock properties.	
		1.1.5	Determine coal devolatilization rates as a function of coal type.	
		1.1.6	Study the effects of inherently present inorganic constituents on	
			product quality and quantity, and process conditions.	
		1.1.7	Study possible role of inherently present mineral matter or externally	
			added inorganics on the thermoplastic properties of coal.	
	1.2		Study the mechanisms and the kinetics of pyrolysis reactions.	
P6		1.2.1	Study the chemistry and the mechanisms of pyrolysis reactions to learn	
			where products come from and to minimize unwanted secondary reactions.	
		1.2.2	Conduct systematic studies to learn: a) effects of particle size, b)	
			effects of surfaces on nature of secondary reactions, and c) roles of	
		122	free radicals.	
		1.2.3	Determine reaction kinetics of pyrolysis by defining the time and temperature history of coal particles.	
P 7		1.2.4	Define the chemistry and the mechanisms of steam-enhanced pyrolysis,	
• •			under both subcritical and supercritical conditions for steam.	
P3		1.2.5	Compare products and yields of pyrolysis with and without reactive	
			atmospheres (CO, CO2, H2O, H2O, to understand the roles of these gases	
			in the devolatilization of coal.	
		1.2.6	Develop models to interpret coal devolatilization data.	
	1.3		Determine the effects of pretreating the coal feedstock.	
PB		1.3.1	Study the effects of moisture in coal and physicochemical changes that	
		122	occur during drying or rewetting of coal. Study steam pretreatment of coal, especially the effect on carbon	
		1.3.2	conversion and liquid yields.	
		1.3.3	Study effects of feedstock comminution method on product properties and	
			yields.	
		1.3.4	Study effects of alkali addition to coal feedstock on reactions and	
			processes.	
Pi	1.4		Study the chemistry and the mechanisms of catalytic hydropyrolysis.	
	1.5		Characterize the liquid products of pyrolysis processes and their	
		1 = 1	properties.	
		1.3.1	Characterize pyrolysis products for cleaned coals. Investigate the combustion characteristics of pyrolysis liquids.	
		1.5.3	Define the potential toxicological and carcinogenicity problems with	
			pyrolysis liquids.	
	1 6		Characterine anatomic star and its assess?	

- 1.6 Characterize pyrolysis char and its properties.
 - 1.6.1 Work on methods for characterizing reactivity of char for combustion and gasification.
 - 1.6.2 Study the fundamental aspects of combustion of char and char-coal mixtures (e.g., ignition flammability, flame stability, and slagging characteristics.

RESEARCH BREAKDOWN STRUCTURE TECHNOLOGY AREA -- PYROLYSIS

Type

Category

- No. Description of Research Need
- 1.6.3 Define the relationship between the devolatilization conditions of the coal and the reactivity of the resulting char.
- 1.6.4 Study the slagging characteristics of char (and the nature of the corresponding coal).

2.0 APPLIED

2.1 Conduct process studies for further development of pyrolysis processes.

- 2.1.1 Investigate the separation of fine suspended solids from liquid products.
- 2.1.2 Study possible use of low-cost inorganic additives as scavengers for sulfur or nitrogen.

P5#

- 2.1.3 Study staged catalytic hydropyrolysis.
- 2.1.4 Determine distributions of heteroatoms/pollutants as a function of process conditions and coal type.
- 2.1.5 Identify factors controlling product selectivity.
- 2.1.6 Determine effects of reactor design and make design improvements.
- 2.1.7 Assess early low-temperature pyrolysis processes with a view of mitigating their negative attributes by varying process conditions.
- 2.1.8 Study the sensitivity of system performance as a function of process variables.
- 2.2 Investigate novel pyrolysis processes.
 - 2.2.1 Investigate the use of high-energy fields, such as corona discharge, laser techniques, microwaves, to decompose heavier tar fractions, activate H2O molecules, etc.
 - 2.2.2 Investigate radio frequency (RF) or microwave volumetric heating as a potentially useful technique.
- 2.3 Conduct economics studies of pyrolysis processes.

P4

2.5

- 2.3.1 Conduct systems analysis of pyrolysis and hydropyrolysis coupled with qasification/combustion.
- 2.3.2 Assess the sensitivity of process economics (e.g., to changes in the prices of fuels or product compositions).
- 2.3.3 Perform a systems study on the transport, effluents, and handling of pyrolysis liquids, keeping in mind the potential for liberating carcinogens into the environment.
- 2.4 Conduct char utilization and upgrading studies.
 - 2.4.1 Examine alternative uses of char, such as its combustion in fluidized-bed combustors.
 - 2.4.2 Investigate methods and systems for handling hot fresh char.
 - 2.4.3 Study how to create multi-phase, high-density fuels with micronized char.
 - 2.4.4 Study the treatment of char to remove heteroatoms and mineral matter.

 Develop methods for upgrading pyrolysis liquids into useful products.
 - 2.5.1 Develop low-cost novel poison— and coke-resistant catalyst systems for reducing N and S compounds in coal liquids.

RESEARCH BREAKDOWN STRUCTURE TECHNOLOGY AREA -- COPROCESSING

Type			
	Catego	ory	
		No.	Description of Research Need
i.O FUI	NDAMENTA	\ L	
C1#	1.1		Study the fundamental chemistry of coal/oil reactions for coprocessing.
		1.1.1	Study the interaction of alicyclic petroleum-type molecules and coal-type compounds.
	1.2		Study the fundamentals of hydrogen-donor chemistry in coprocessing.
		1.2.1	Study the effects of hydrogen donors in coprocessing.
	1.3		Develop methods for analyzing coprocessing products.
		1.3.1	
2.0 APF	PLIED		
	2.1		Investigate scale-up methods for coal/oil coprocesses.
		2.1.1	Investigate scale-up procedures, problems, and opportunities for combining coal with non-coal-derived heavy organic solvents.
C2	2.2		Conduct process studies to develop coprocessing.
		2.2.1	Study the effects of different feeds on reactivity and product quality.
		2.2.2	Study the influence of residua and coal composition.
	2.3		Develop coprocessing catalysts.
		2.3.1	Optimize the catalyst used for coprocessing.

RESEARCH BREAKDOWN STRUCTURE

TECHNOLOGY AREA -- BIOLIQUEFACTION

Туре

Area

No. Description of Research Need

2.0 APPLIED

- 810 2.1 Identify useful microoganisms and enzyme systems.
 - 2.1.1 Identify nonaqueous enzyme systems to degrade three-dimensional structure (by enhancing solubility and swelling).
 - 2.1.2 Identify optimal organisms for bioconversion of syngas to ethanol.
 - 2.1.3 Investigate potential of microorganisms and biomaterials to decompose nitrogen and sulfur compounds and to clean (pyrolysis) liquid products. Conduct process studies to develop bioreactor systems.
 - 2.2 Conduct process studies to develop bioreactor systems.2.2.1 Develop design of bioreactors to handle solids as feeds.
 - 2.2.2 Optimize reactor design for mass transfer, heat removal, and product preparation.
 - 2.3 Conduct assessment and economic studies of bioprocesses.
 - 2.3.1 Develop reactor and total system design for economic optimization.

RESEARCH BREAKDOWN STRUCTURE DIRECT CONVERSION OF METHANE

Type

Category

No. Description of Research Need

1.0 FUNDAMENTAL

- 1.1 Study the reaction chemistry, mechanisms, and catalysis of the partial oxidation of methane to H2/CO, C2+ hydrocarbons, methanol, and formaldehyde with emphasis on novel approaches to achieve high selectivity.
 - 1.1.1 Study the oxidation of methane to heteropoly oxometalates.
 - 1.1.2 Investigate new low-temperature routes to direct conversion of methane to oxygenates.
- 1.2 Study the reaction chemistry, mechanism, and catalysis for the synthesis of ethylene via the catalytic oxidative coupling of methane with emphasis on approaches to achieve high selectivity.
 - 1.2.1 Study the oxidative coupling of methane over promoted magnesium oxide catalyst.
 - 1.2.2 Study the conversion reactions of methanol and methane over zeolites and aluminophosphates (ALPOs).
 - 1.2.3 Investigate promoted oxidative coupling of methane (including halogen-promoted).
 - 1.2.4 Study the oligomerization of lower olefins to octane enhancers and distillate-range olefins by nickel-based homogeneous and supported catalysts.
 - 1.2.5 Investigate new low-temperature routes to direct conversion of methane to C2+ hydrocarbons.

2.0 APPLIED

- 2.1 Conduct process development studies to develop oxidative coupling processes.
 - 2.1.1 Conduct R&D on fluidized-bed process for oxidative coupling of methane, including high-density fluid beds.
 - 2.1.2 Assess the engineering aspects of alternative routes for the conversion of natural gas.
 - 2.1.3 Evaluate materials of construction to minimize halogen corrosion in direct conversion of methans.
- 2.2 Conduct economic studies to assess processes for the direct conversion of methane.
 - 2.2.1 Perform computer process simulation studies of direct conversion processes.
 - 2.2.2 Investigate coproduction of energy, fuels, and chemicals.