Gas-to-Liquid Technology Research at TAMUQ and its Potentials

Nimir O. Elbashir

Texas **A&M U**niversity at **Q**atar

February 15, 2015

Water & Energy Workshop

HBKU, Education City, Doha, Qatar

Qatar Foundation

مؤسسة قطر
Qatar Foundation

❖ Founded in 1995 by His Highness the Emir Sheikh Hamad bin Khalifa Al-Thani.

❖ Chaired by Her Highness Sheikha Mozah bint Nasser Al-Missnad.

An independent, chartered, nonprofit organization committed to the development of Qatar and its people.

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Weill Cornell Medical College in Qatar

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جامعة تكساس إي أند إم في قطر

VCUQatar Virginia Commonwealth University in Qatar

Northwestern University in Qatar

جامعة كارنيجي ميلون في قطر
Carnegie Mellon Qatar

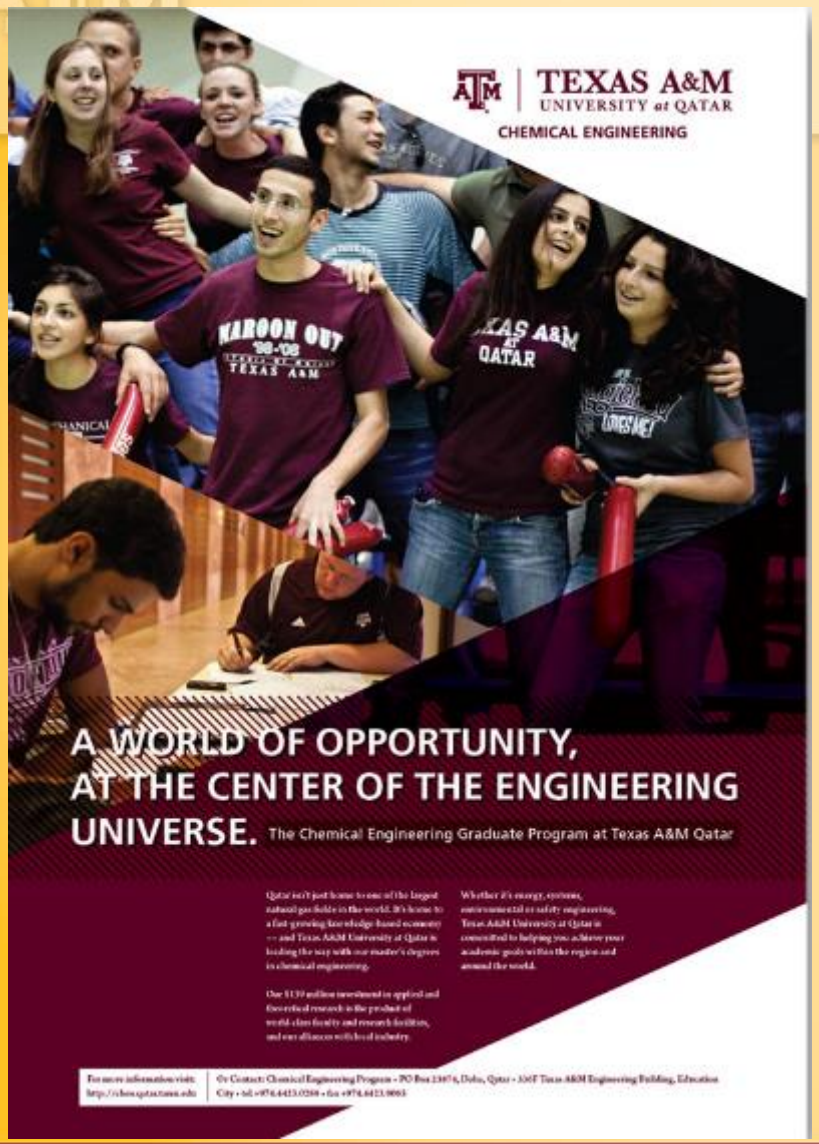
جامعة جورجتاون
GEORGETOWN UNIVERSITY
كلية الشؤون الدولية في قطر
SCHOOL OF FOREIGN SERVICE IN QATAR

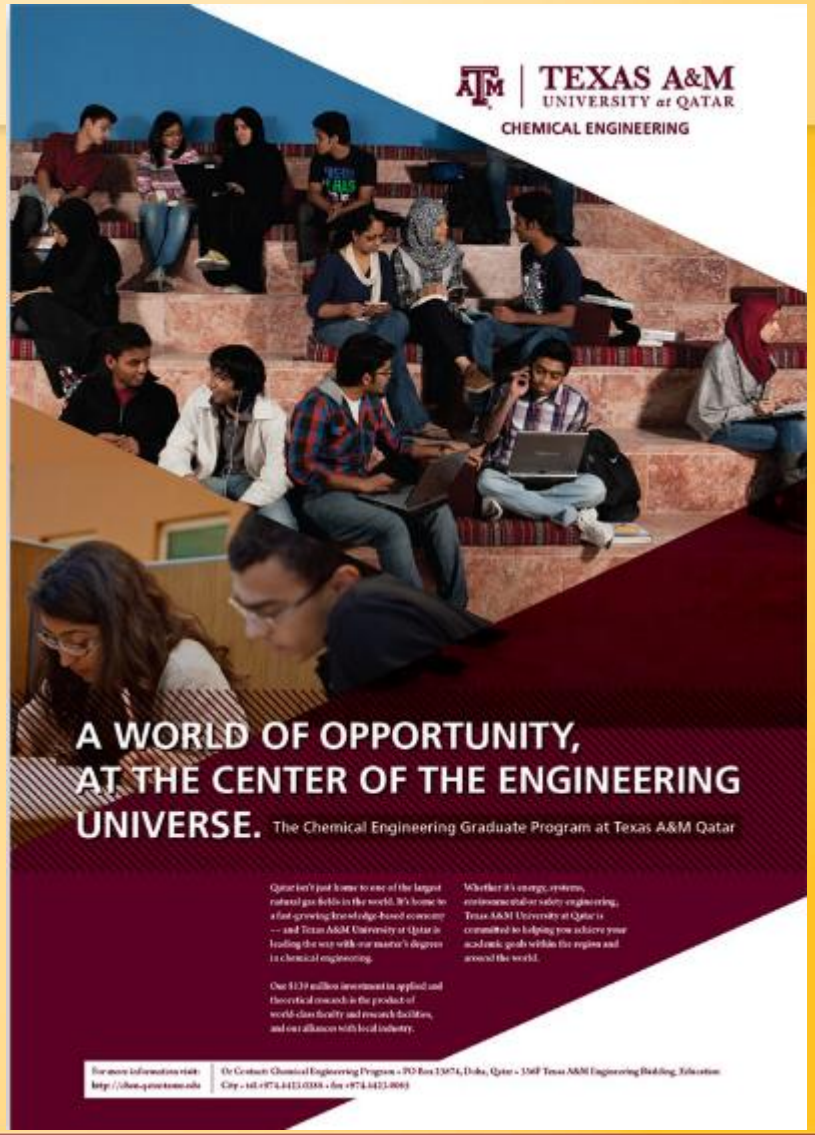
Texas A&M Qatar built on A&M University Heritage

Texas A&M Qatar

550 Students in four majors CHEN, PETE, ELECT, MEEN since 2003

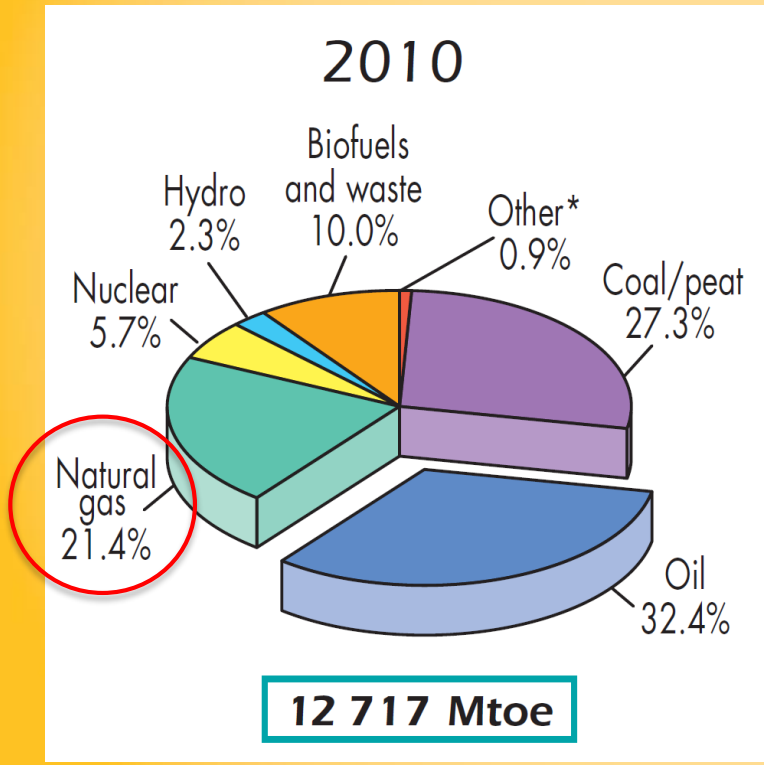
Life in Campus





Qatar's role in the energy market

World's Primary Energy Supply



Natural gas

Producers	bcm	% of world total
Russian Federation	677	20.0
United States	651	19.2
Canada	160	4.7
Qatar	151	4.5
Islamic Rep. of Iran	149	4.4
Norway	106	3.1
People's Rep. of China	103	3.0
Saudi Arabia	92	2.7
Indonesia	92	2.7
Netherlands	81	2.4
Rest of the world	1 126	33.3
World	**3 388**	**100.0**

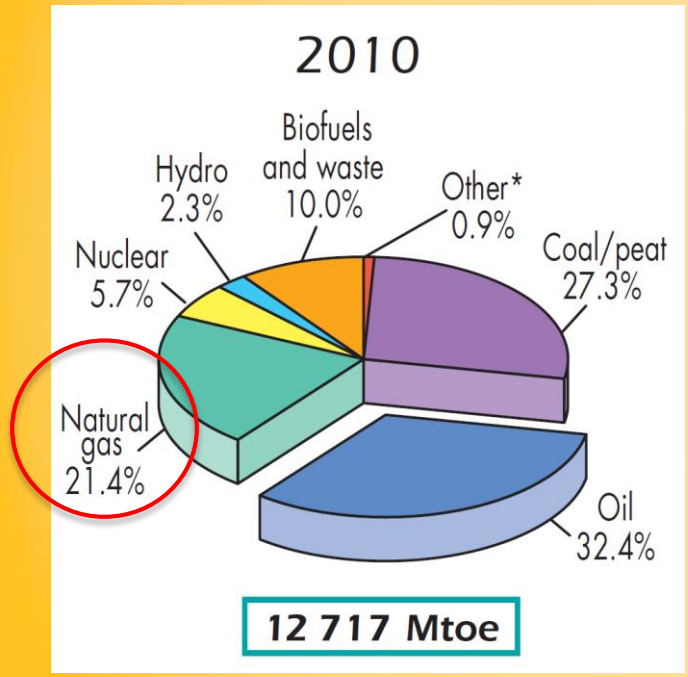
2011 data

Net exporters	bcm
Russian Federation	196
Qatar	119
Norway	99
Canada	63
Algeria	49
Indonesia	46
Netherlands	33
Turkmenistan	29
Nigeria	26
Malaysia	22
Others	152
Total	**834**

2011 data

Source: International Energy Agency
www.iea.org

Natural gas monetization in Qatar



Transportation

Physical

1/600 volume

Chemical

Pipeline

LNG

GTL

Qatar's aspiration to become the "World Gas Capital" led to the building the largest GTL and LNG plants in the world.

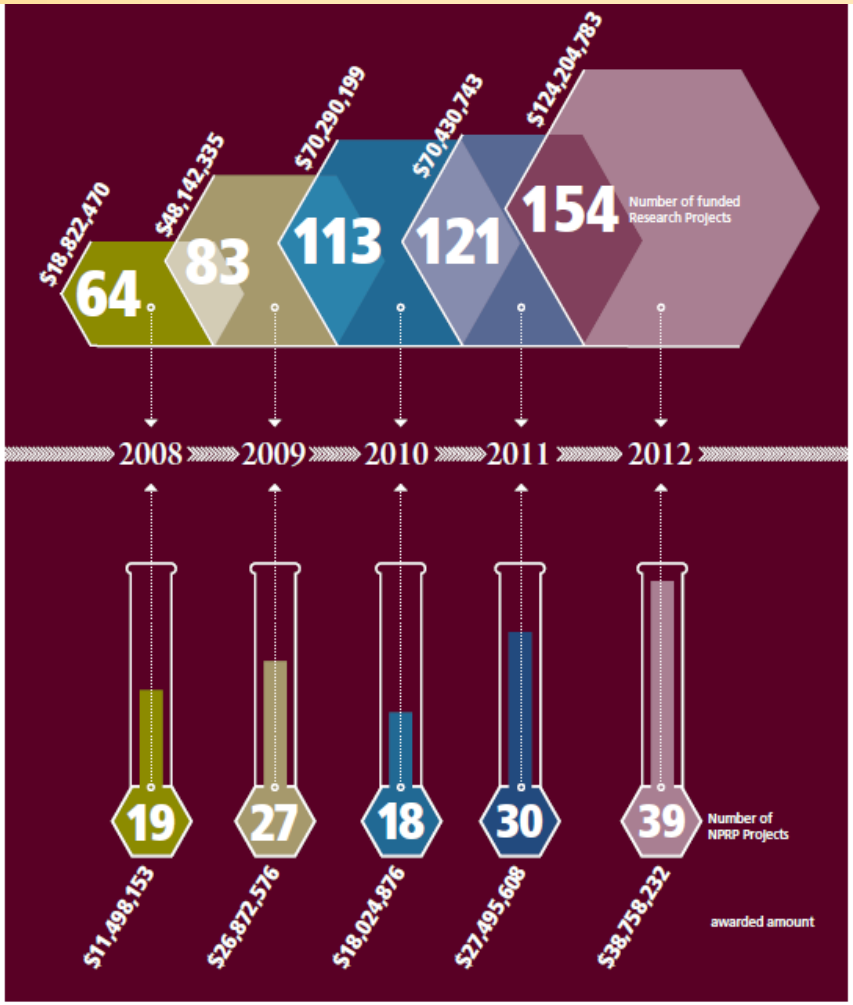
QAPCO- QP & TOTAL

QatarGas Project

Shell Pearl GTL Plant

ExxonMobil Support LNG Facilities

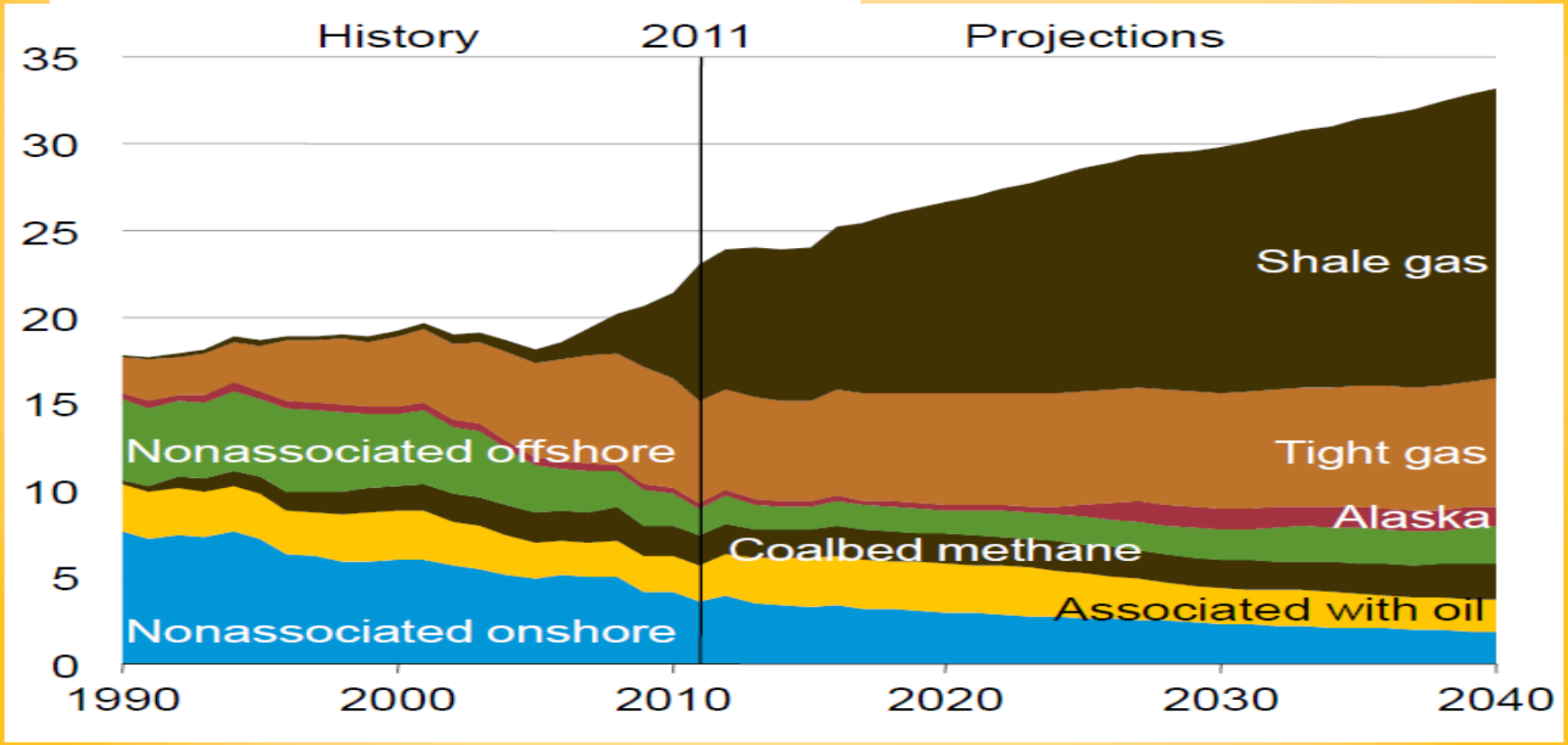
Research Funding



More than 200m US$ in 2014

World natural gas production

U.S. dry natural gas production by source, 1990-2040 (trillion cubic feet)



U.S. Energy Information Administration | Annual Energy Outlook 2013 Early Release Overview

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TEXAS A&M ENGINEERING EXPERIMENT STATION

TEXAS A&M UNIVERSITY | TEXAS A&M UNIVERSITY at QATAR

TEES Gas and Fuels Research Center

Nimir Elbashir (Director)
Mahmoud El-Halwagi (Managing Director)
Ioannis Economou (Co-Director)

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Shale Gas Potential

What is Texas A&M's expected role in the shale oil and gas revolution?

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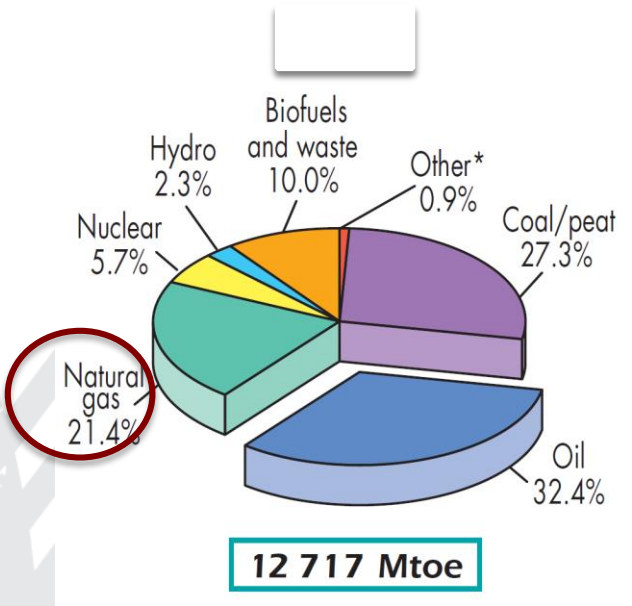
Role of Natural Gas in the Energy Market

World's primary energy supply



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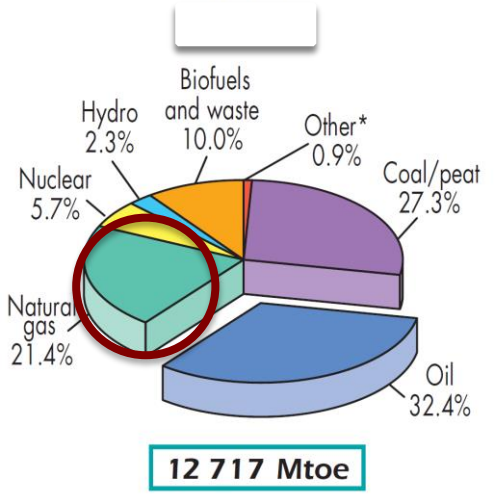
http://www.gfrc.tamu.edu

Qatar is the "World Gas Capital"



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Pipeline

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1/600 volume

LNG

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GTL

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Shale Gas Potential for Gulf of Mexico Region and U.S.

Expected growth in U.S. chemical/other industry by 2030 ≈ $110 billion

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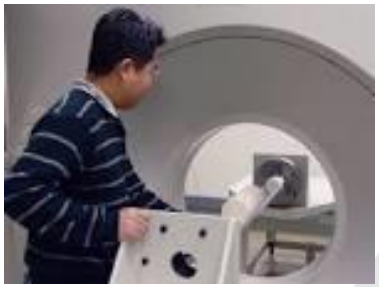

It's time to bring together Texas A&M's expertise to advance shale/natural gas exploration, production, treatment and processing.

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NSF-sponsored workshop

Gas and Fuels Research Initiative

TEES | TEXAS A&M UNIVERSITY | TEXAS A&M UNIVERSITY at QATAR

Short Course and Workshop on

Shale Gas Monetization

Potential Opportunities in the US and Lessons Learned from the Qatari Experience with Natural Gas

March 26-28, 2014
La Torretta, Lake Conroe, Montgomery
Texas - USA

Sponsor

Overview
The substantial growth in shale gas production in the US is expected to entail significant investments and gains to the US energy, chemical, and petrochemical industries. Substantial opportunities exist for shale gas monetization. The identification and planning of these opportunities require collaborative efforts among governmental, industrial, and academic entities. Additionally, the academic institutions must adapt to provide industry with skilled engineers and scientists capable of supporting and to advancing this emerging market.
The purpose of this workshop is to bring together experts from academia, industry, and government to discuss opportunities and needs in shale gas monetization in the US. The workshop will also discuss lessons learned from Qatar's experience in natural gas monetization. Qatar's current reserves of natural gas are estimated to be around 22 trillion cubic meters, the third largest in the world. The State of Qatar monetized its rich non associated natural gas reserves in several ways to become the "The Gas Processing World Capital". The country has attracted major global corporations to invest in shale gas monetization. Examples include the world's largest facilities in gas-to-liquid (GTL) and liquefied natural gas (LNG) production in addition to a well-integrated supply chain of chemicals and petrochemicals.

Short Course
A short course in the form of two tutorials will be given on the first day (March 26, 2014) to cover the following topics:
Tutorial I: "Natural Gas Monetization: Technology Fundamentals and the Potentials" by Dr. Nimir Elbashir, Texas A&M University-Qatar
Tutorial II: "Theoretical and Experimental Evaluation of Natural Gas Properties" by Dr. Mert Atilhan, Qatar University

Workshop
The workshop (March 27-28, 2014) will offer the following:
Discussion of supply chain, environmental, and safety issues associated with the emerging shale gas industry in the US.
Review of recent progress in natural gas monetization highlighting Qatar's experience its relevance to the US shale gas industry.
Identification of future educational, workforce training, and research opportunities, directions, and emerging trends in shale gas monetization.
Description of current and future challenges in developing, adapting, and commercializing emerging technologies in the area shale gas monetization.
Networking and discussion opportunities among junior and senior academic, industrial, and government attendees.

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Processing

Fuels and chemicals formulation, processing, characterization

Catalysis, reaction engineering, reactor deign

Thermodynamics and phase behavior (experimental and modeling)

Safety

Control

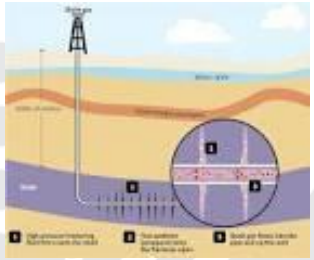
Process integration, synthesis, simulation, design, operation, and optimization, techno-economic analysis, sustainable process design, and molecular/product design

Reservoir simulation and modeling

Design and evaluation of hydraulic fracture treatments

Performance of advanced and stimulated wells

Hydraulic fracture mechanics



Shale-gas fluid behavior modeling

Computational design of materials and processes

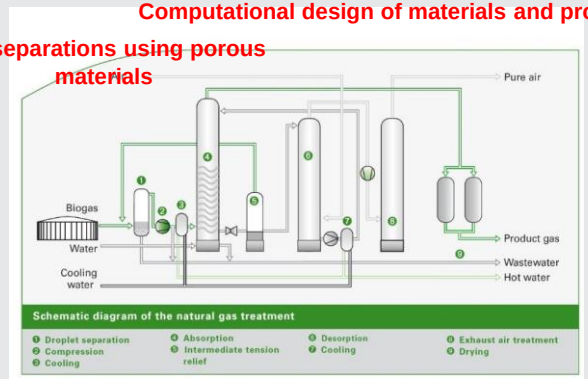
Gas separations using porous materials

Production

Systematic modeling of heat transfer in wellbores

Wellbore integrity analysis

Gas properties



Treatment

Monetization

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Texas A&M at Qatar Faculty Affiliates

Professor Nimir Elbashir
Director
Reaction Engineering and Reactor Design
Chemical Engineering

Professor Ioannis Economou
Co-director
Molecular Thermodynamics
Chemical Engineering

Professor Mert Atilhan
Natural Gas Properties
Chemical Engineering

Professor Dragomir Bukur
Catalysis and Reaction Engineering
Chemical Engineering

Professor Marcelo Castier
Thermodynamics and Phase Behavior
Chemical Engineering

Professor Ken Hall
Hydrocarbon Processing
Chemical Engineering

Professor Reza Sadr
Thermofluids and Combustion
Mechanical Engineering

Professor Reza Tafreshi
Engine Testing and Emissions
Mechanical Engineering

Professor Luc Vechot
LNG Safety
Chemical Engineering

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Texas A&M University Faculty Affiliates

Professor Mahmoud El-Halwagi
Managing Director
Process Integration and Optimization
Chemical Engineering

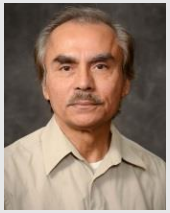
Professor Jim Holste
Thermodynamics
Chemical Engineering

Professor Jorge Alvardo
Fuels Combustion
Mechanical Engineering

Professor Perla Balbuena
Computational Material Design
Chemical Engineering

Professor Maria Barrufet
Reservoir Simulation and Modeling
Petroleum Engineering

Professor Faruque Hasan
Computational Energy Analysis
Chemical Engineering



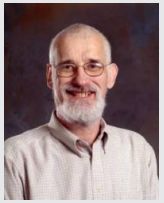
Professor A. Rashid Hasan
Gas Production
Petroleum Engineering

Professor Mark Holtzapple
LNG, Fuels and Thermodynamics
Chemical Engineering

Professor Nazmul Karim
Control
Chemical Engineering

Professor Sam Mannan
Safety
Chemical Engineering

Professor Andrea Strezlec
Combustion, Kinetics and Engines
Mechanical Engineering



Professor Peter Valkò
Design of Hydraulic Fracture Systems
Petroleum Engineering

Professor Benjamin Wilhite
Reaction Kinetics and Simulations
Chemical Engineering

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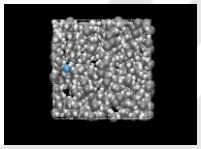
GFRC Capabilities and Resources



Molecular Thermodynamics and Simulation Group (Qatar)

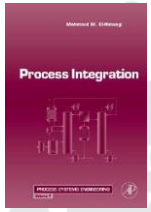
Fuel Characterization Lab (Qatar)

TEES Mary O'Connor Process Safety Center

Qatar

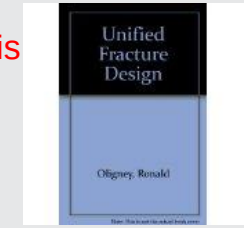
College Station

Engine testing and fuels combustion behavior

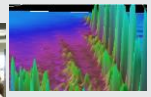


Process integration and optimization

Material synthesis and simulations



Naturally Fractured/Integrated Reservoir Studies Laboratory



Applied catalysis and reaction engineering (College Station and Qatar)

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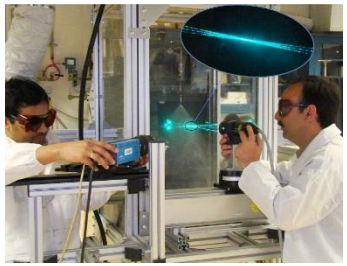
GFRC Impact



Training future generation of highly skilled engineers

Collaboration with academia/research institutions

Continuing education

Institutional collaboration

Support Qatar and Texas economies

Global impact

Collaboration with industry and funding agencies

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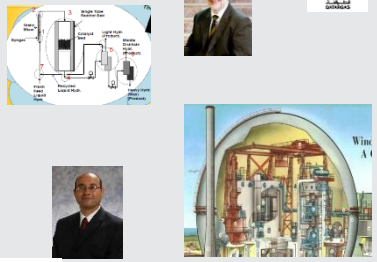
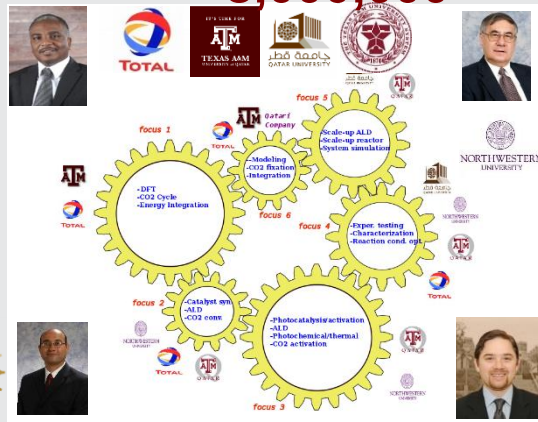
Current Successful Internal Collaborations and the Potentials





≈5,000,000

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Major Industry Collaborations in Qatar & USA

Platinum

ORYX GTL

Synthetic Fuels & Lubricants, Engine Tests; Trainings

GE Oil & Gas

Fuel blends, engine & emissions

sasol reaching new frontiers

Synthetic Fuels

Reactor, Synthetic Fuels, Lubricants

TOTAL

قطر للبترول Qatar Petroleum

Catalysts

ExxonMobil

Gas production

RasGas

MAERSK OIL

Gas Production and Process Optimization

وقود WOQOD

Fuels & Lubricants

Chevron

Gas Processing Technologies

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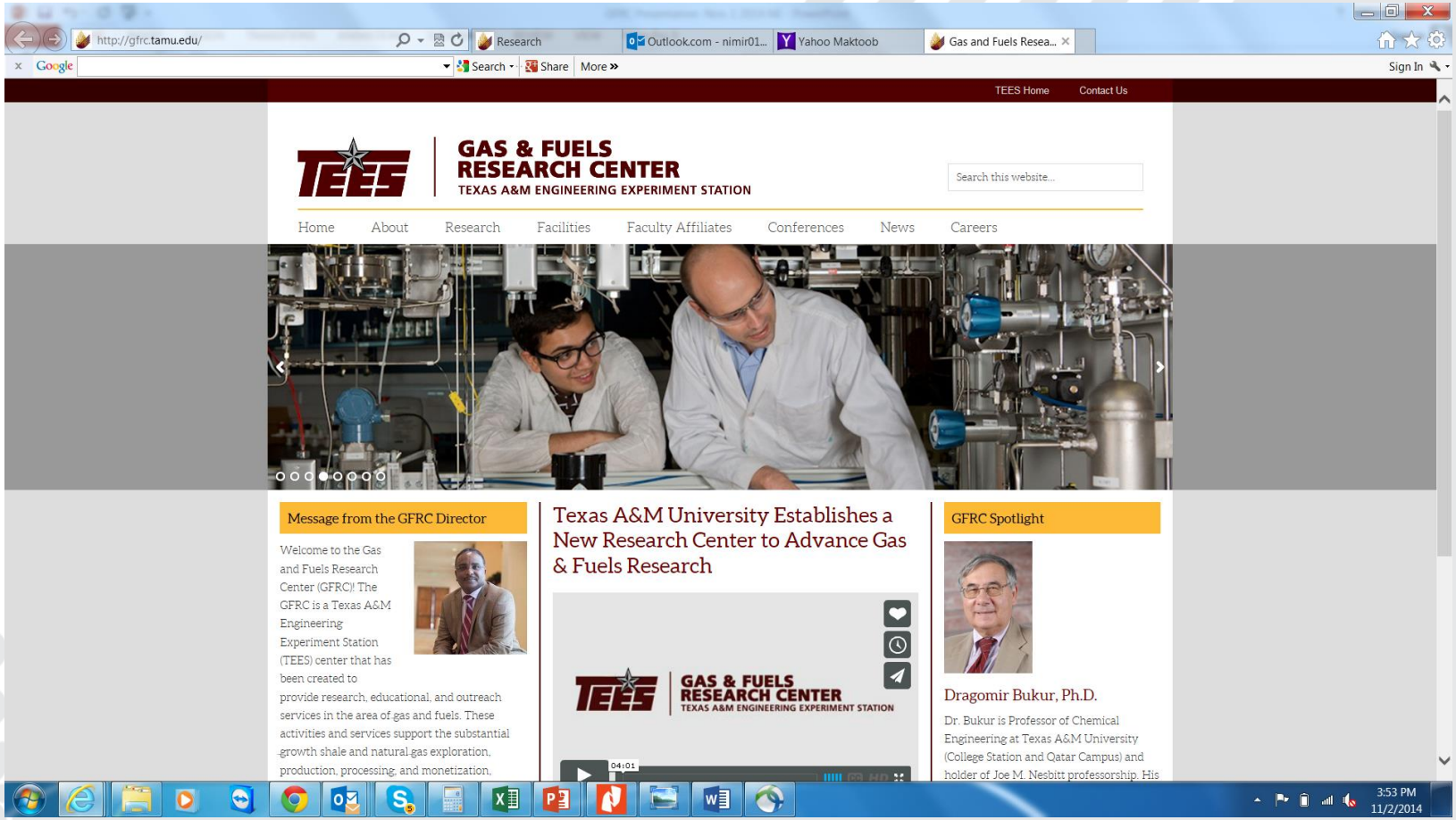
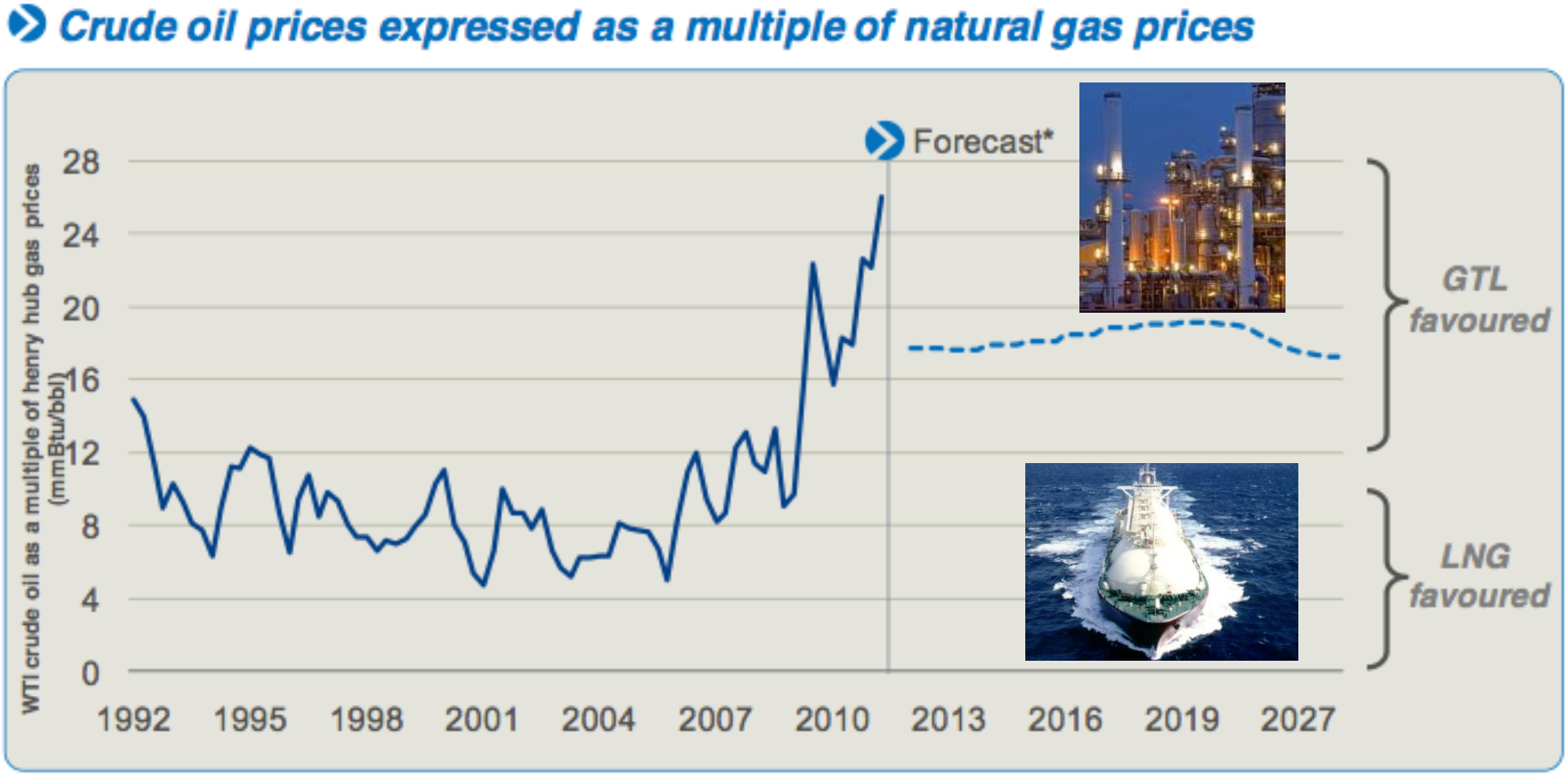
http://gfrc.tamu.edu



LNG vs. GTL, which option is better?



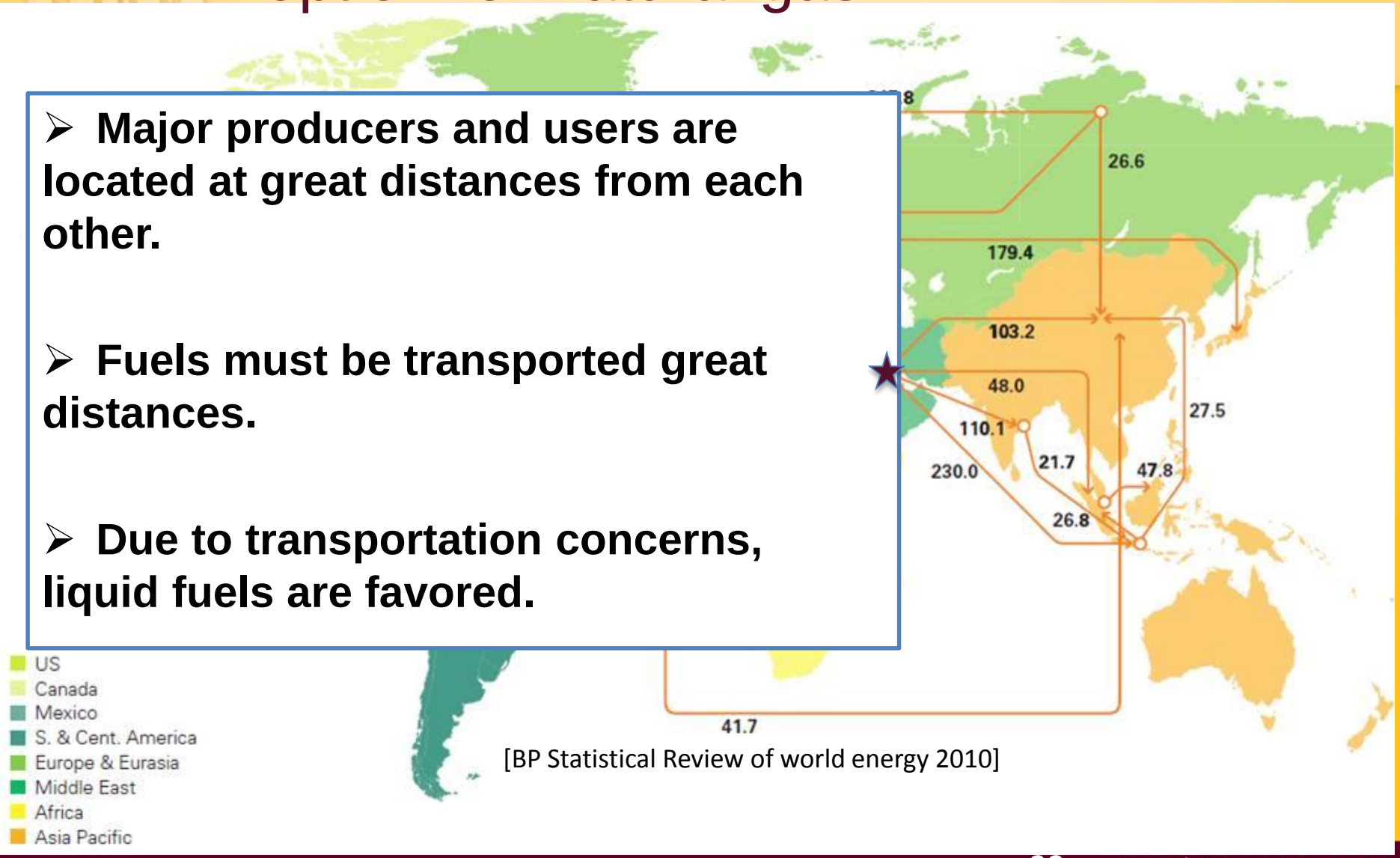
From Mike Nel (Sasol) Presentation at the XTL World Summit in London – June 2011.

* source: EIA

Copyright © 2011, Sasol New Business Development

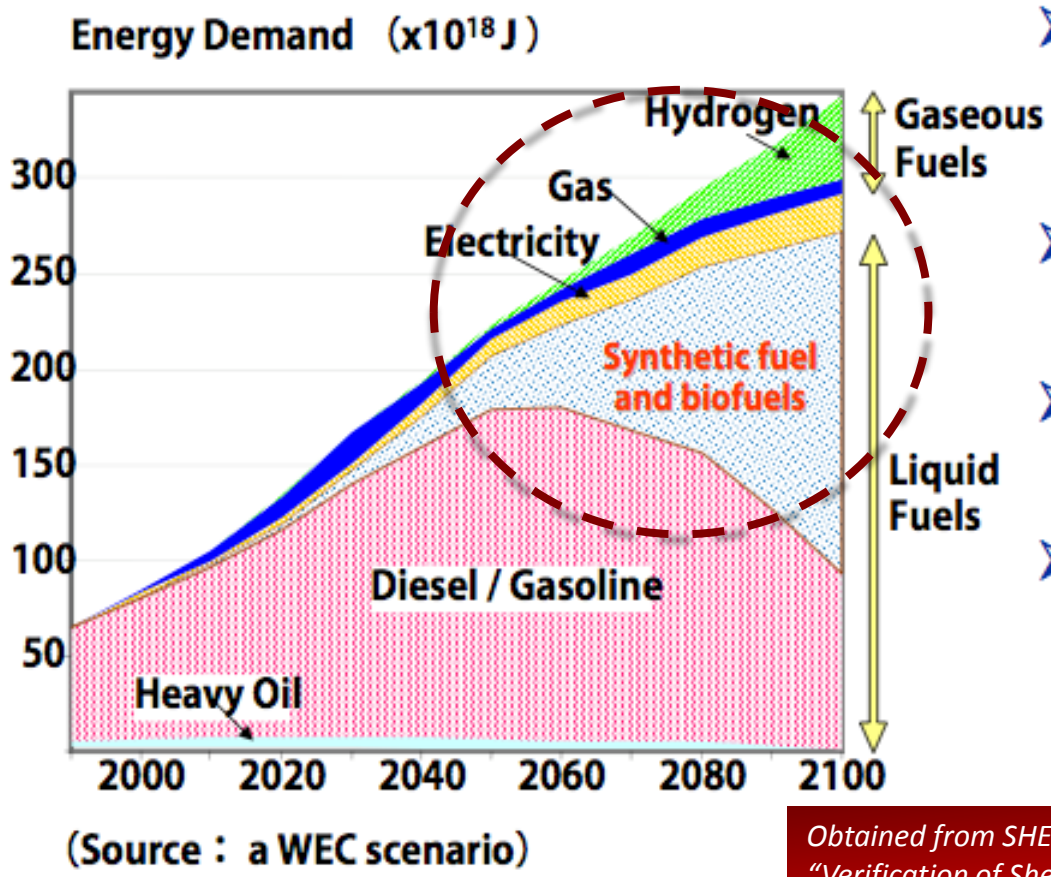
Is LNG or pipeline transportation is best option for natural gas?

- **Major producers and users are located at great distances from each other.**
- **Fuels must be transported great distances.**
- **Due to transportation concerns, liquid fuels are favored.**



[BP Statistical Review of world energy 2010]

Synthetic fuels have bright future!

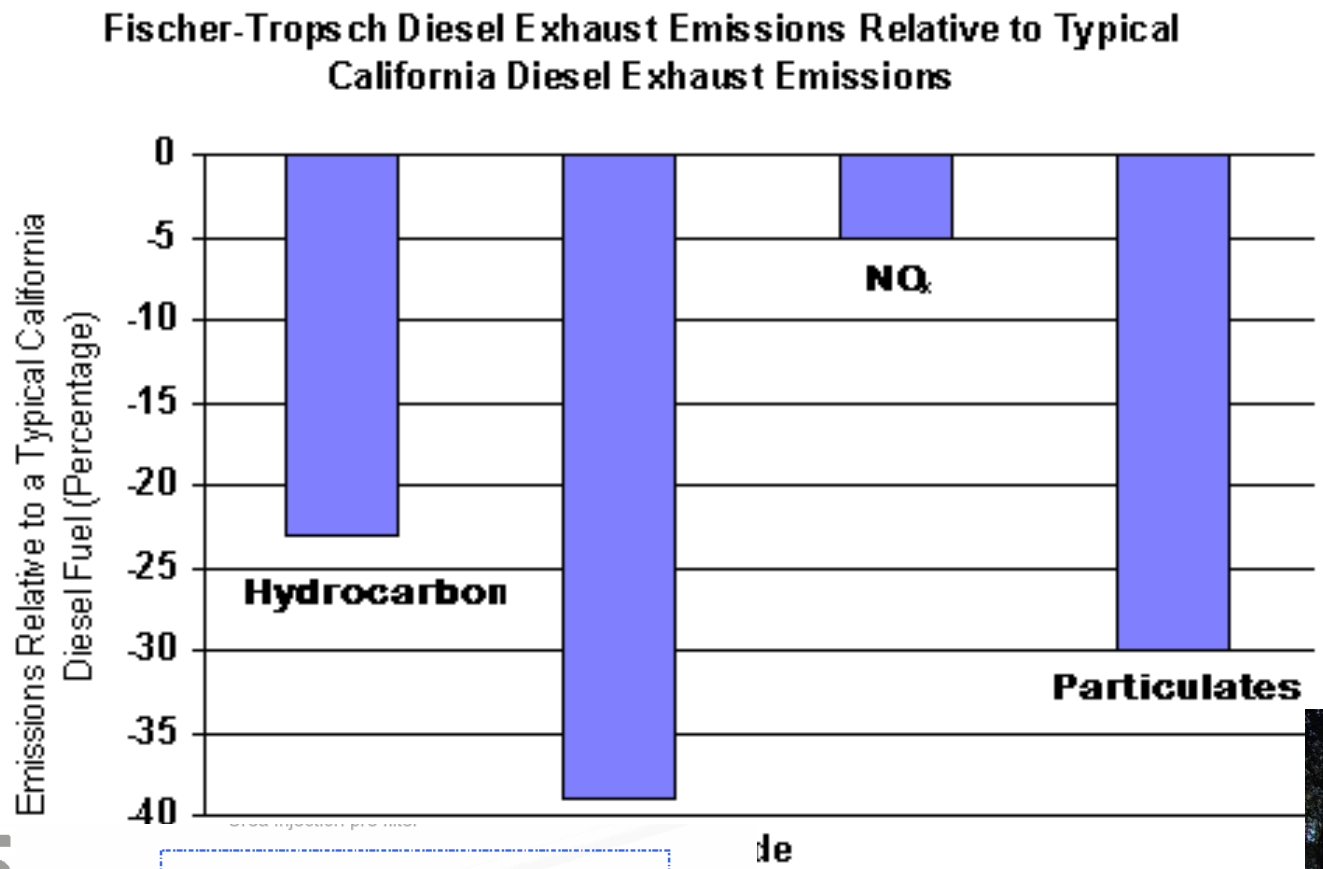


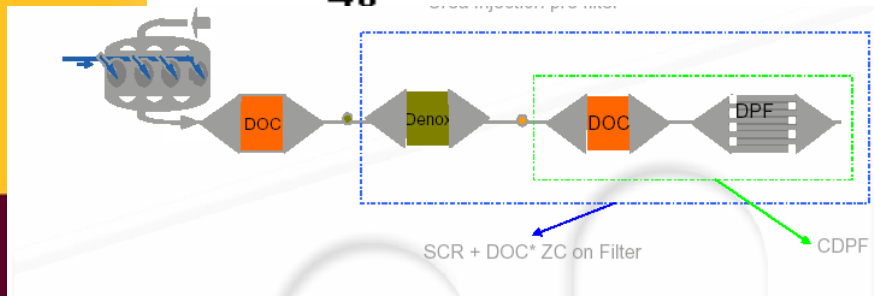
- Significant uncertainty in plateau of 'conventional oil mountain'
- Increased environmental pressures
- Plethora of potential vehicle-fuel solutions
- Common denominator ought to be cost effectiveness.

Obtained from SHELL Global Solutions, 2007. Cherillo, et al. "Verification of Shell GTL Fuel as CARB Alternative Diesel"

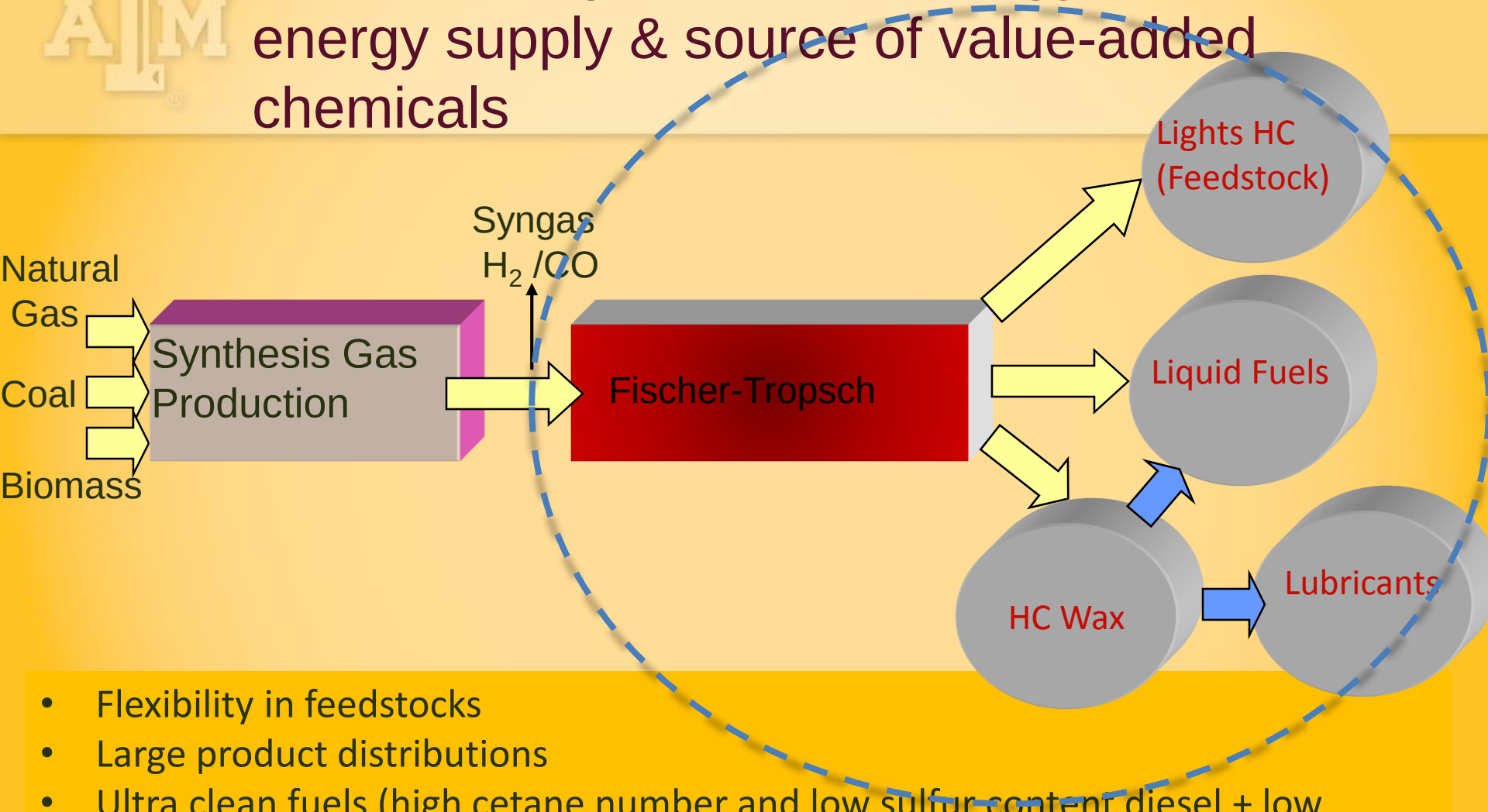
GTL fuels environmentally attractive

Extremely low (0-5-ppm) sulfur, aromatics, and toxics



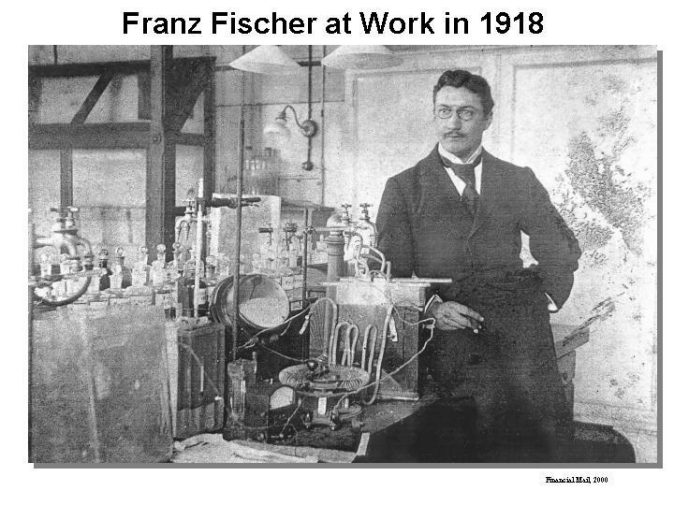


Gas-to-Liquid Technology: Alternative energy supply & source of value-added chemicals



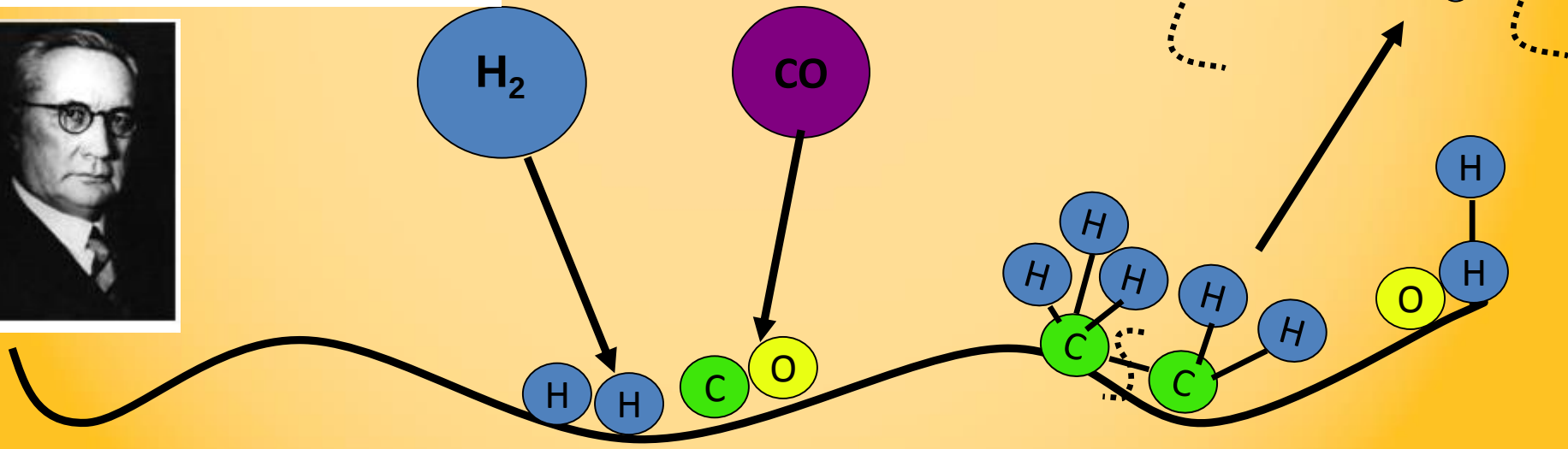
- Flexibility in feedstocks
- Large product distributions
- Ultra clean fuels (high cetane number and low sulfur content diesel + low octane gasoline) & value added chemicals

Fischer-Tropsch chemistry facilitates the conversion of syngas into liquids



α-olefins+ Gasoline + Jet Fuel+ Diesel +wax

C_nH_{2n} and C_nH_{2n+2} + CO_2, H_2O, oxygenates



Catalyst Surface: Cobalt, Iron, Ruthenium, etc

GTL technology in Qatar

145,000 bpd
1 million tons of kerosene/ year
+ base oil

24,000 bpd diesel
+ 9,000 bpd naphtha
+1,000 bpd LPG

Oryx GTL – The F-T reactors

- 60 m tall
- Could hold the water from the 3 Olympic swimming pool
- Weights 2,100 tones

Shell Multi-tubular Fixed-Bed Reactors

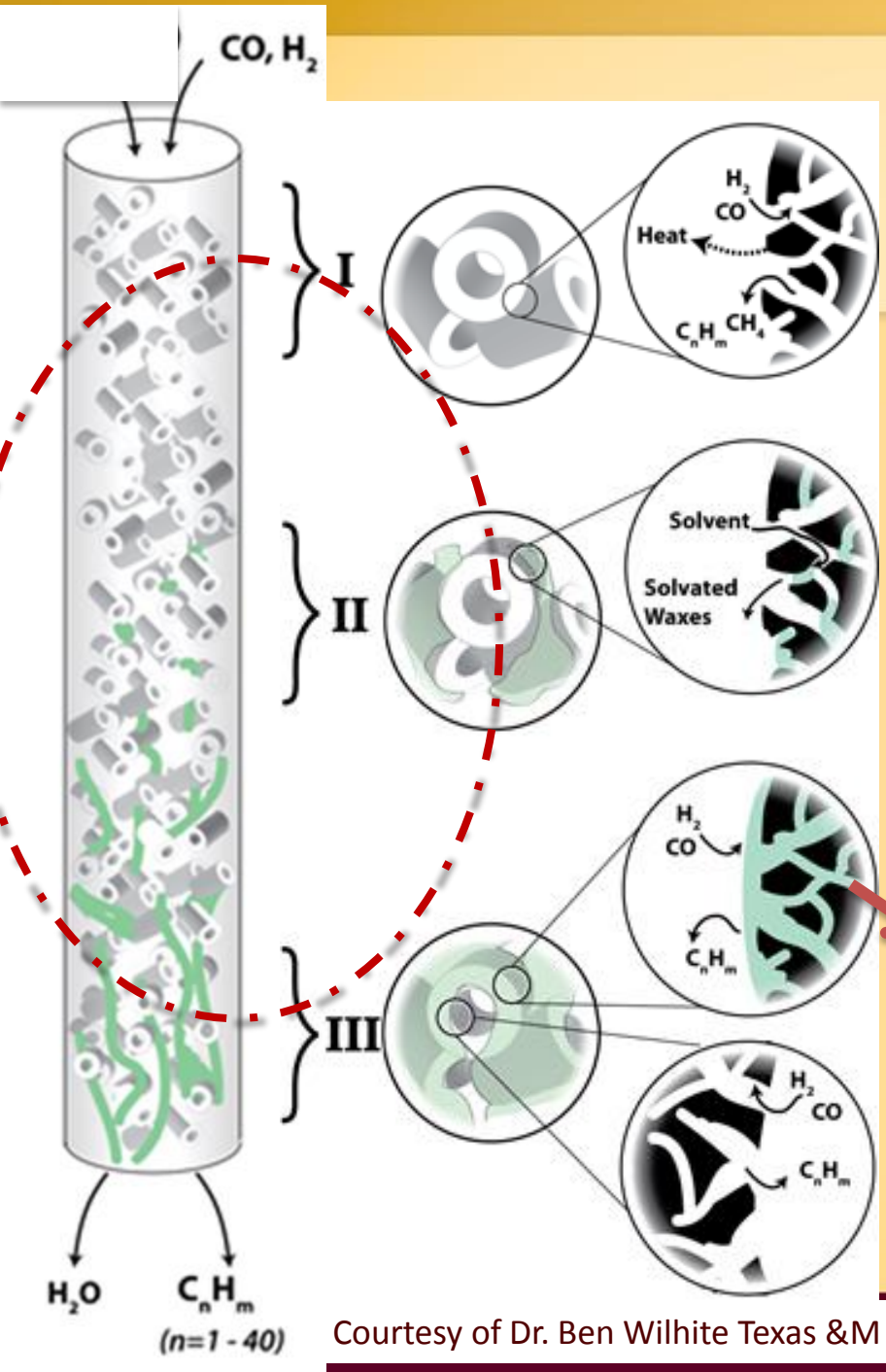
Comparison between FTS reactors

Desired Characteristics	Packed bed reactor (gas phase)	Slurry phase reactor (liquid phase)
Operational Consideration	↓	↑
High Catalyst hold-up	↑	↓
High heat transfer rate	↓	↑
Wide product spectrum	↑	↑

The ideal FTS reactor should combine the advantages of the two major reactor technologies; **fixed-bed reactors** of high reactant diffusivity and reaction rates coupled with steady performance to that of the **slurry reactor** of well-mixed phase and excellent temperature distribution inside the reactor bed coupled with higher overall productivity.

→ **One more feature is the capability of controlling the hydrocarbon product distribution.**

↑ Advantage ↓ Disadvantage

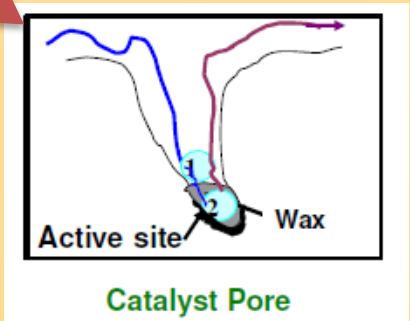


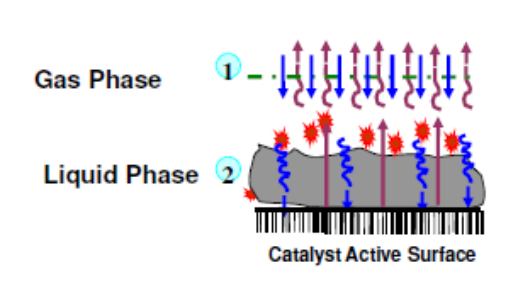
Courtesy of Dr. Ben Wilhite Texas &M University

Region 1: Exothermic reaction occurring in single phase – focus on hot spot prevention

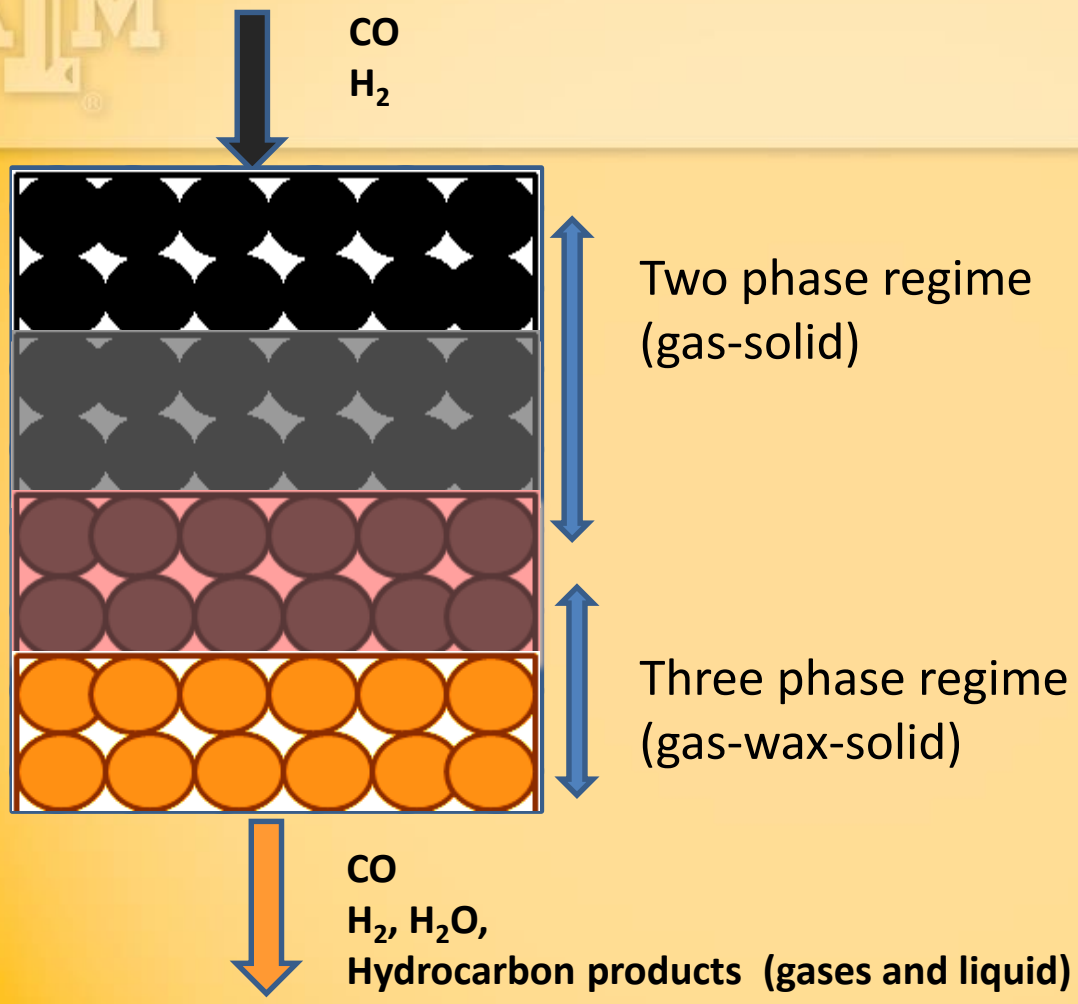
Region 2: Wax formation – tailor pore structure to facilitate wax extraction from catalyst

Region 3: Trickle bed regime – tailor pore structure and surface wettability to maximize secondary reactions





Gas-Phase FTS in fixed bed reactor

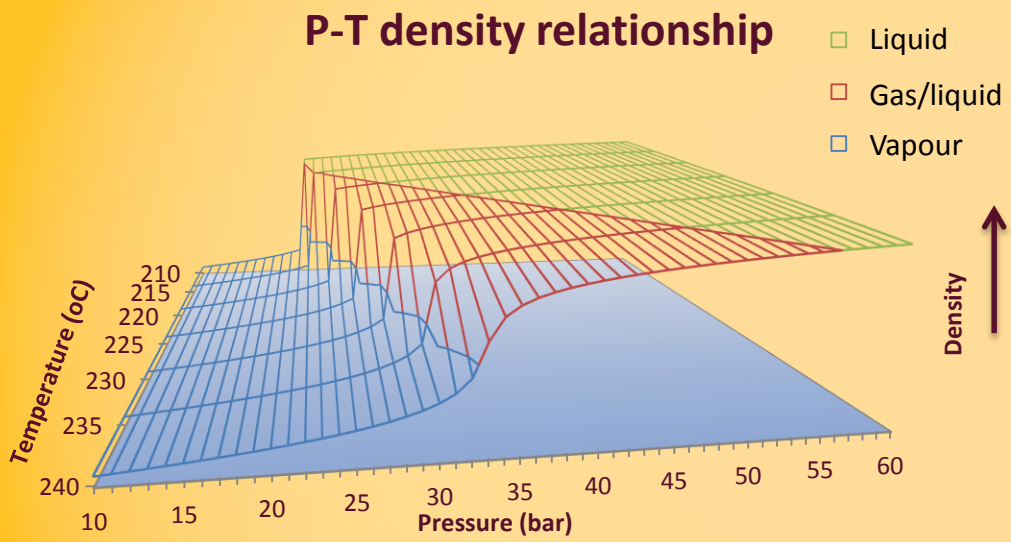


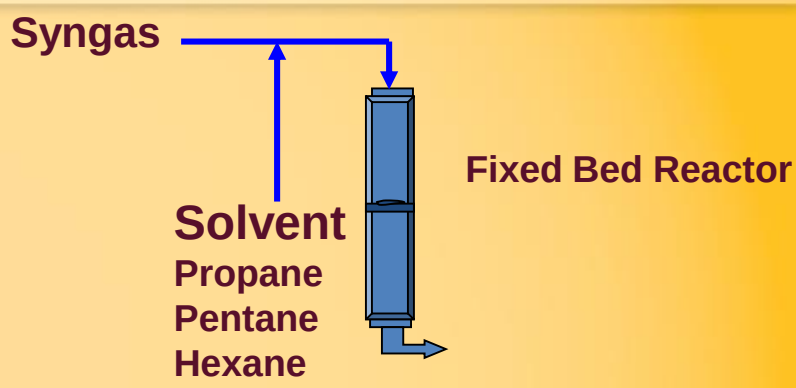
Syngas

Wax

Ref: L.Caldwell, D.S.van Vuuren. *Chemical Engineering Science* 41(1) (**1986**) 89-96

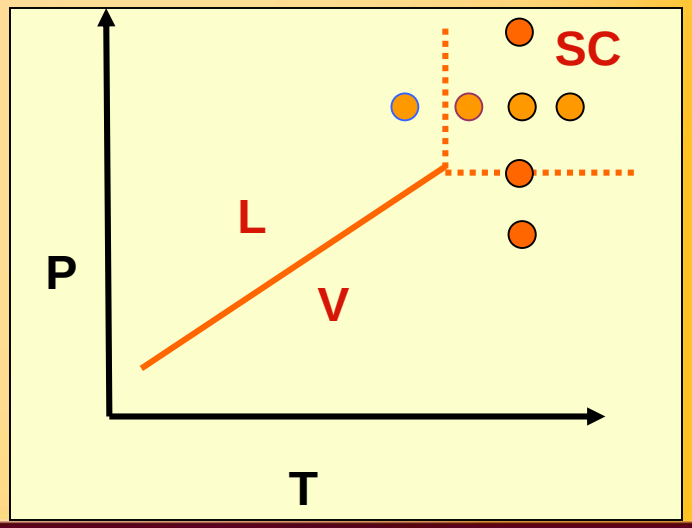
Introduction of supercritical hydrocarbon solvent in FTS



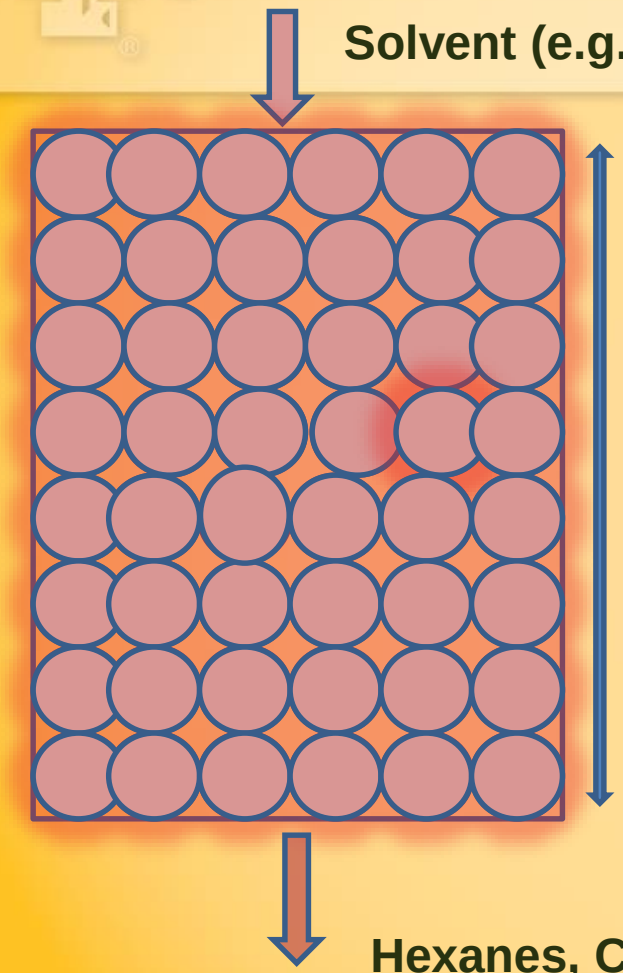


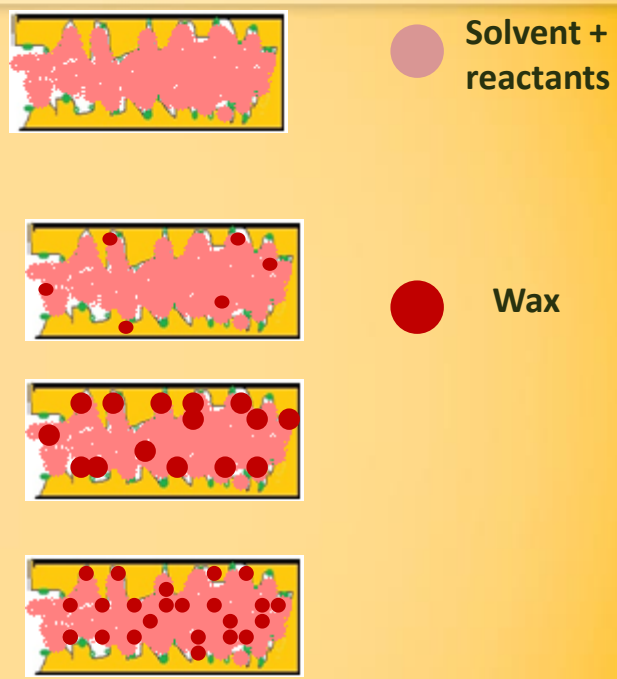
- ***Liquid-like density and heat capacity***
- ***Gas-like diffusivity and transport properties***

Elbashir, Bukur, Durham, Roberts. 2010 AIChE J. 56 (3) 997.



Supercritical Phase FTS

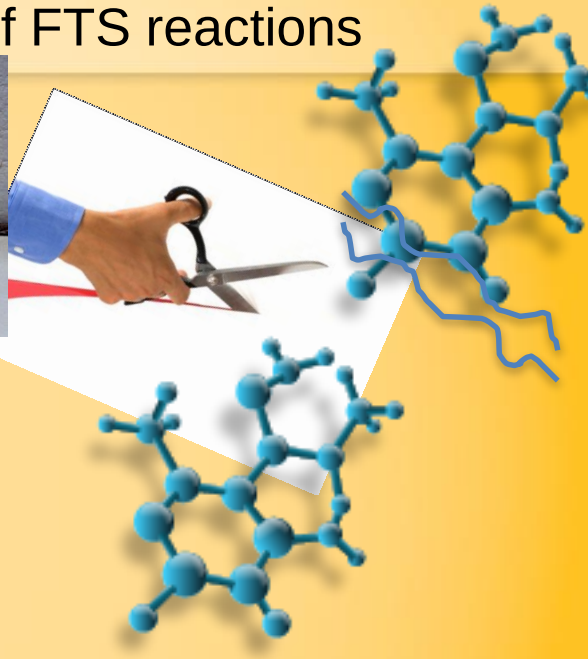




Ref: Biquiza, Claeya, van Steen. *Fuel Proc. Tech.* 91 **(2010)** 1250-1255.

Why is the selective control of Fischer-Tropsch products important?

Start with the control of the polymerization nature of FTS reactions

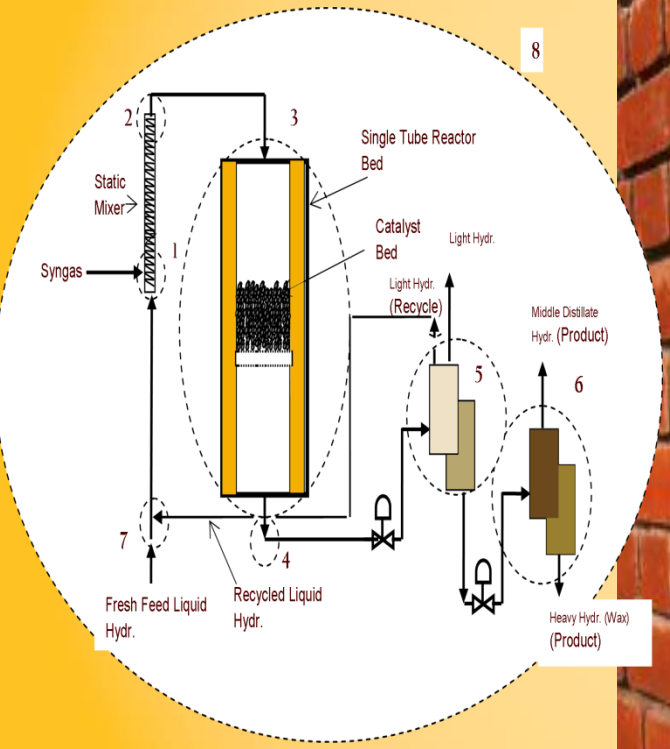


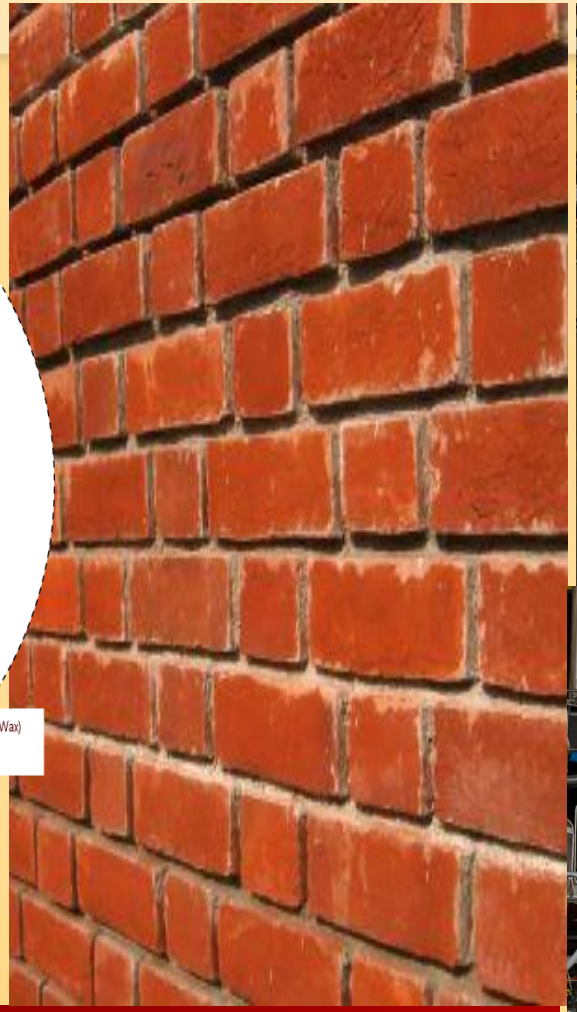
Improve product yields and purity

Simplify separation processes

Minimize production cost

What it takes to design a novel reactor technology?





Elbashir, Eljack. 2010 in Advances in Gas Processing: Elsevier ©, vol. 2; 369.

The design phases of a novel reactor

Process Design: Energy Integration & Optim

Phase Behavior & Thermodynamics

Process Control

Products Processi

Kinetics & Product Distribution

Reactor Design & Experimental Camp

In situ Reactor Behavior

Advisory

Elbashir, Eljack. 2010 in Advances in Gas Processing: Elsevier ©, vol. 2; 369.

Microscale studies:

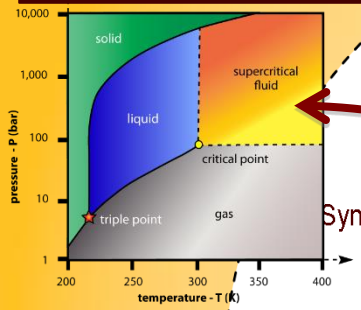
Simulation & Experimental

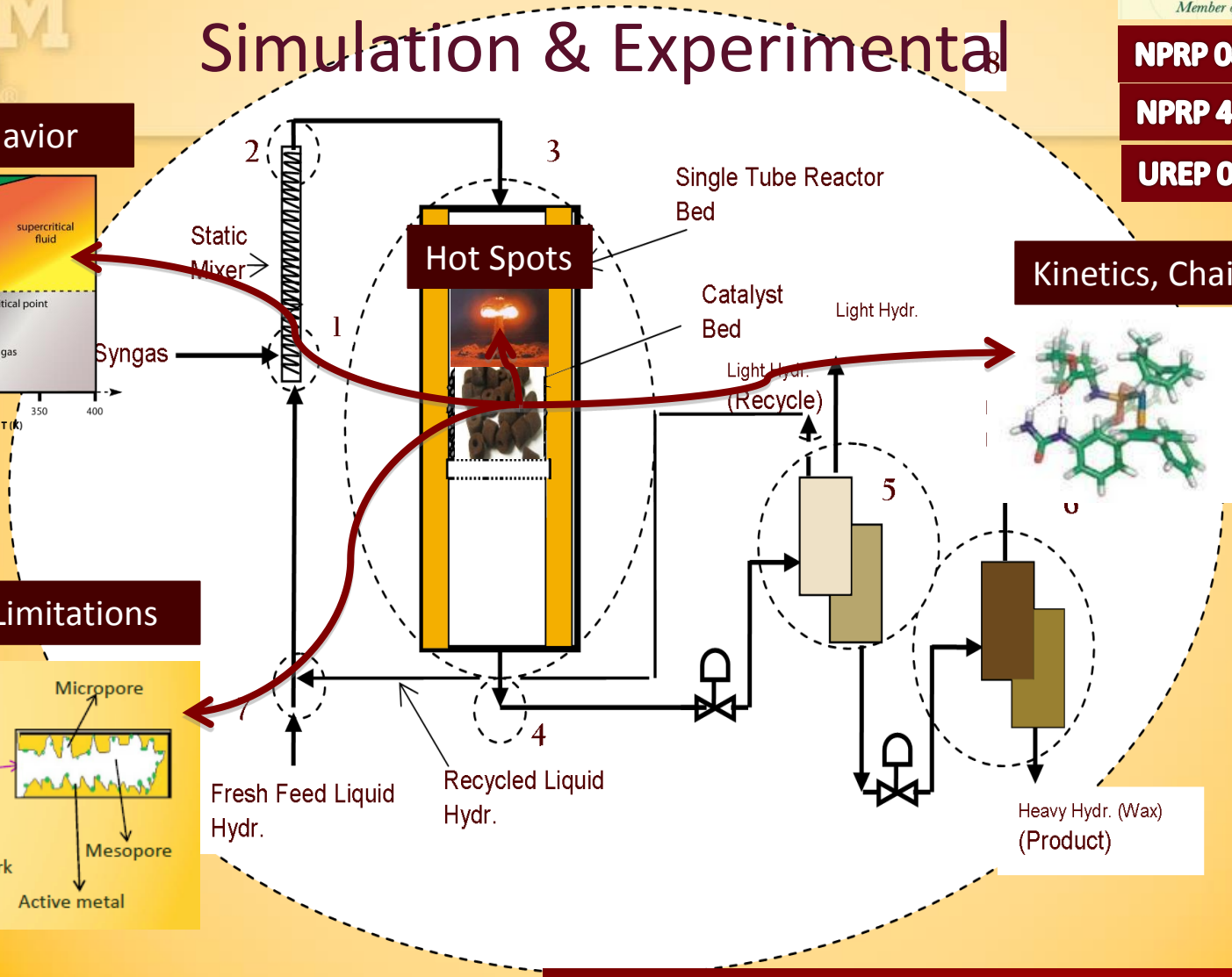
NPRP 08 - 261 - 2 - 082

NPRP 4 - 1484 - 2 - 590

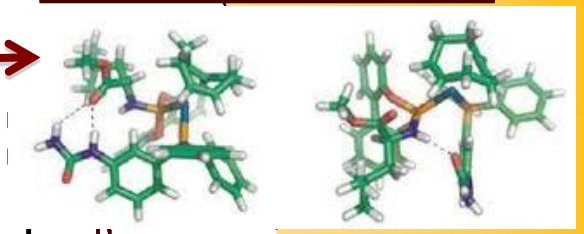
UREP 07 - 055 - 2 - 012

Phase Behavior

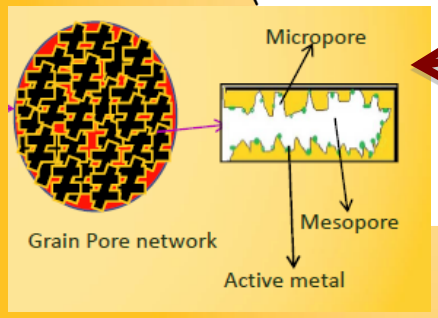




Kinetics, Chain growth



Diffusion Limitations



Bao, El-Halwagi, Elbashir 2010. Fuel Processing Technology 91(7) 703-713.

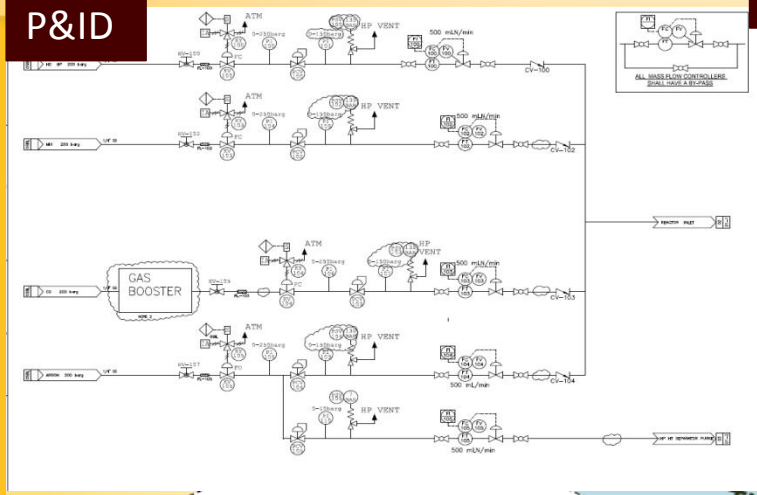
Macroscale studies

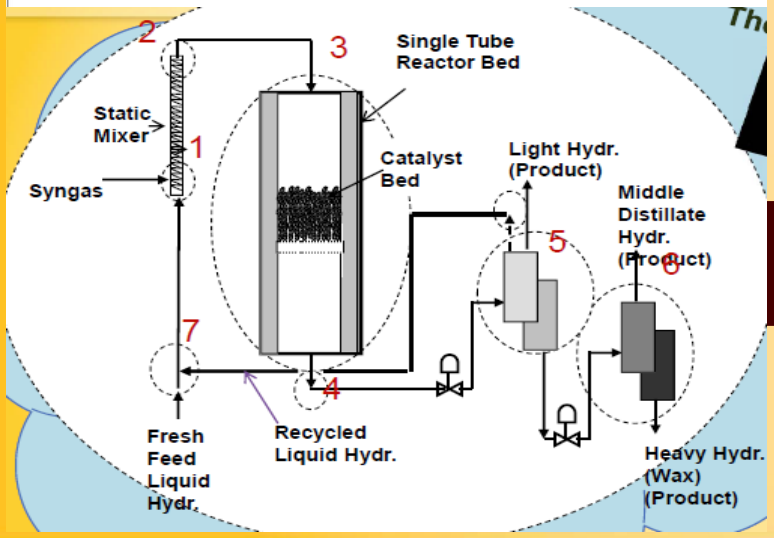
NPRP 08 - 261 - 2 - 082

NPRP 5 - 066 - 2 - 023

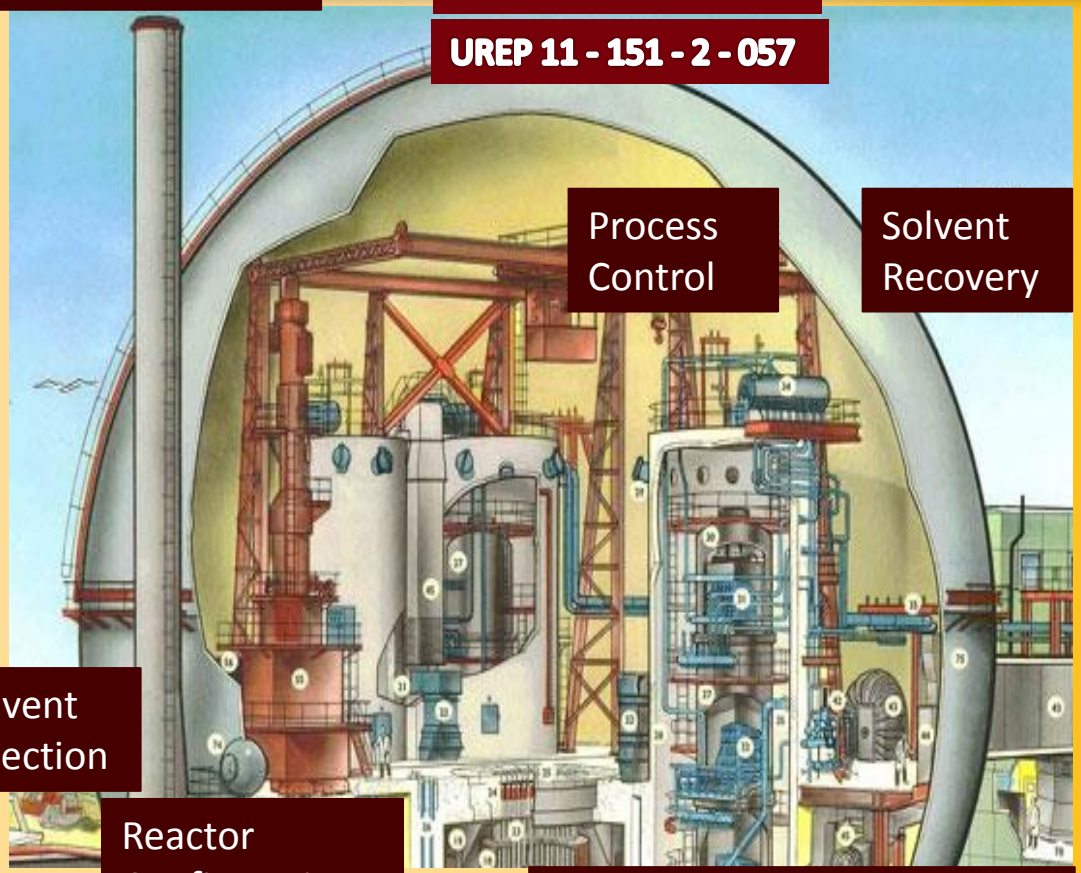
UREP 11 - 151 - 2 - 057

P&ID





Energy Optimization



Process Control

Solvent Recovery

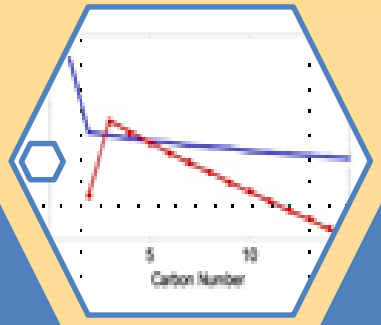
Solvent Selection

Reactor Configuration

Synthetic Fuels Formulation & Characterization

Building blocks

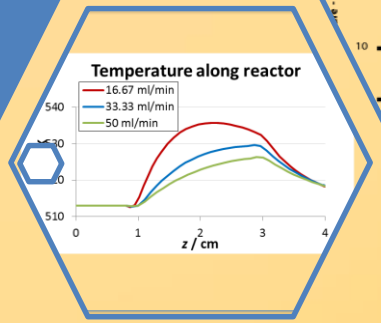
Mechanistic modelling



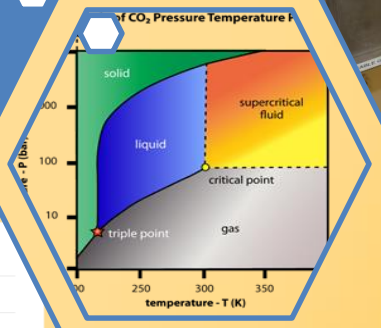
Intraparticle transport phenomena

Reactor bed modeling

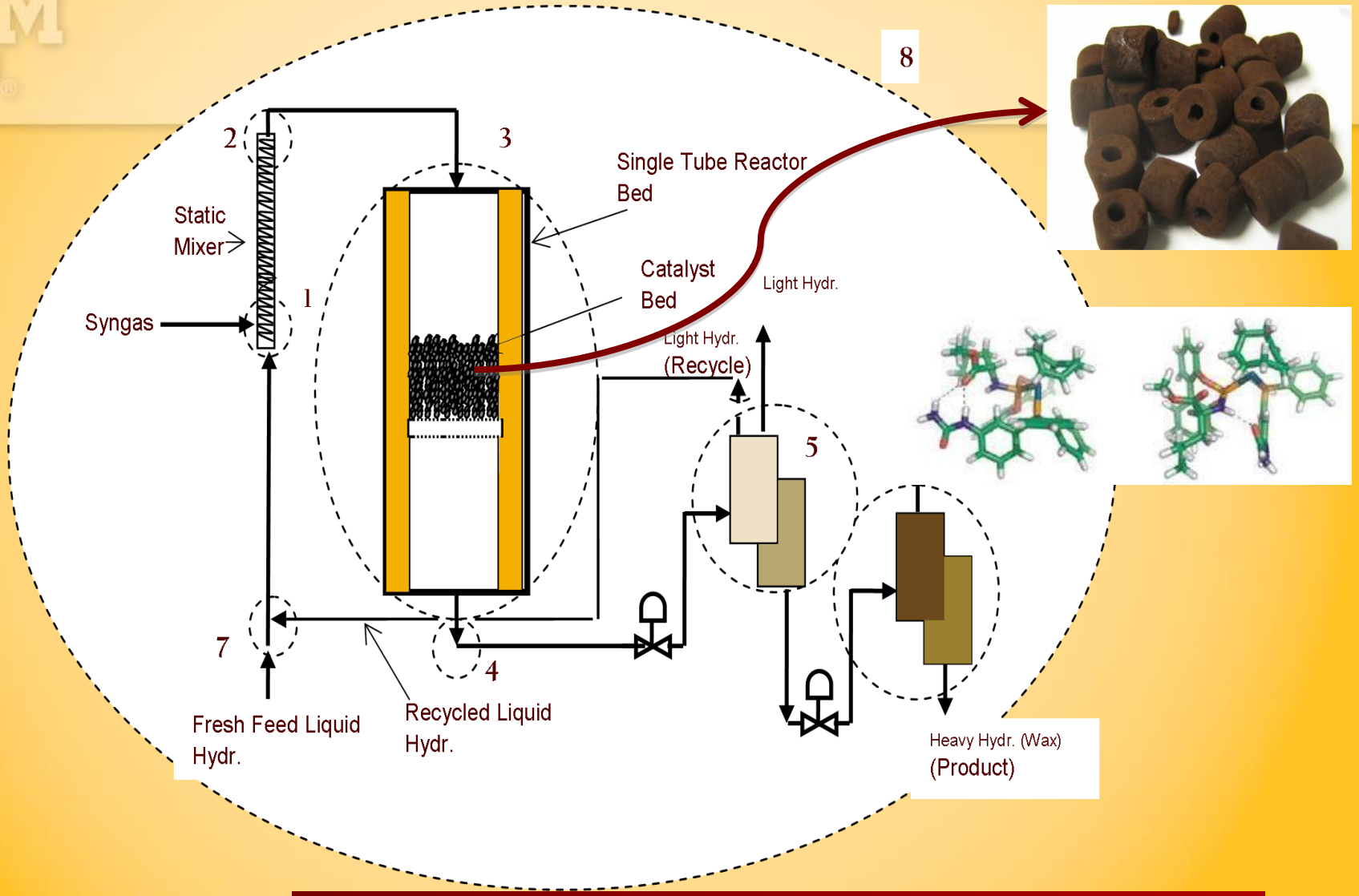
Thermo dynamics



Experimental validation

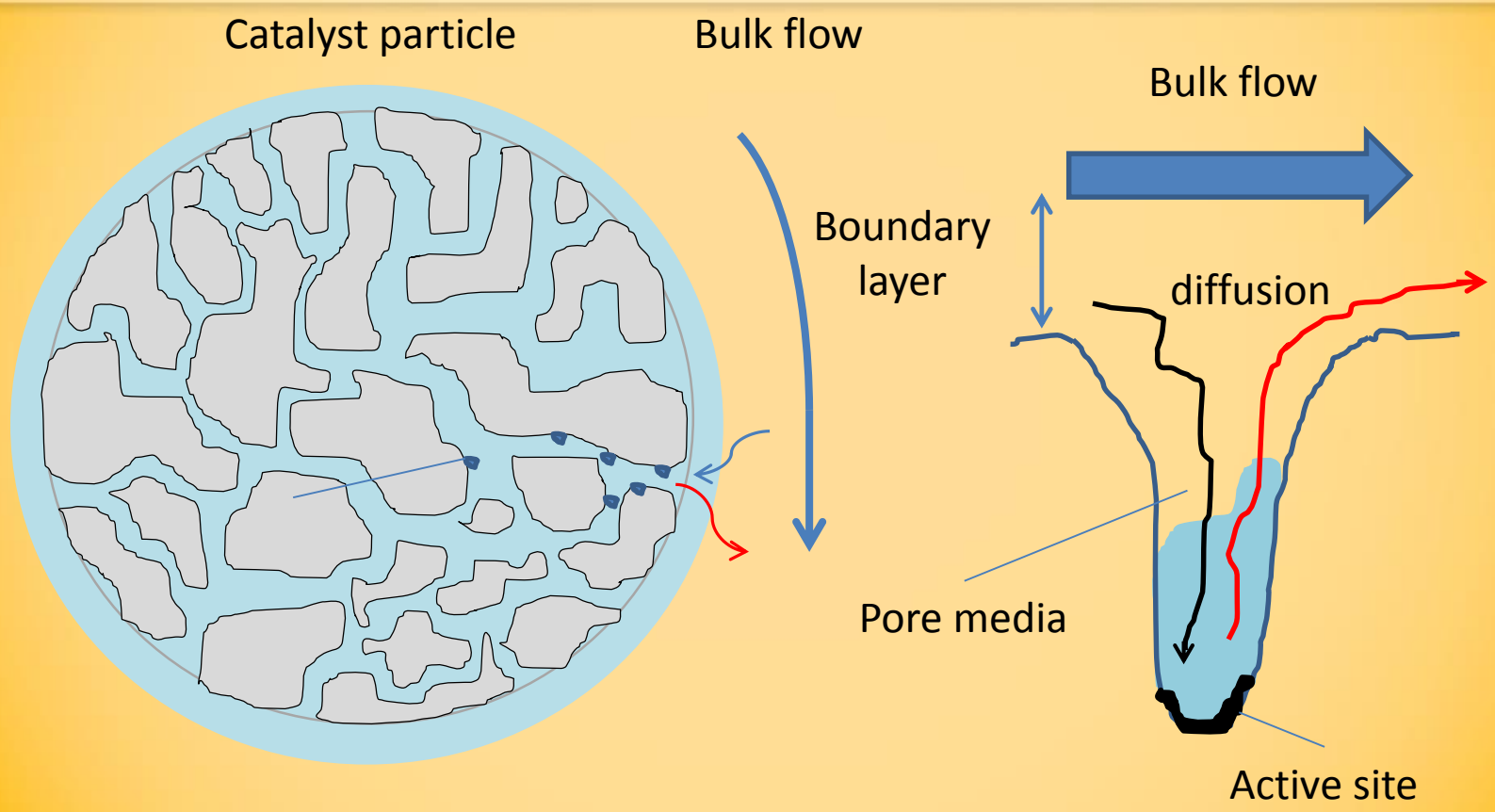


Catalyst bed behavior in SCF-FTS



Mogalicherla , Elmalik& Elbashir (2012) Chem. Eng. Prog.: Proc. Intes. 62, 59-68.

Modeling catalyst particle effectiveness



Modeling catalyst particle effectiveness

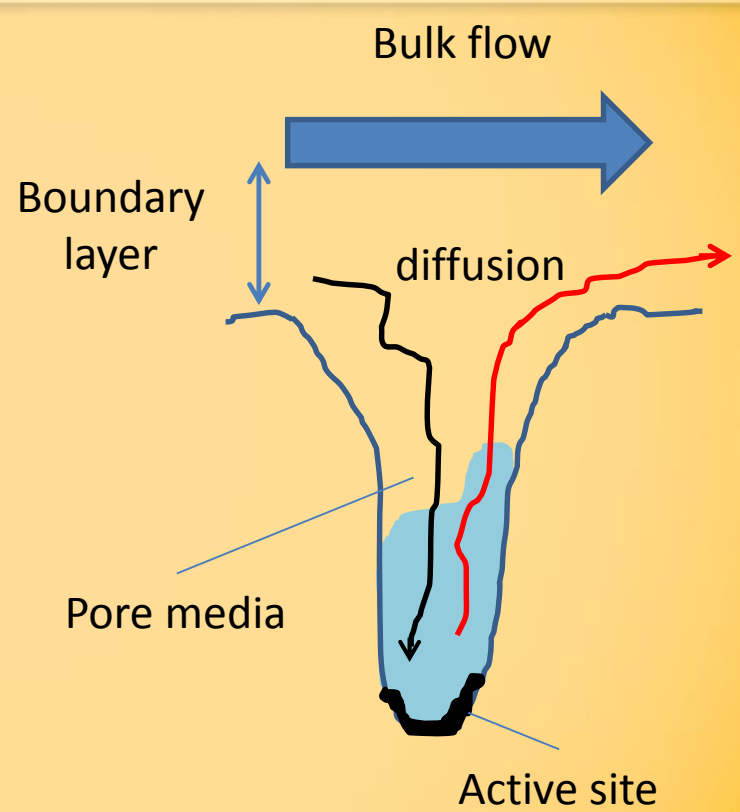
$$\frac{\lambda^e}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) = (-r_{CO})\rho_{cat.}(\Delta H)_r$$

$$\frac{D^e_{CO}}{r^2}\frac{d}{dr}\left(r^2\frac{df_{CO}}{dr}\right) = RT(-r_{CO})\rho_{cat.}$$

Mass transfer

$$\frac{\lambda^e}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) = (-r_{CO})\rho_{cat.}(\Delta H)_r$$

Heat transfer



BC. 1: $r = Rcat \rightarrow \left.\frac{dfco}{dr}\right|_{r\ =\ Rcat} = f_{co_{bulk}}$

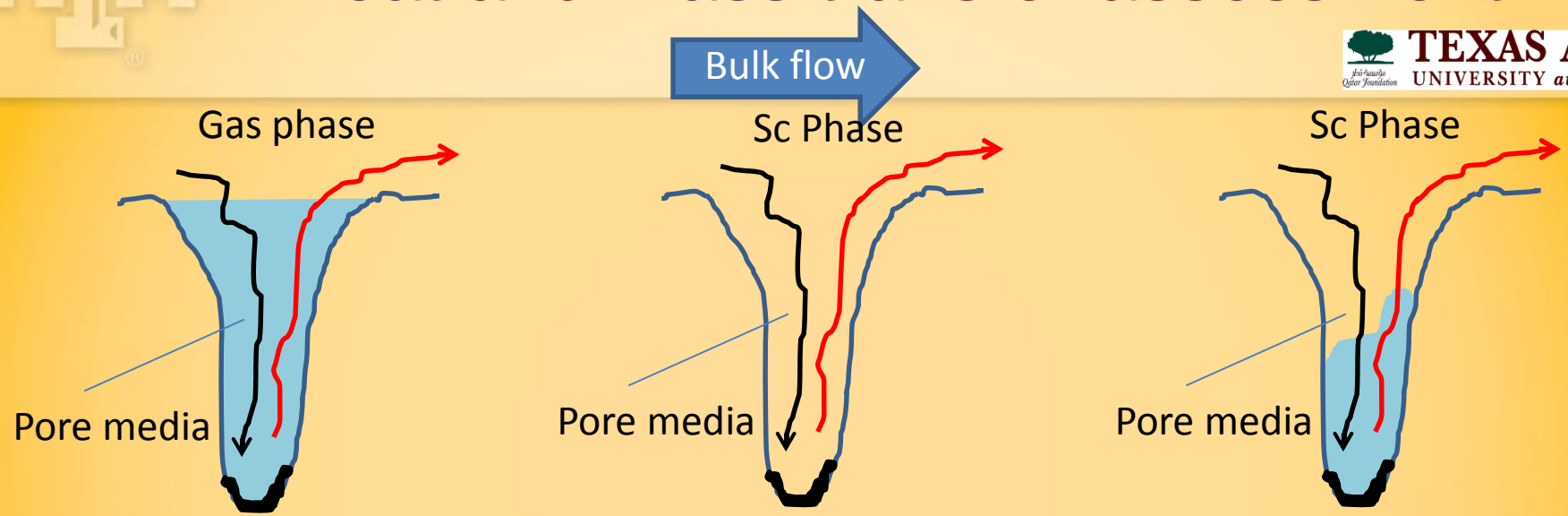
BC 2.: $r = 0 \rightarrow \frac{df_{co}}{dr} = 0$

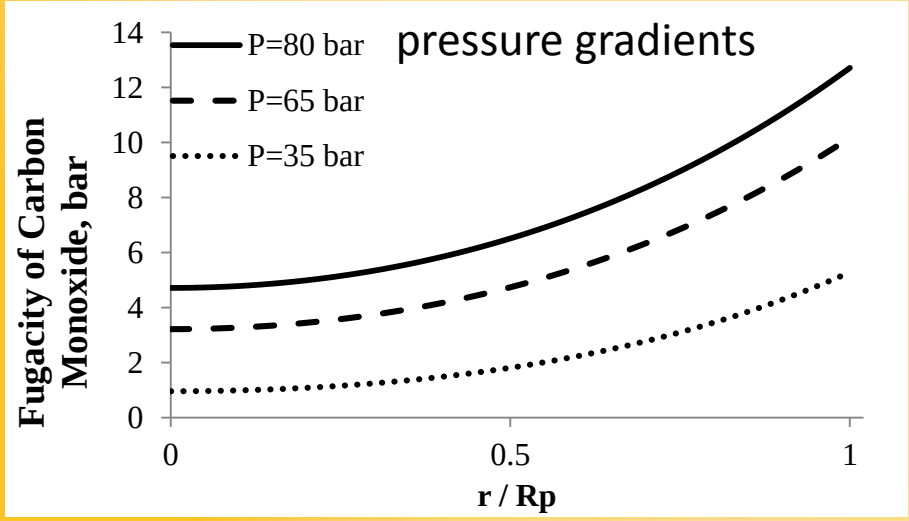
BC. 1: $r = Rcat \rightarrow \left.\frac{dfco}{dr}\right|_{r\ =\ Rcat} = k_m\left(f_{co_{bulk}} - f_{co_{surface}}\right)$

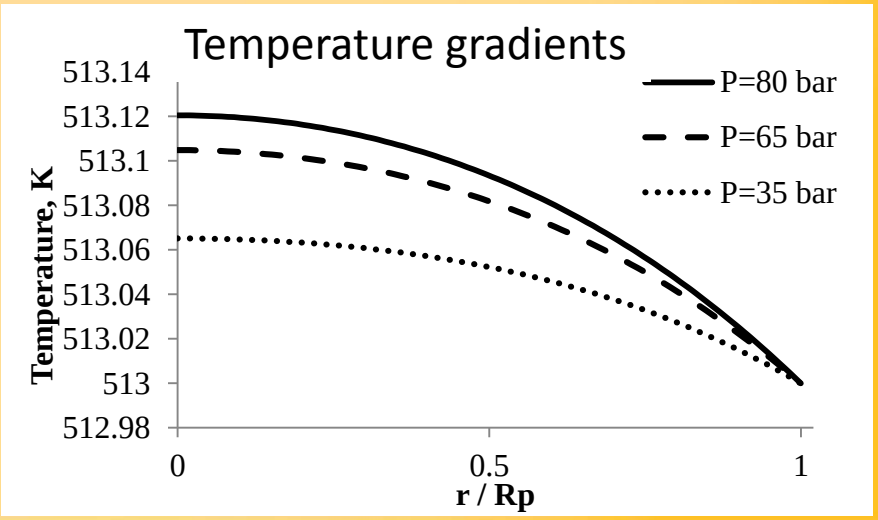
BC 2.: $r = 0 \rightarrow \frac{df_{co}}{dr} = 0$

Hussain et al. (2013) in Weichold, Hall, and Masad "'Development of gas-to-liquid technologies from macro- to micro-scale' Chapter 3, pg. 25.

Intraparticle diffusion and simultaneous heat and mass transfer assessment

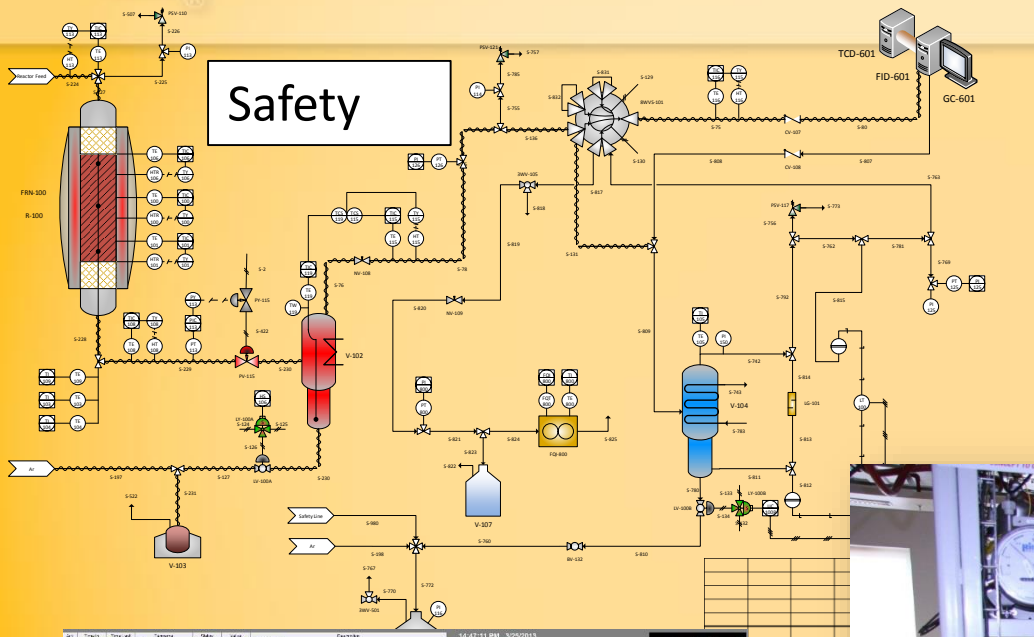


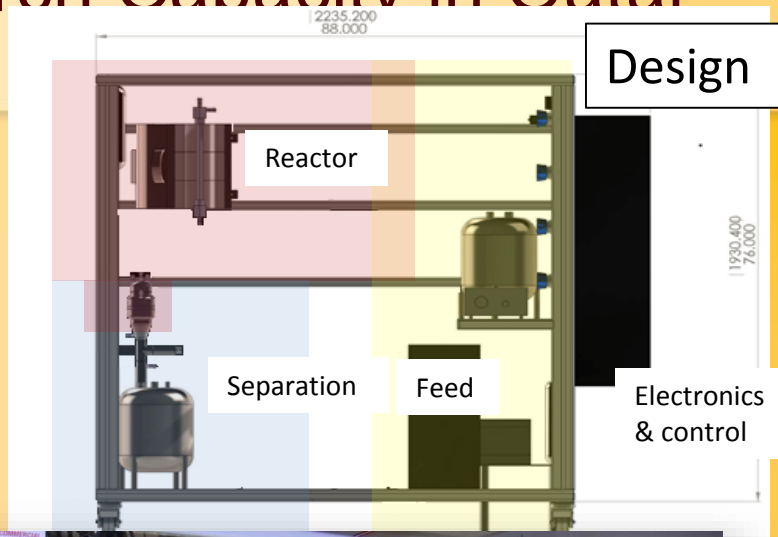


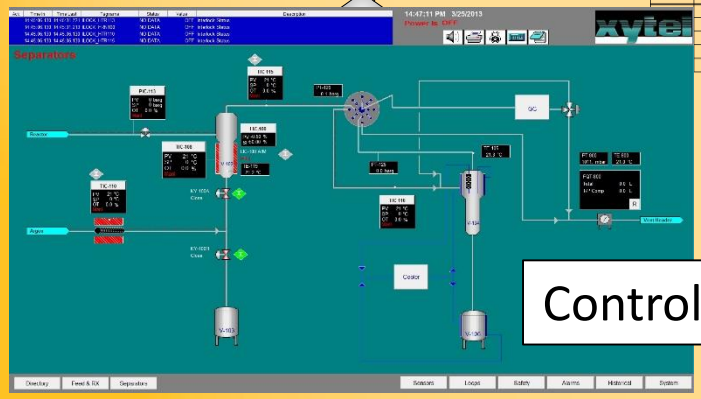


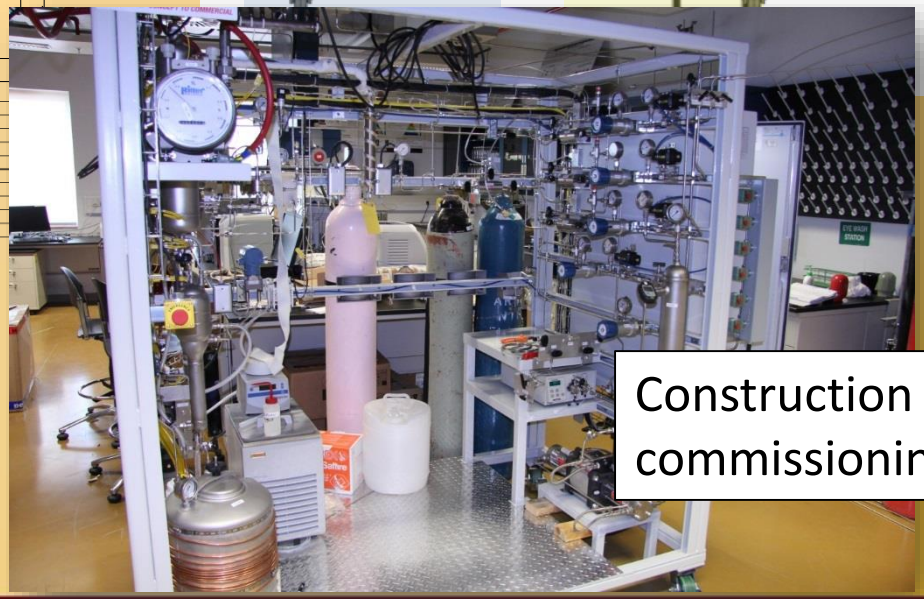
Rig design and commissioning

Development of Research Capacity in Qatar



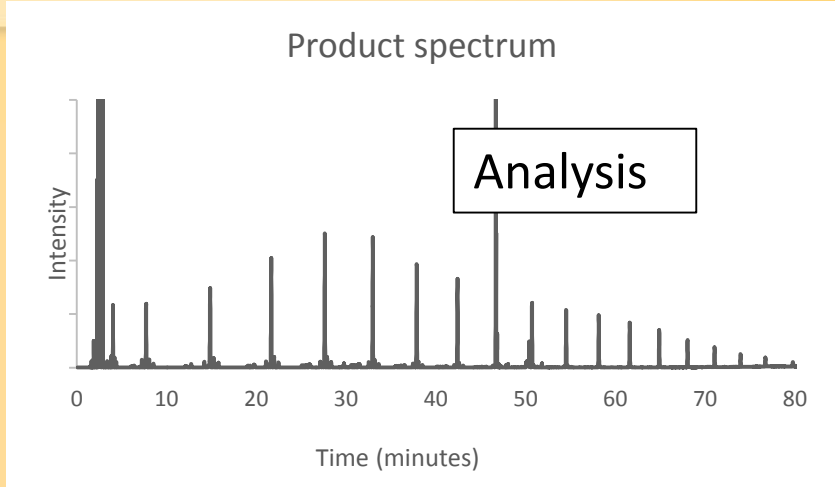




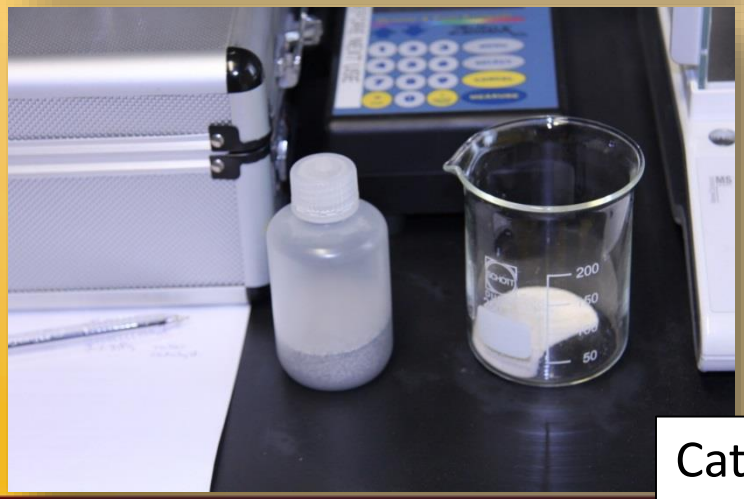


Experimental verification of the modeling results

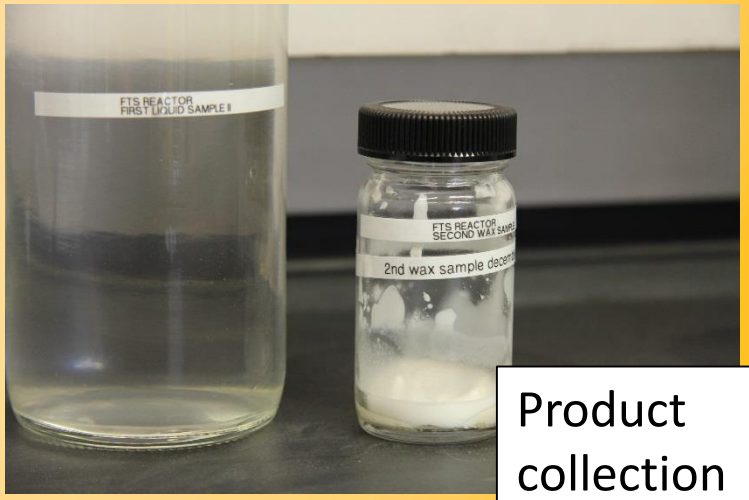
Testing



Analysis



Catalyst synthesis



Product collection

The link between micro scale and macro scale calculations is essential

- Local activity dependent on local conditions
- The sum of all local interactions lead to “bulk” activity
- Use 1-D Model
- Local regimes can be identified and taken into account:
  - Trickle bed behavior
  - Boundary layers
  - Turbulent v laminar flow
  - Diffusion v convection

Bed conductivity needs to be measured

interlinked

Bulk flow

diffusion

Diffusion coefficients

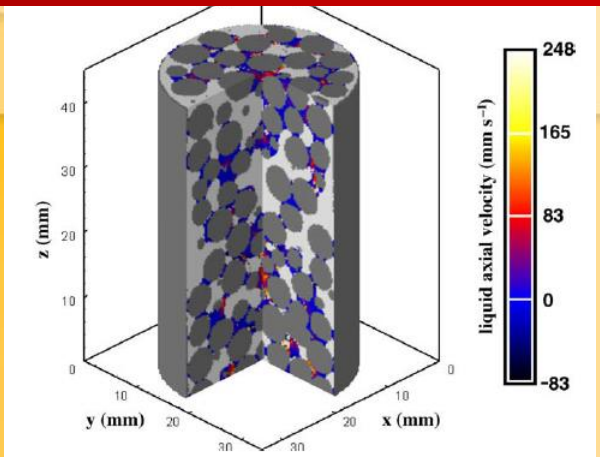
Liquid hold-up

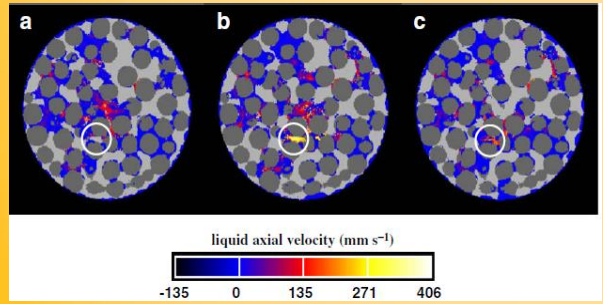
Active site

Velocity profiles

MRI studies

Velocity Profile and Phase Distribution

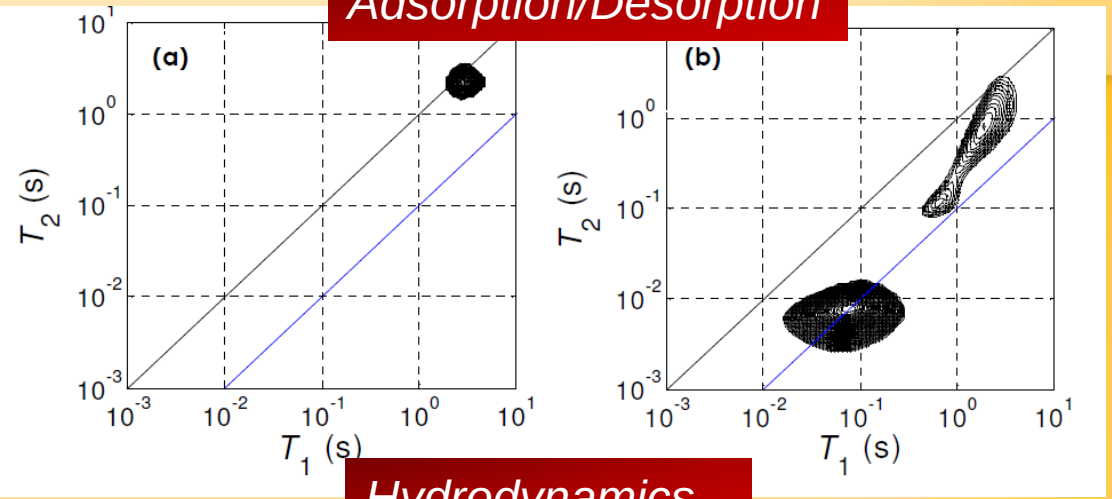




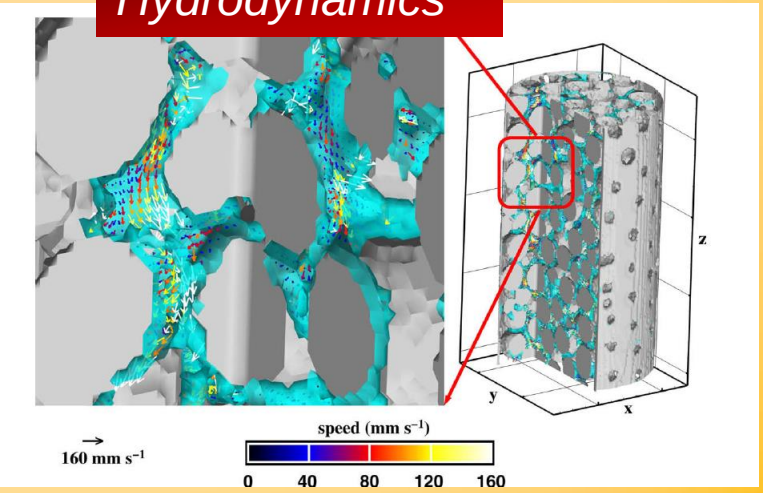
NMR Relaxometry

Gladden, et al. 2009. J Phys. Chem. C 113, 6610.

Adsorption/Desorption



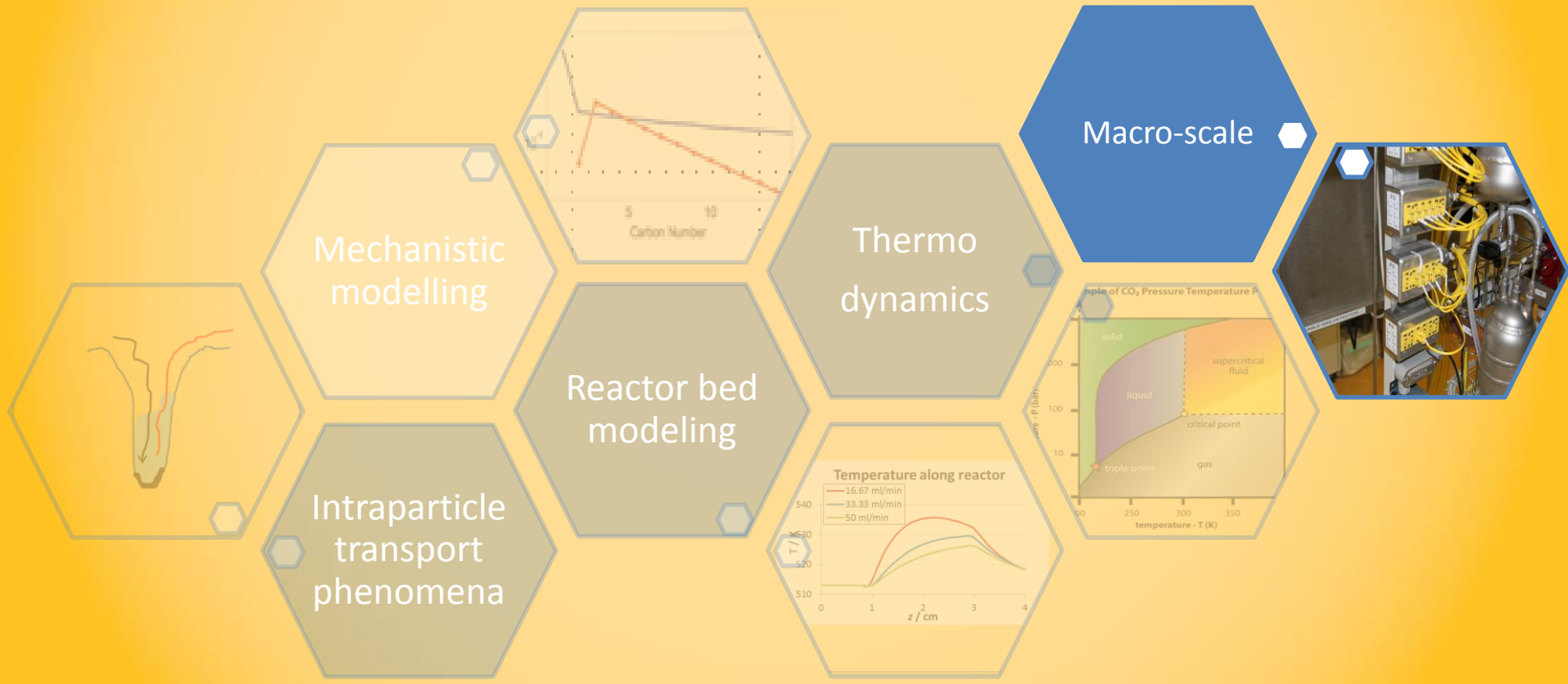
Hydrodynamics



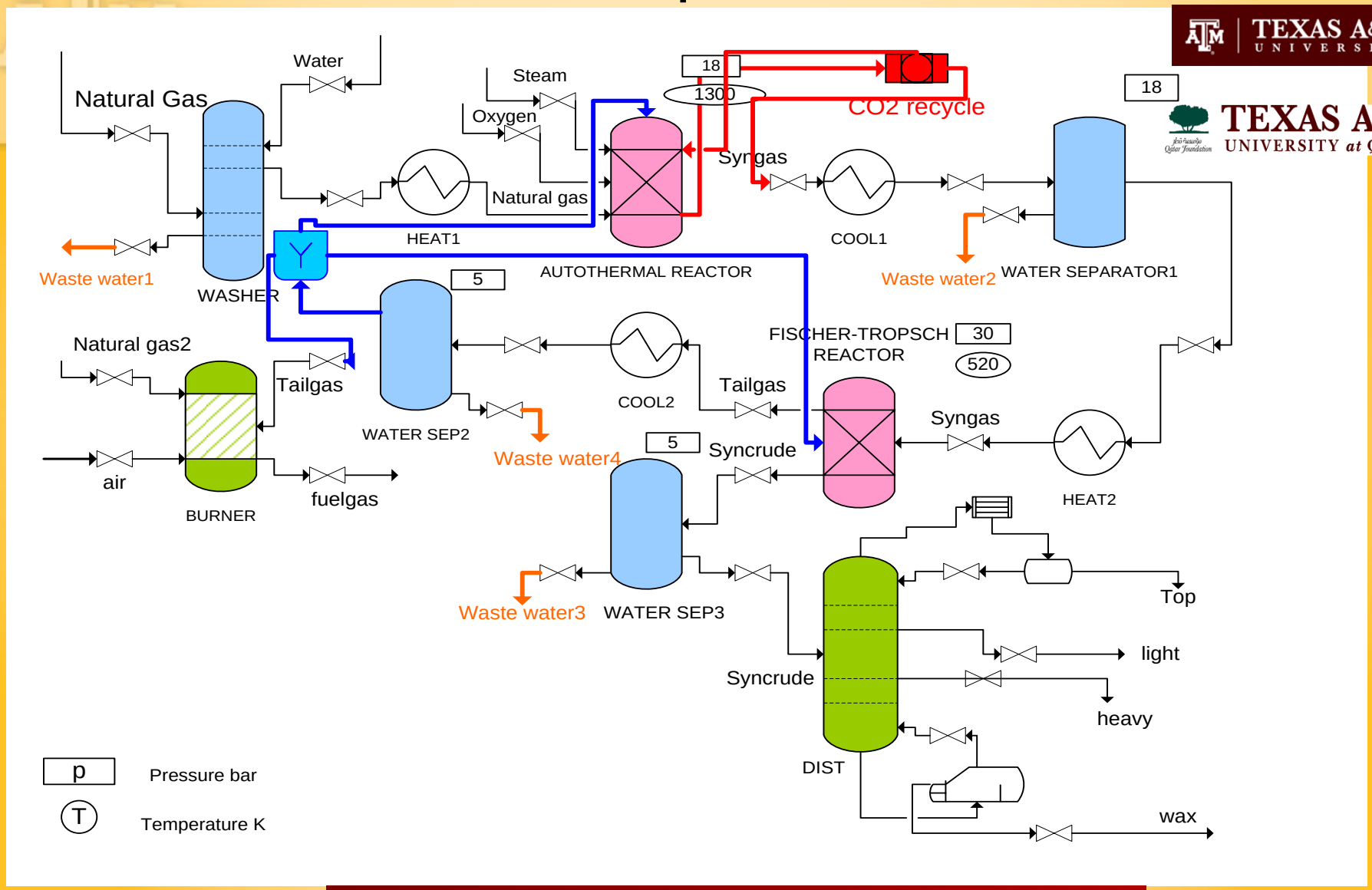
Liquid & gas velocity profile 3D visualization

Gladden et al. 2009. JMR 196, 142.

Building blocks



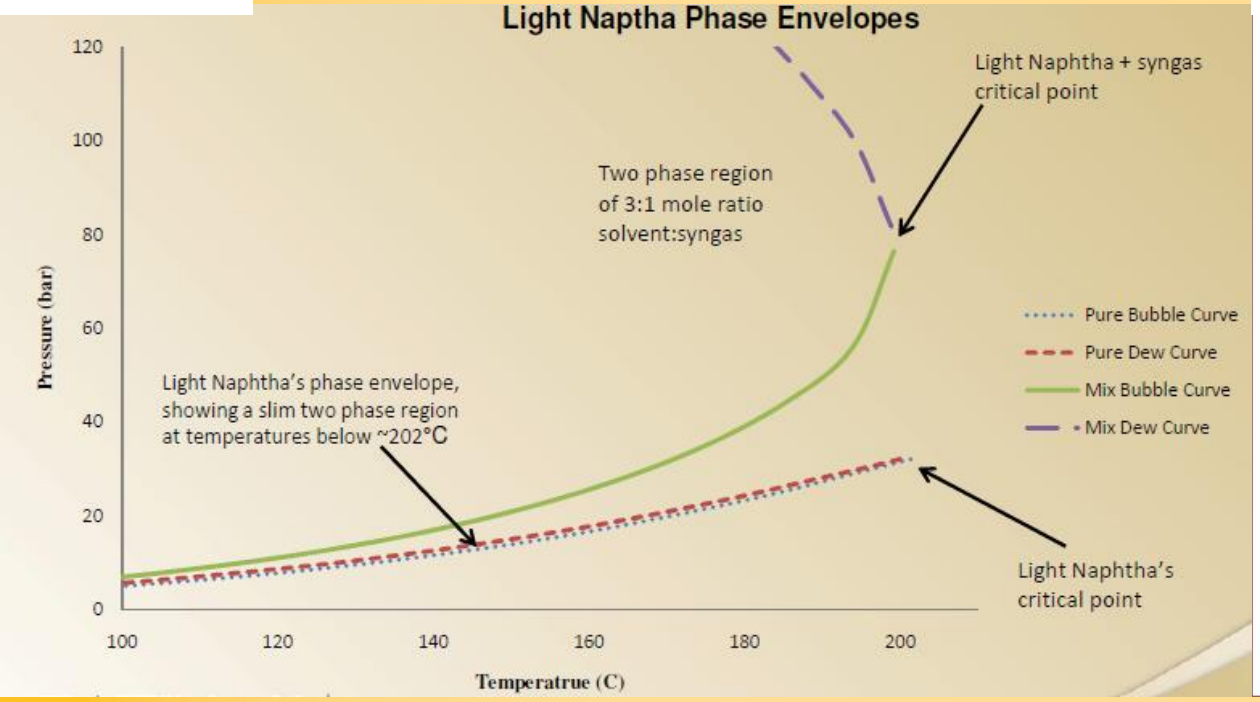
Simulation: GTL plant with SCF-FTS



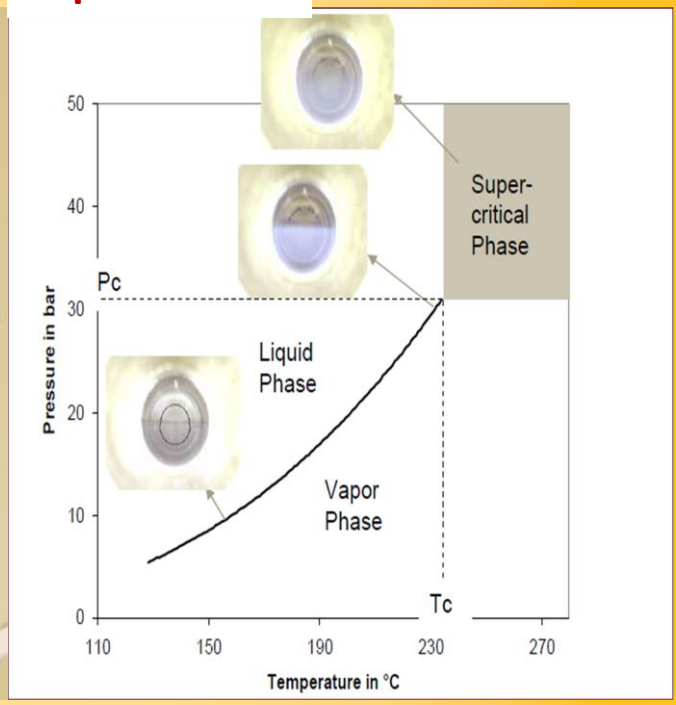
Bao, El-Halwagi, Elbashir 2010. Fuel Processing Technology 91(7) 703.

Examining the most applicable solvent for commercial SCF-FTS

Simulation

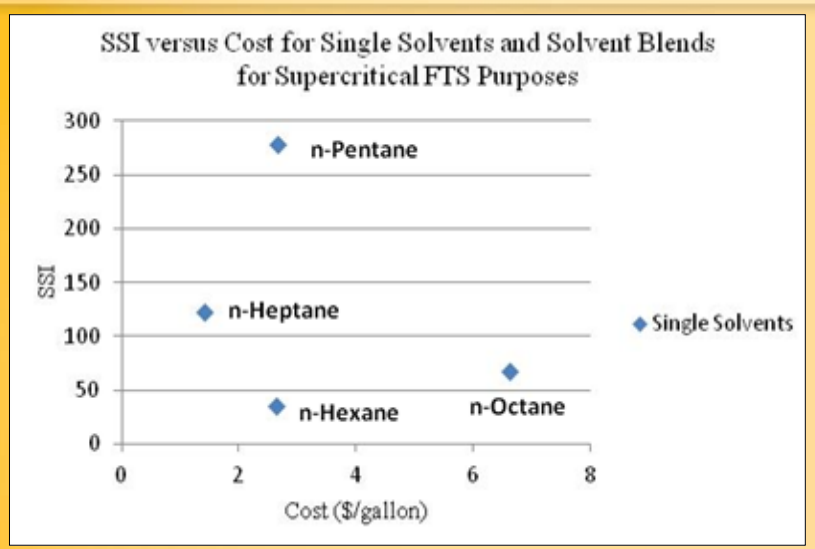


Experimental



Elmalik, Tora, El-Halwagi, Elbashir 2011 Fuel Proc. Techn., 92; 1525.

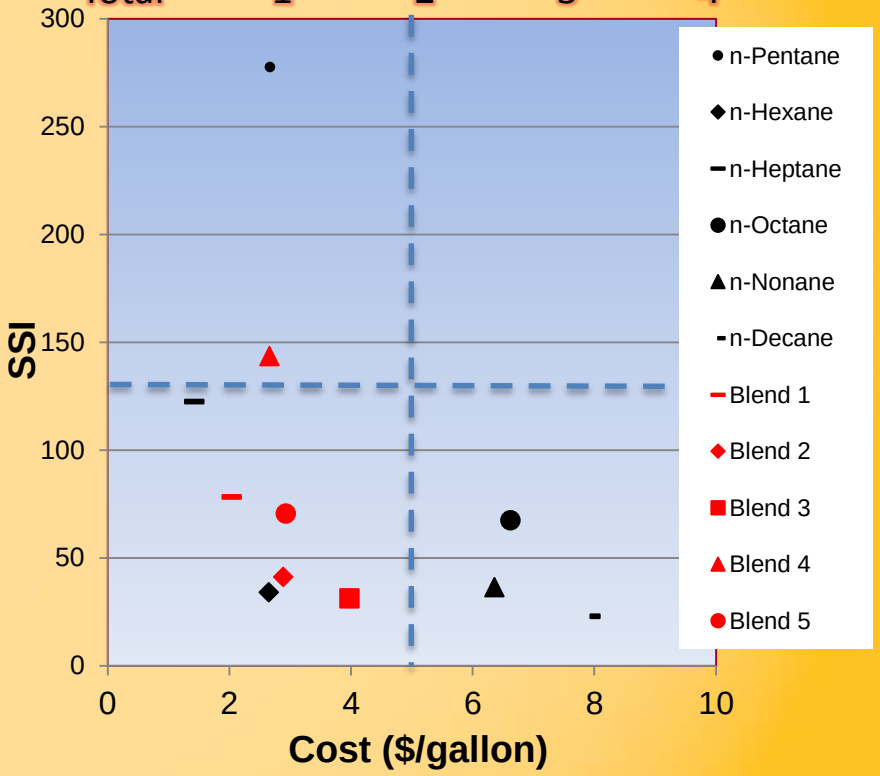
Examining the most applicable solvent for commercial SCF-FTS



Solvent	Price ($ per tonne)*
n-Pentane	989 - 1055
n-Hexane	955 - 985
Light Naphtha	720 - 775
Naphtha	690 - 761
Solvent Naphtha	875 - 885
Gasoline	722 - 745

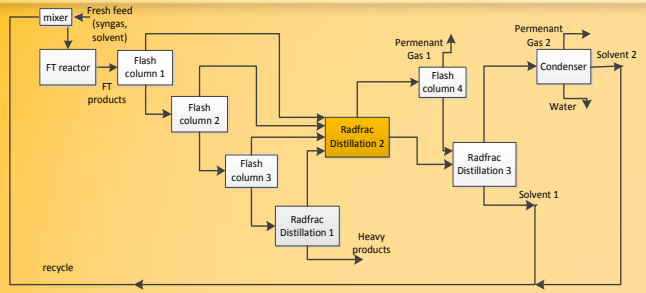
Elmalik, Tora, El-Halwagi, Elbashir (2011) Fuel Proc. Techn., 92; 1525.

$$SSI_{Total}=SSI_1+SSI_2+SSI_3+SSI_4$$

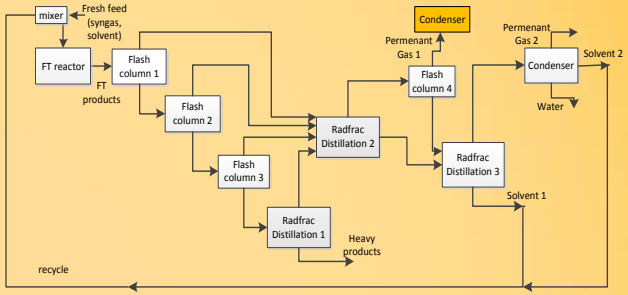


Hamad, El-Halwagi, Elbashir, Manann (2012) J. Loss Prevention in the Process Industries, online.

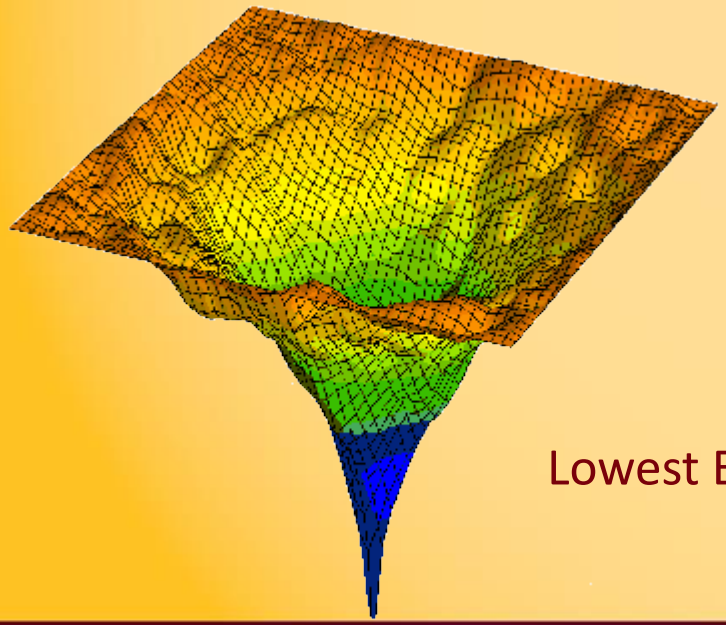
Design of optimized sequence for solvent separation & recycle



Replace RadFrac column with flash column

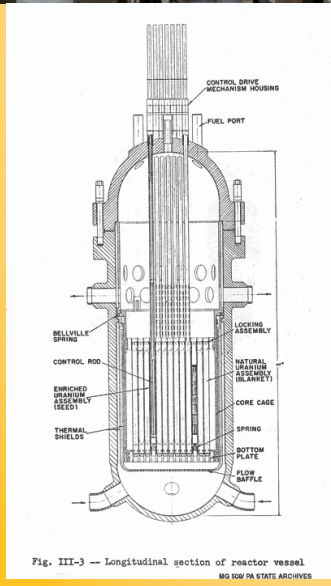


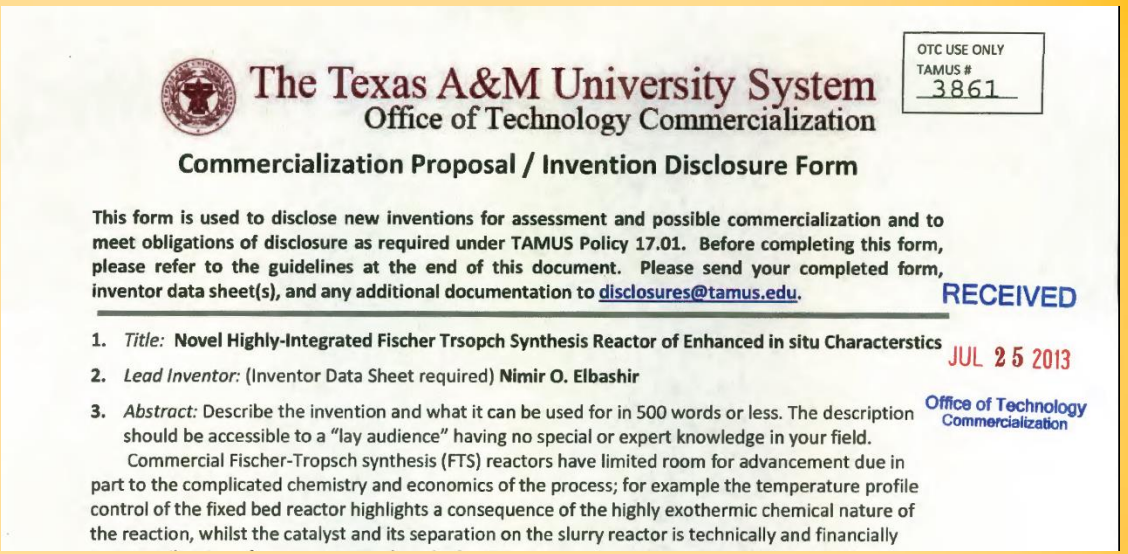
Add a condenser after the flash column



Lowest Energy and Higher Efficiency

Invention Disclosure





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This form is used to disclose new inventions for assessment and possible commercialization and to meet obligations of disclosure as required under TAMUS Policy 17.01. Before completing this form, please refer to the guidelines at the end of this document. Please send your completed form, inventor data sheet(s), and any additional documentation to disclosures@tamus.edu.

RECEIVED
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Office of Technology Commercialization

1. *Title:* **Novel Highly-Integrated Fischer Trsopch Synthesis Reactor of Enhanced in situ Characterstics**
2. *Lead Inventor:* (Inventor Data Sheet required) **Nimir O. Elbashir**
3. *Abstract:* Describe the invention and what it can be used for in 500 words or less. The description should be accessible to a "lay audience" having no special or expert knowledge in your field.

Commercial Fischer-Tropsch synthesis (FTS) reactors have limited room for advancement due in part to the complicated chemistry and economics of the process; for example the temperature profile control of the fixed bed reactor highlights a consequence of the highly exothermic chemical nature of the reaction, whilst the catalyst and its separation on the slurry reactor is technically and financially

This is a schematic <u>but</u> not representing the actual art since it is still under processing.

Cleaner skies

- ***Qatar Airways makes historic journey with first GTL fueled commercial flight from London Gatwick to Doha***

- ***New Gas-to-Liquids fuel offers diversity of supply and better local air quality at busy airports***

Consortium

- A unique collaboration between industry and academia partners.
- Each partner works on specific topics and collaborate towards the overall objective.
- The testing is split up as follows:

Funding Agencies

Technical Guidance

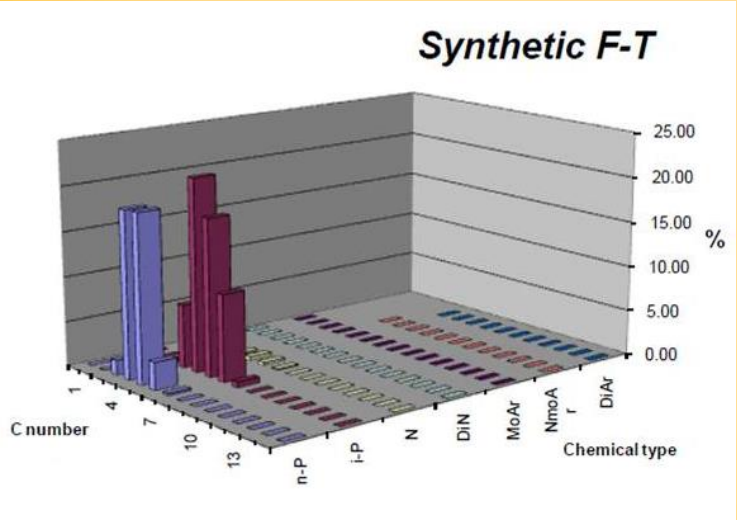
Properties Testing

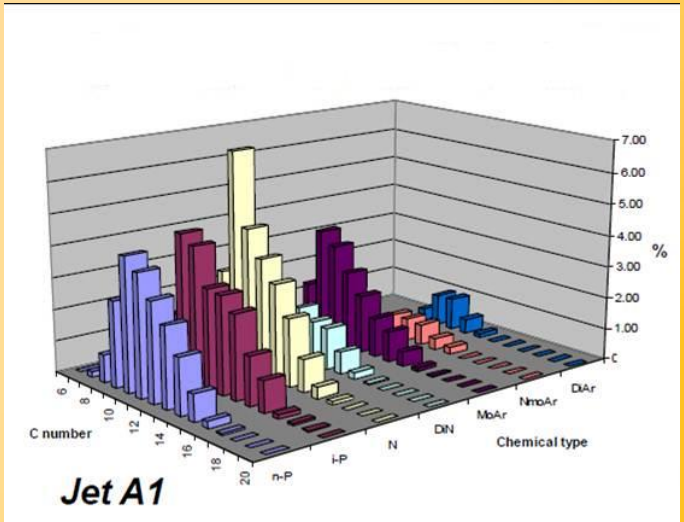
Combustion Testing

Performance Review

Jet Fuels Hydrocarbon Stucture

Species & Carbon Number distribution in a conventional jet fuel (Jet A-1) versus a synthetic GTL kerosene (SPK).





*GCxGC data provided by Shell

Overview of TAMUQ Fuel Characterization Lab

- State-of-the-art experimental facilities

OryxGTL Green Diesel Fuels Campaign!

GE (Oil & Gas) Future Blends of Synthetic Fuels

Summary

- The first phase of the micro & macro scale design successfully completed and resulted in an advanced SCF-FTS lab scale reactor.
- The second phase is focused on experimental verification and the Visualization of the in situ behavior of the reactor bed.
- Energy optimization and process integration efforts continued to identify scale up challenges.
- Design of synthetic fuels and chemicals obtained from natural gas is a major focus of our research activities.
-
- This research work is part of Texas A&M building center of excellence in Catalysis, Reactor Design and ***Advancement of GTL Technologies***.

Acknowledgements

Collaborators

Prof. Mahmoud El-Halwagi

Prof. Juergen Hahn (currently RPI)

Prof. Ben Wilhite

Prof. Christopher Roberts

Prof. Bruce Tatarchuk

Prof. Manfred Aigner

Prof. Fadwa Eljack

Prof. Lynn Gladden

Prof. Chris Wilson

Prof. Rafiqul Gani

Prof. Dragomir Bukur

Prof. Marcelo Castier

Industry Collaborators & Advisory Board

Dr. Joanna Baulready
Paul Bogers
Willem Scholten

Dr. Jim Rigby

Dr. Ernest De Toit (former)

Rashid Al-Rashdi

John Moran

Research Outcome:

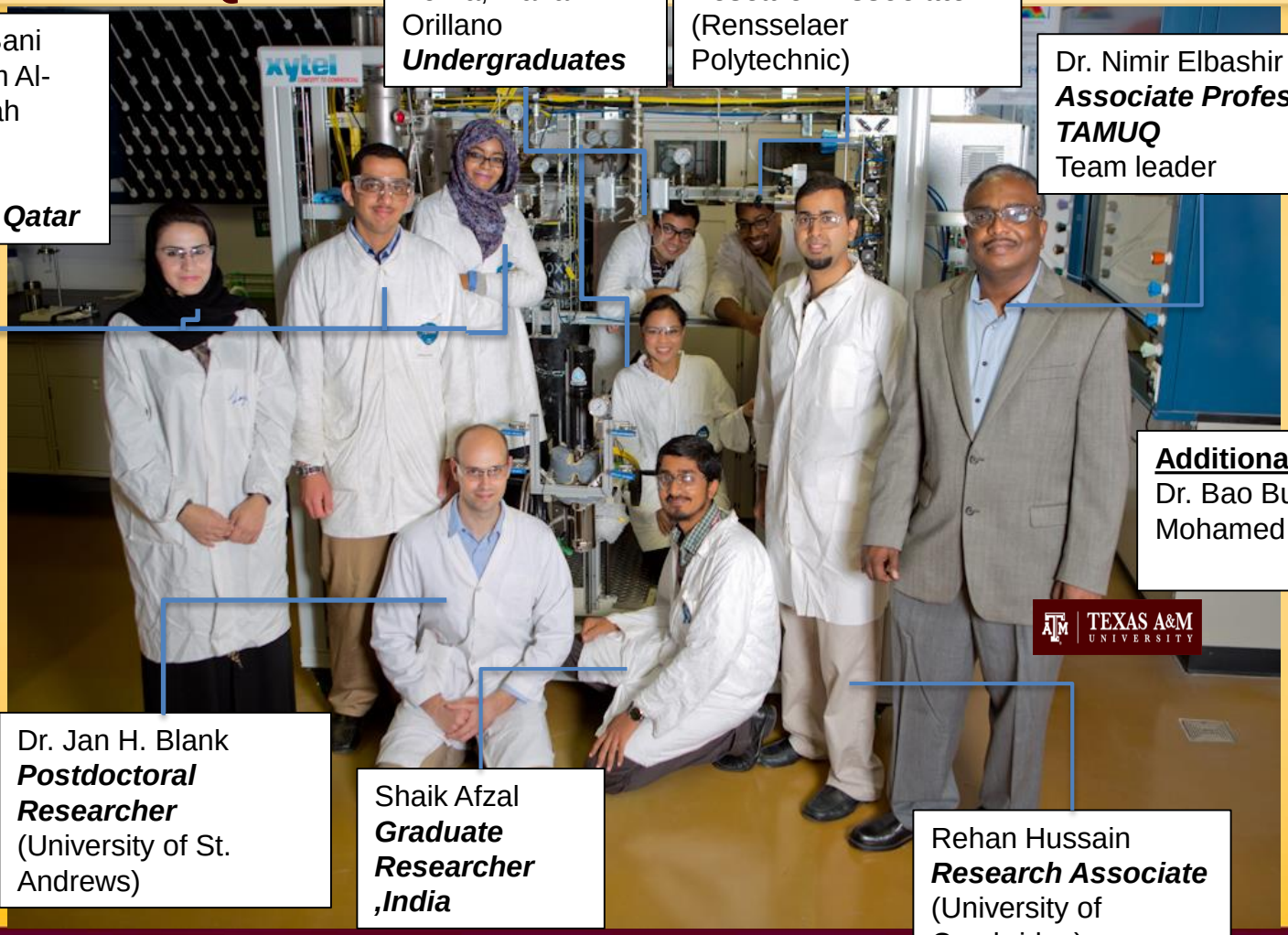
Development of Research Capacity in Qatar

L to R: Laial Bani Nassr, Ibrahim Al-Nuaimi, Samah Warrag
Graduate Researchers Qatar

L to R: Moiz Bohra, Maria Orillano
Undergraduates

Elfatih Elmalik
Research Associate
(Rensselaer Polytechnic)

Dr. Nimir Elbashir
Associate Professor, TAMUQ
Team leader



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UREP 07 - 055 - 2 - 012

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National Priorities Research Program
NPRP

UREP

Thank you

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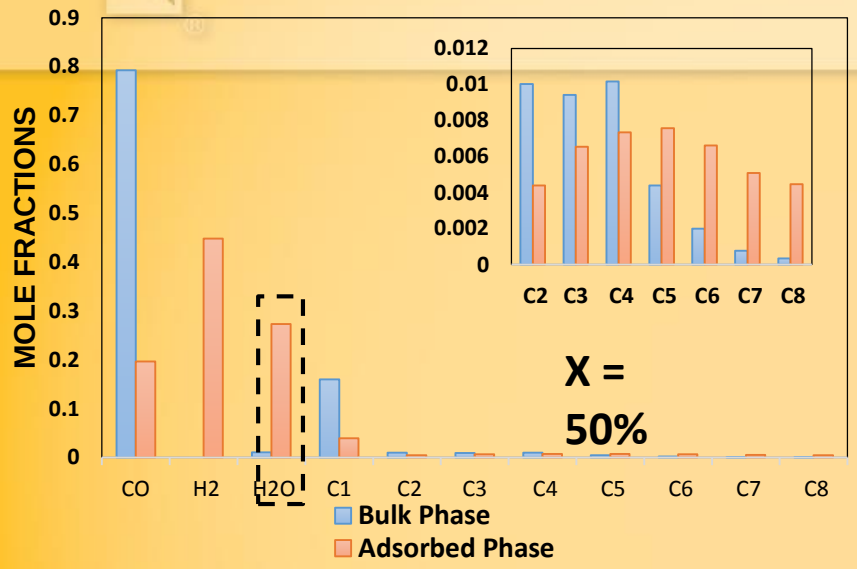
Backup Slides

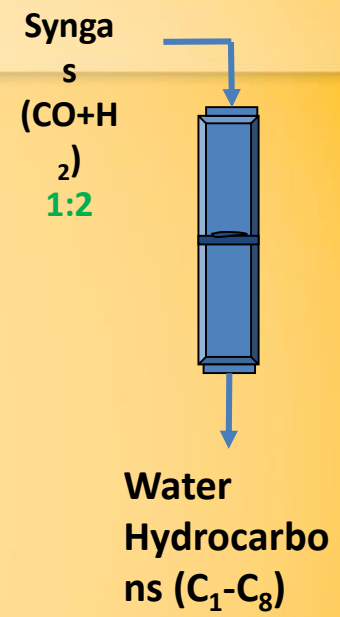
Results & Discussion : Conventional Gas Phase at 20 bar

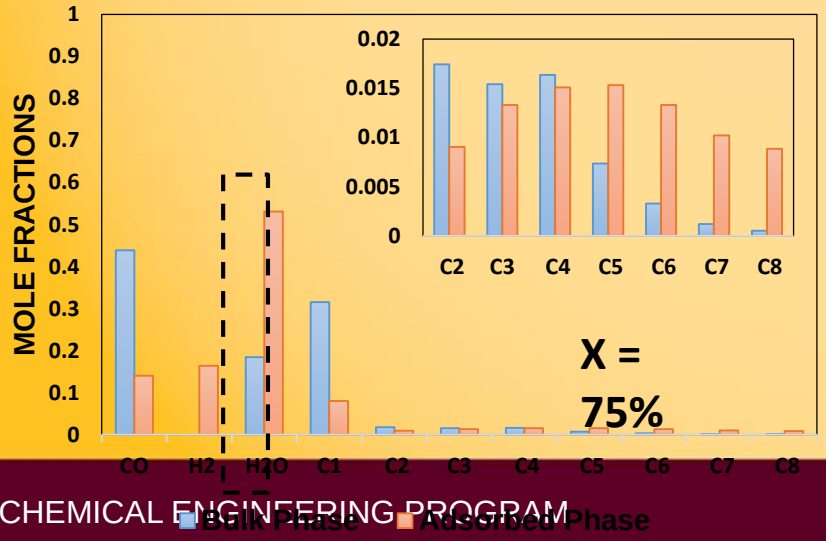


Temperature = 513K

Total Pressure = 20 bar

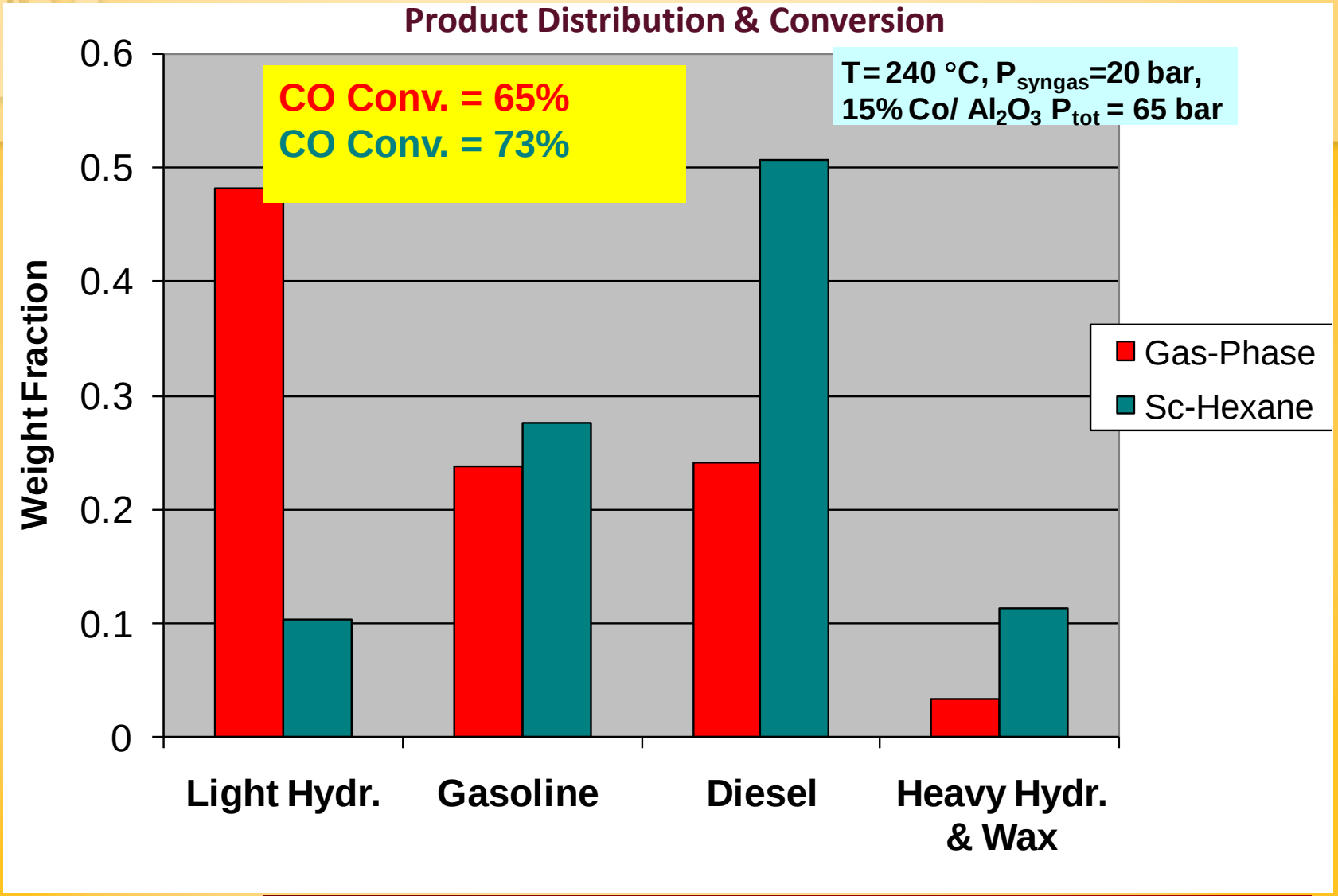
- Increased fraction of water inside the pores.
- Gas-like density in both phases





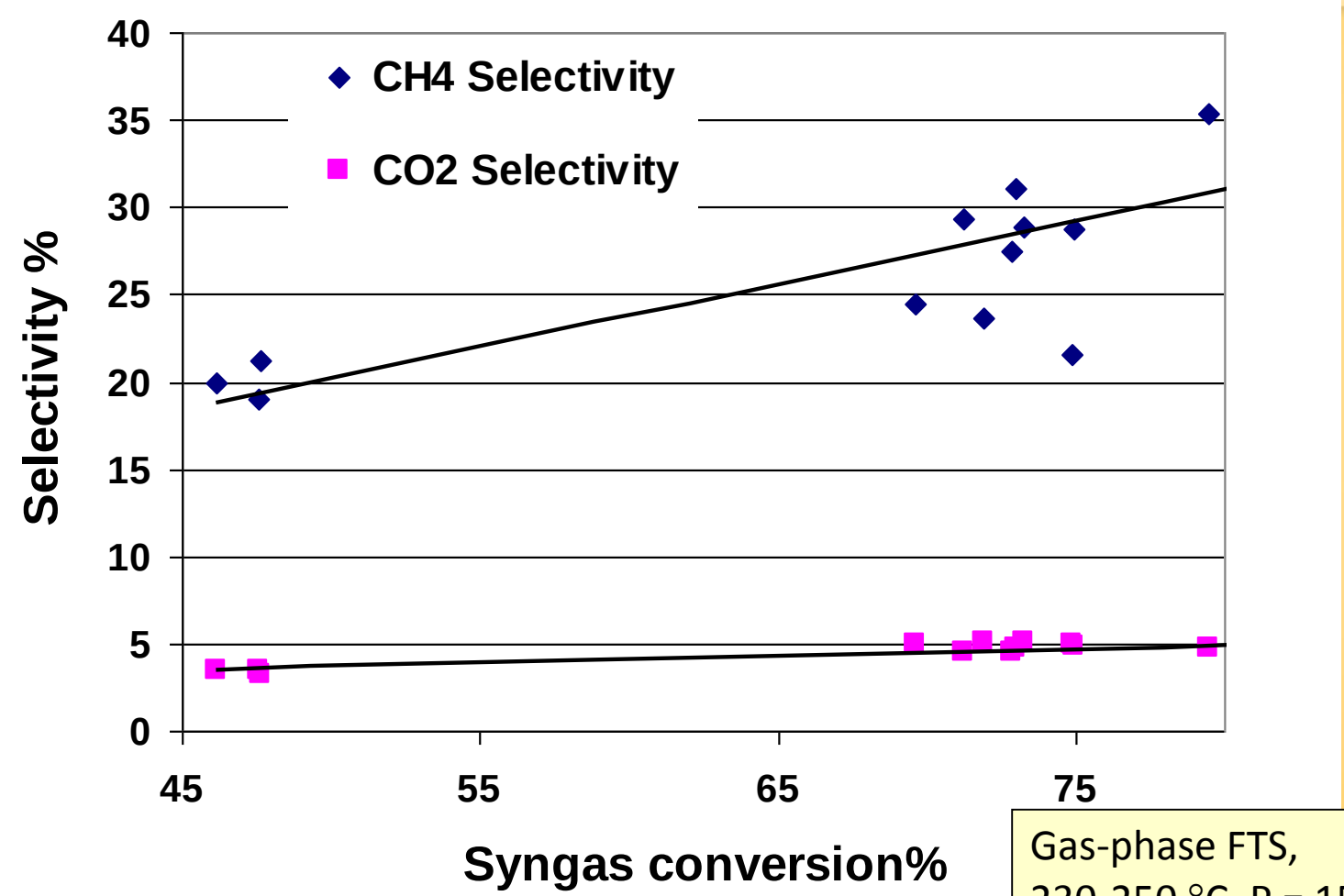
Phase	Bulk Phase	Adsorbed Phase
50% Conversion		
Compressibility Z	1.00	-
Density (Kg/m³)	12.58	71.40
75% Conversion		
Compressibility Z	74 0.99	
Density		

Comparison SCF-FTS & Gas Phase FTS



Huang, Elbashir , Roberts 2005. Industrial & Engineering Chemistry Research 43, 6369.

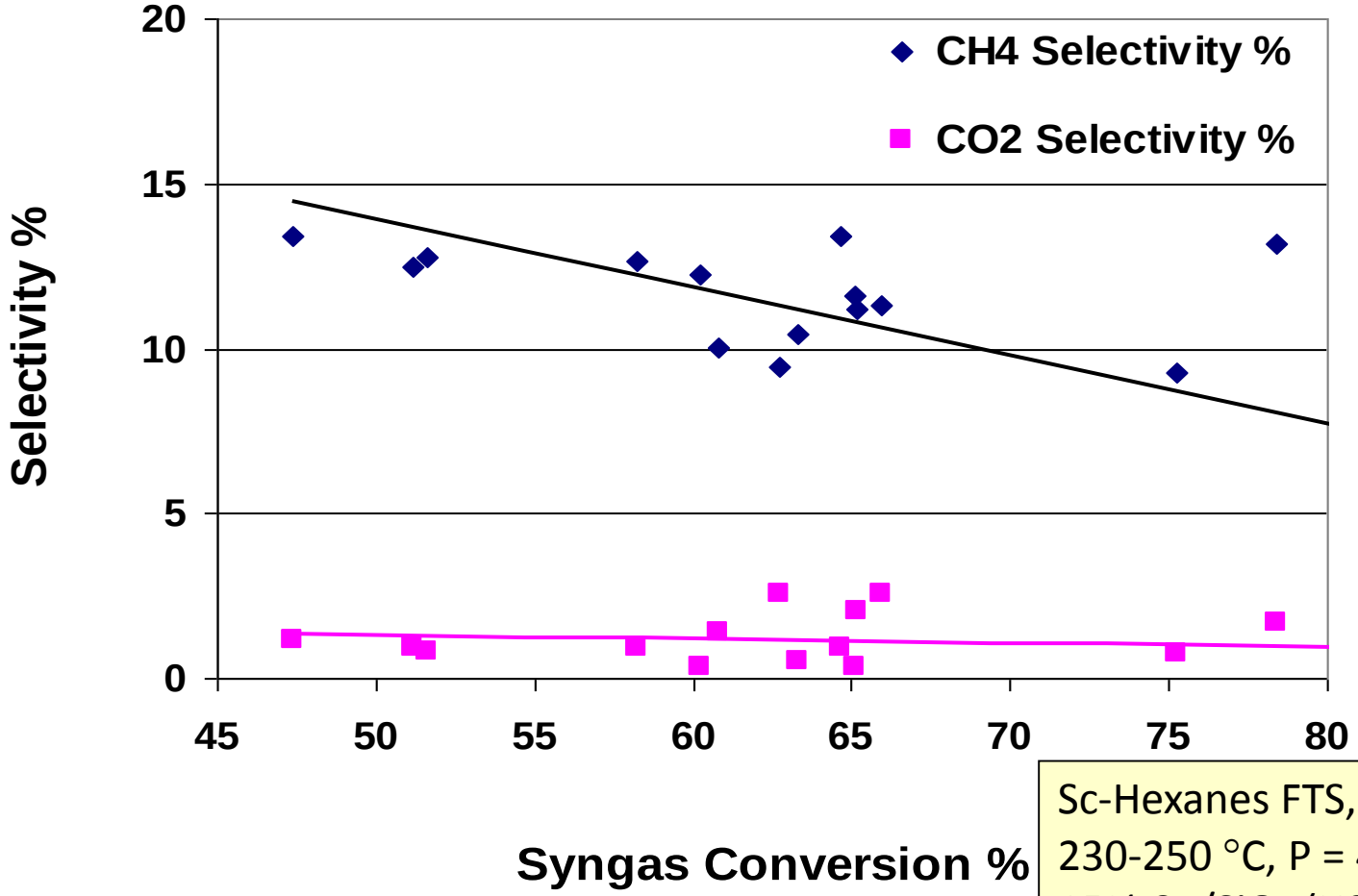
Comparison SCF-FTS & Gas Phase FTS Selectivity vs. Conversion



Gas-phase FTS,
230-250 °C, P = 15-20 bar
15% Co/SiO_2 (HSA),
Syngas FR = 50-100 sccm/g_{cat}

Elbashir , Dutta, Seehra, Roberts 2005. Applied Catalysis A: General 285, 169.

Comparison SCF-FTS & Gas Phase FTS Selectivity vs. Conversion



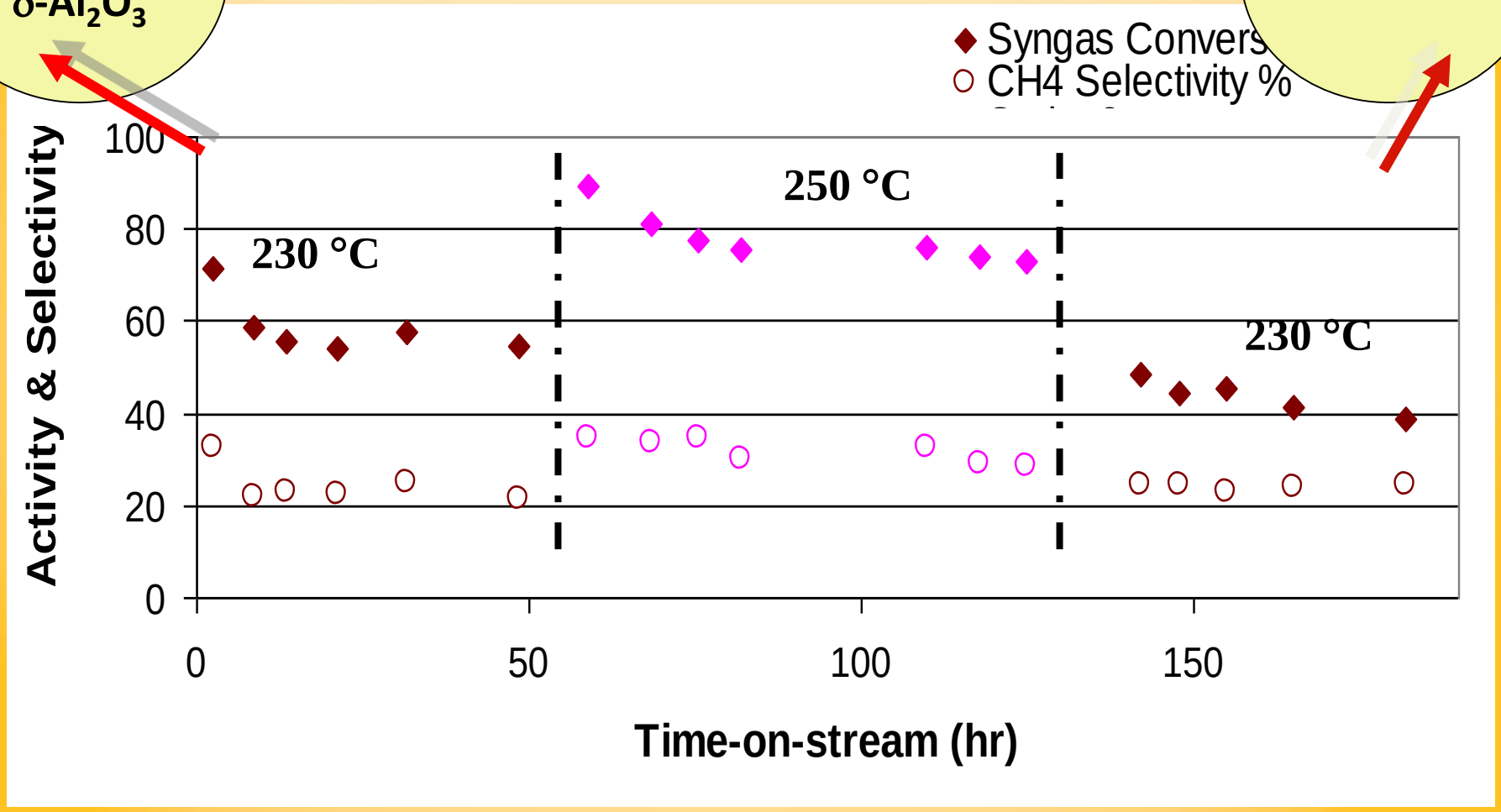
Sc-Hexanes FTS,
230-250 °C, P = 45-65 bar
15% Co/SiO_2 (HSA),
Hexanes/syngas (molar) = 3
Syngas FR = 50-100 $sccm/g_{cat}$

Elbashir , Dutta, Seehra, Roberts 2005. Applied Catalysis A: General 285, 169.

Stability of the same Catalyst in **Gas-Phase FTS**

Co_3O_4, Co^{+2}
δ-Al_2O_3

Co_3O_4
fcc Co^0

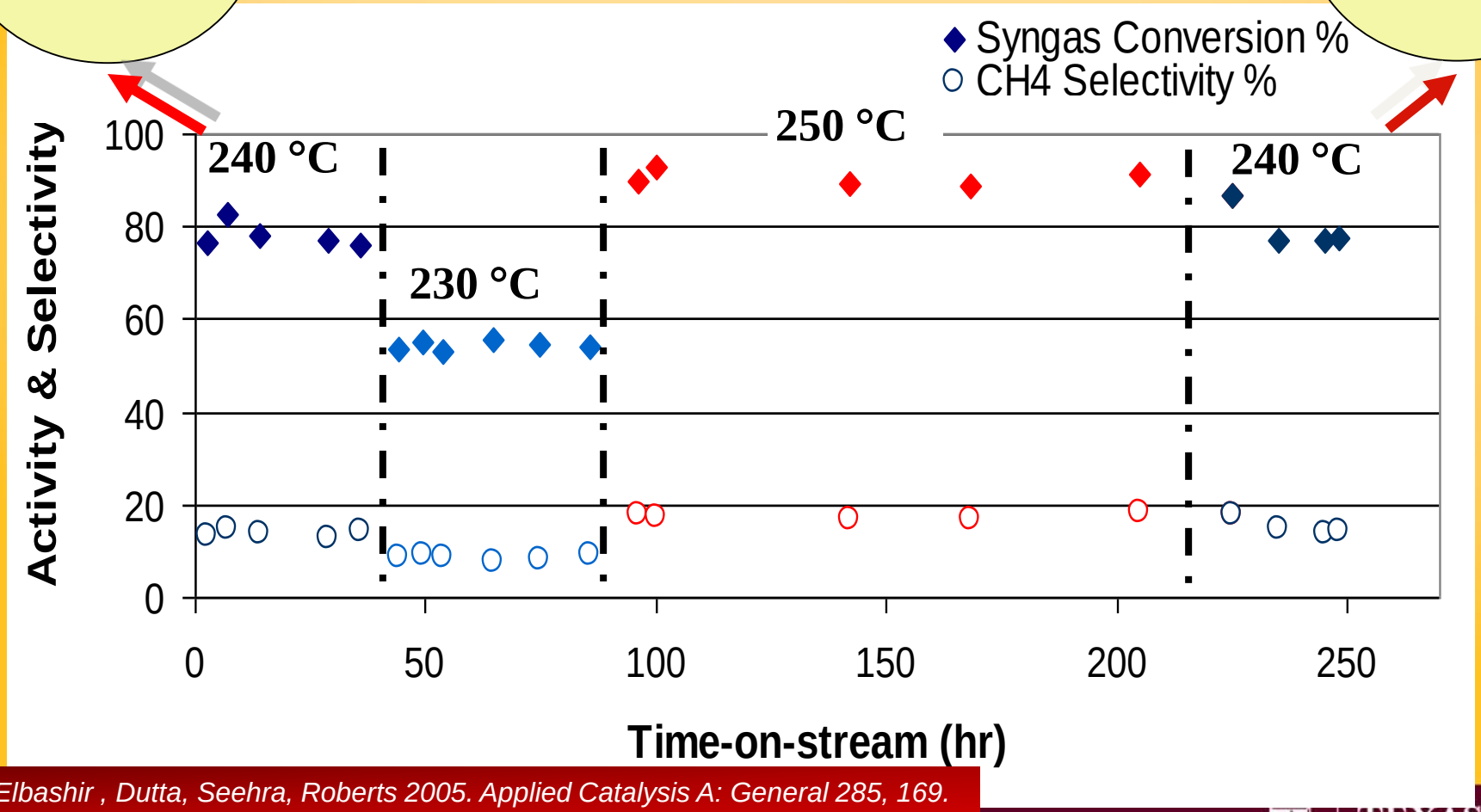


Elbashir , Dutta, Seehra, Roberts 2005. Applied Catalysis A: General 285, 169.

Stability of the same Catalyst in **Supercritical Phase FTS**

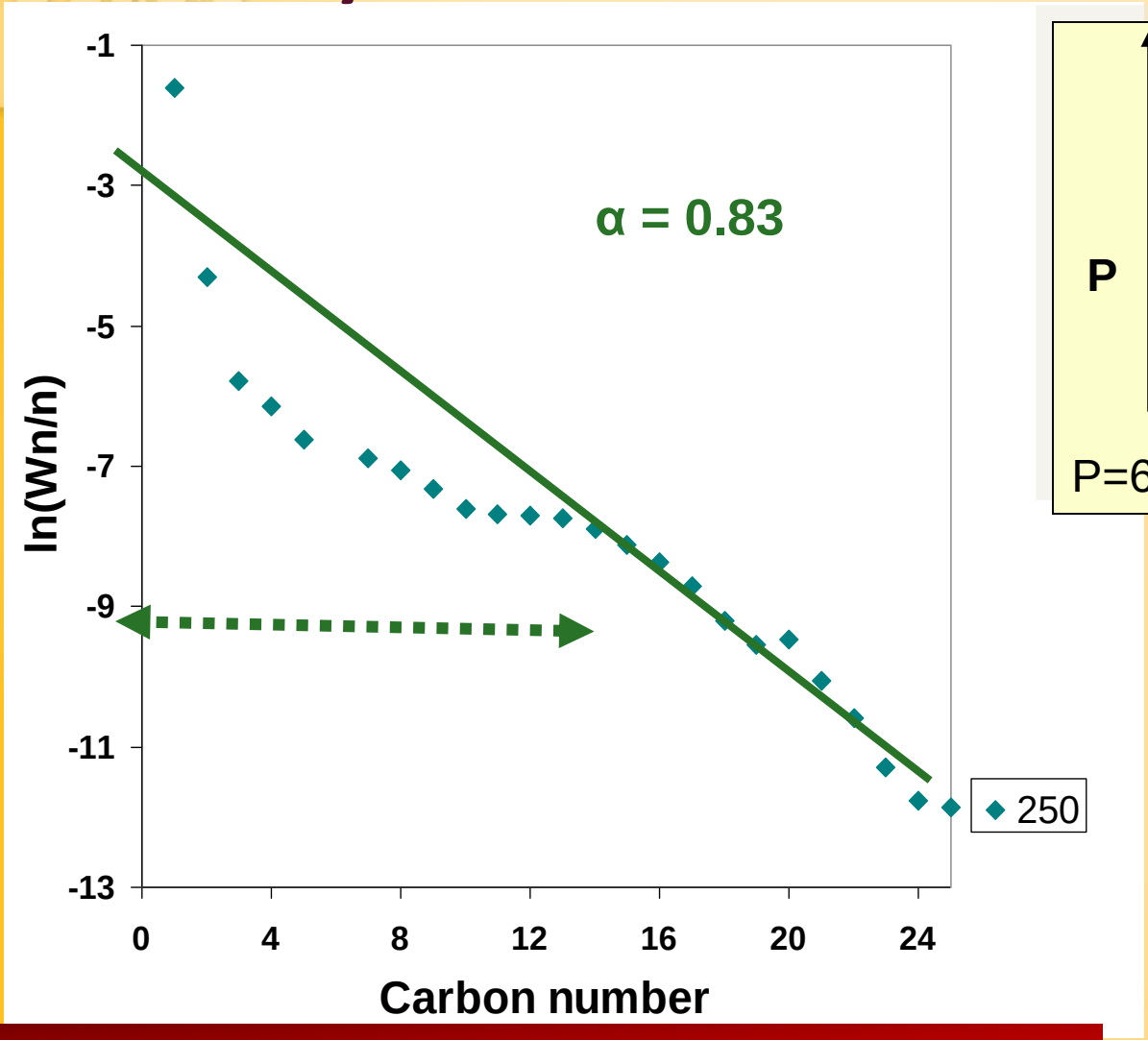
Co_3O_4, Co^{+2}
δ-Al_2O_3

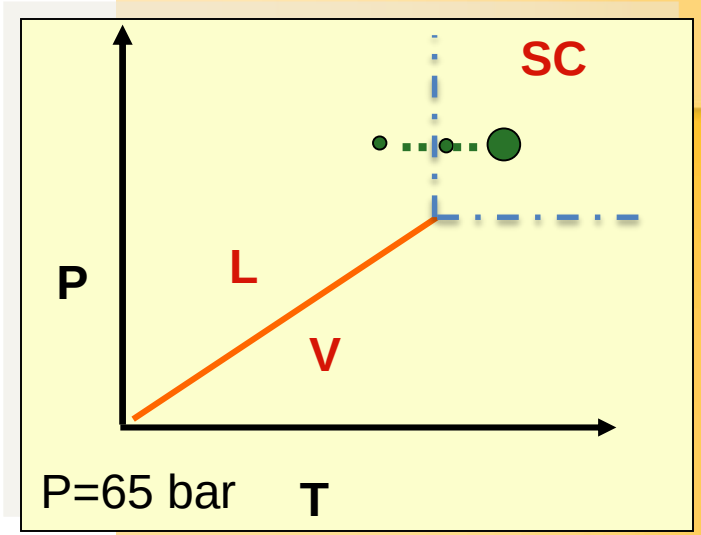
hcp Co^0



Elbashir , Dutta, Seehra, Roberts 2005. Applied Catalysis A: General 285, 169.

Opportunity for Selective Control of Hydrocarbon Product Distribution



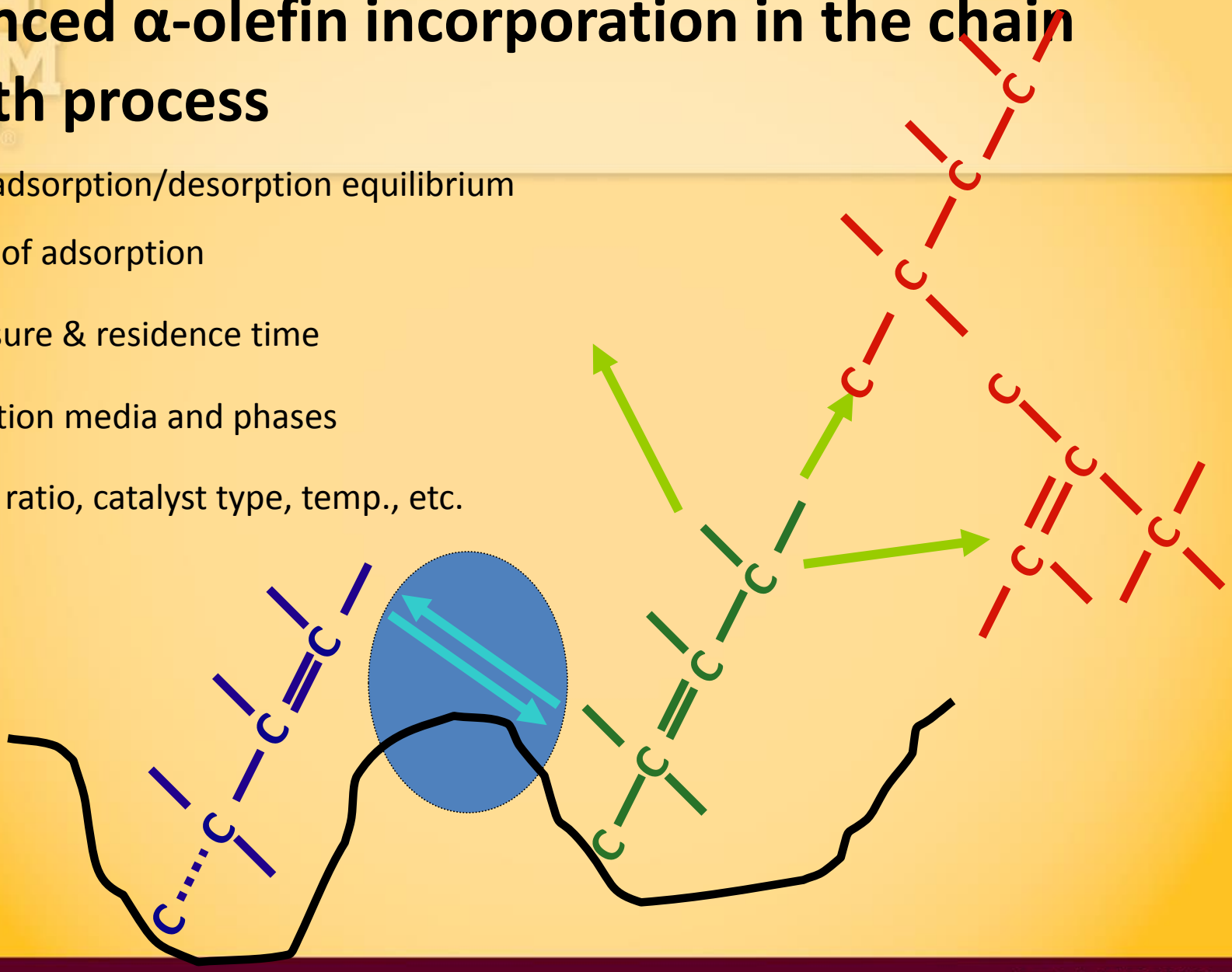


Elbashir , Roberts 2005. Industrial & Engineering Chemistry Research 44, 505.

Enhanced α-olefin incorporation in the chain growth process

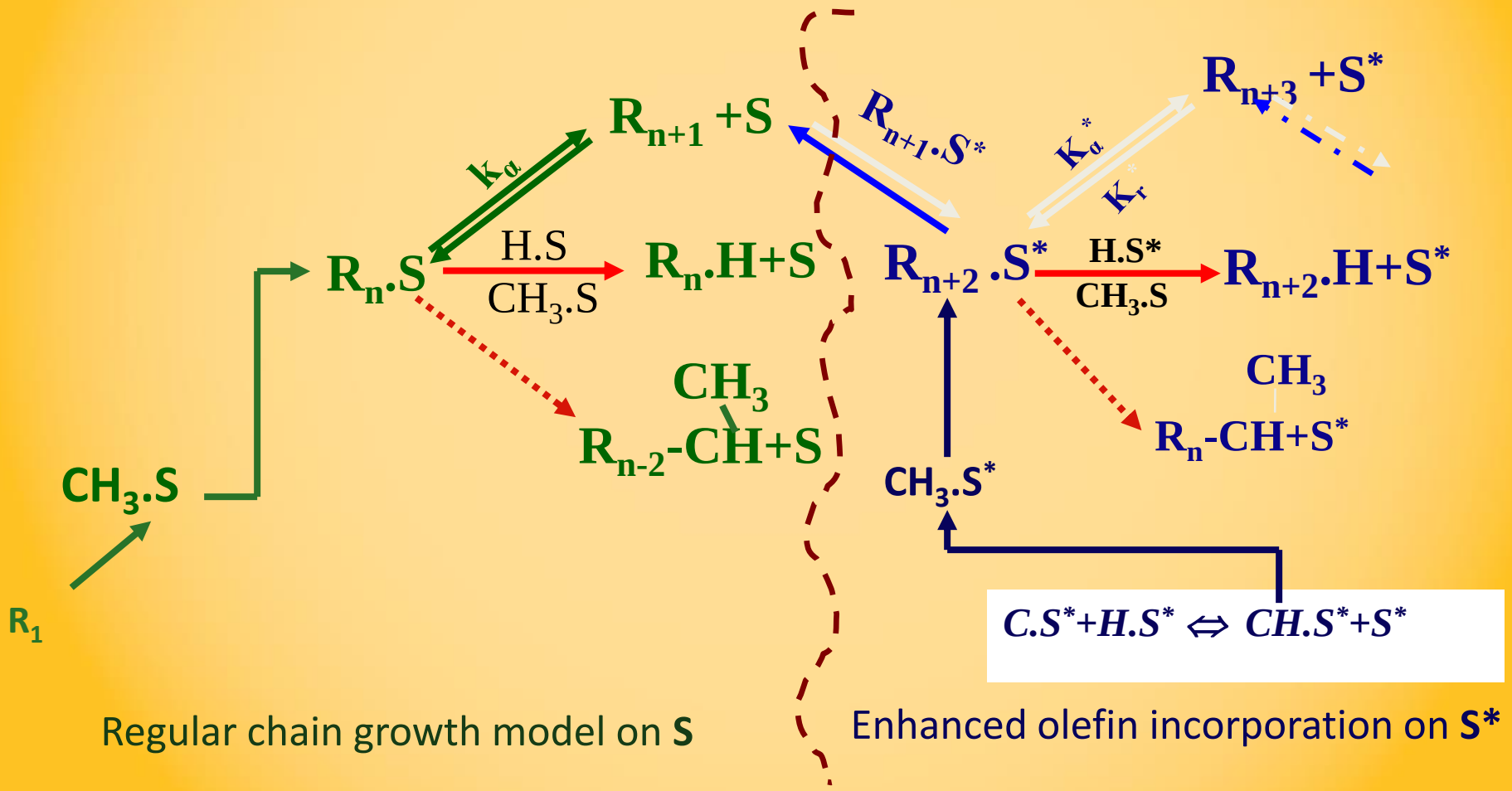
Dynamic adsorption/desorption equilibrium

1. Heat of adsorption
2. Pressure & residence time
3. Reaction media and phases
4. Feed ratio, catalyst type, temp., etc.



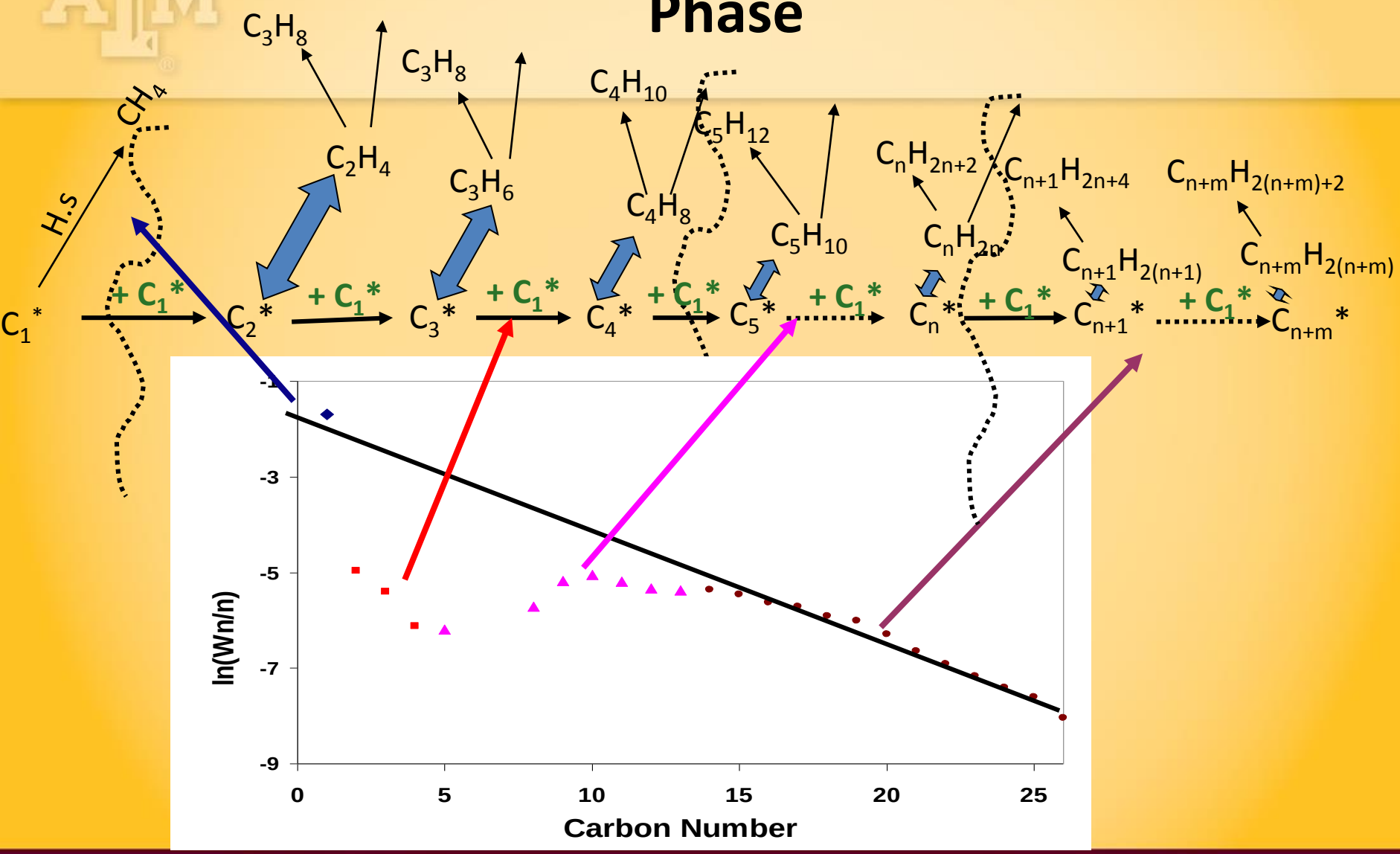
(4) Kinetics of the SCF-FTS

Modified Reaction Pathway and Chain Growth Model for SCF-FTS



TEXAS A&M UNIVERSITY at QATAR

Enhanced incorporation of α-olefins in SCH Phase



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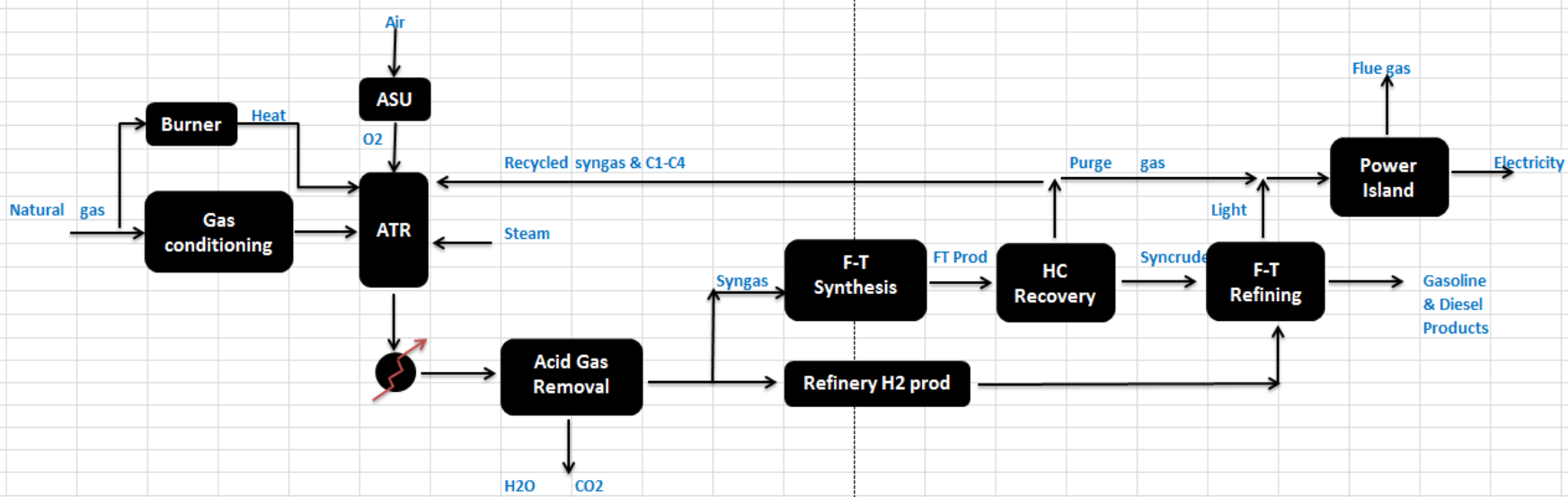
Energy Integration & Overall Techno-economic Assessment



	SCFT					FT
		lb/hr	IN	OUT		
57196.2	2556671	CH4	27104			
	3099153	O2	32855			3711560
	118005	H2O	1251			
	3318277	CO		35178		3973984
remaining	181635	H2		6951		174949
					H2O	2004813
	33808.9					

Techno-economic Assessment of the Optimized Sequence

calculation							1.1223539							Cm=Cxn*0x(S/S	Cm		Cm*(1+B	Cm*(1+in	Cm*(1+BOP%)*(1+indirect%)
Air separation unit	75 bar pressure	Pure O2, t/day	2,202	2500	0.5	105	117.6	15.5	included	a2	33808	14	1324	461	1324	1529	1324	1529	
	O2 compressor	power, MW	10		0.67	7.24	8.1088	included	32	f2	346.45	1	87	87	87	87	115.1	115.104	
	N2 compressor	power, MW	10		0.67	5.41	6.0592	included	32	f2	1266.2	1	155	155	155	155	204.96	204.958	
Auto-thermal reforme	Auto-thermal reformer	input, MM SCF	365	8,000	0.67	29.9	33.488	eq4	32	a1	1601.2	1	90	90	90	101.19	119.04	133.564	
	gas scrubbing & low temp	power, MW	77		0.6	33.2	37.184	15.5	included	a2	38.96	1	25	25	25	28.537	25	28.5374	
FT synthesis	FT fresh feed compressor	power, MW	10		0.67	6.31	7.0672	included	32	f3	126.62	1	39	39	39	39	51.109	51.1091	
	FT synthesis, slurry reacto	input vol flowra	2.5	100	0.75	13.6	15.232	eq4	32	f3	155.84	2	375	336	375	420.69	494.93	555.306	
	Slurry reactor synthesis	BPD	20,000		0.75	49	54.88	eq4	32	f4	120000	1	210	210	210	236.06	277.72	311.538	
	Slurry catalyst pretreatment																		
	Slurry hydroclone after reactor																		
	Slurry catalyst centrifuge																		
	Slurry wax filter																		
	Fixed bed synthesis	BPD	20,000		0.75	82.1	91.952	eq4	32	f4	142702	1	401	401	401	450.41	529.89	594.536	
Syncrude refining	HC recovery plant	HC inlet flow, 1(	14	200	0.7	0.724	0.81088	eq4	32	f3	1425.9	8	31	21	31	35.087	41.279	46.315	
	Wax hydrocracking	wax inlet flow, 1	9	575	0.7	9.3	10.416	eq4	32	f3		1	0	0	0	0	0	0	
	Distillate hydrotreating	distillate inlet fl	2.9	650	0.7	2.49	2.7888	eq4	32	f3	1425.9	3	266	214	266	298.56	351.24	394.094	
	Naphtha hydrotreating	naphtha inlet flc	2.1	650	0.7	0.754	0.84448	eq4	32	f3	97.4	1	12	12	12	13.9	16.353	18.3482	
	Naphtha reforming	naphtha reformi	3.4	750	0.7	5.18	5.8016	eq4	32	f3	1003.2	2	357	311	357	400.58	471.27	528.765	
	C5/C6 isomerization	C5/C6 isomeriz	1.158	250	0.7	0.956	1.07072	eq4	32	f3	246.42	1	46	46	46	51.197	60.232	67.5806	
	Fuel gas compressor	power, MW	10	70	0.67	6.31	7.0672	included	32	f2	58.44	1	23	23	23	23	30.445	30.4451	
	Recycle gas compressor	power, MW	10	70	0.67	6.31	7.0672	included	32	f2	50.648	1	21	21	21	21	27.662	27.6616	
	H2-feed, PSA-feed comp:	power, MW	10	70	0.67	6.31	7.0672	included	32	f2	25.324	1	13	13	13	13	17.386	17.3855	
	H2 recovery	H2 recovery, M	0.033	0.1	0.7	0.833	0.93296	eq4	32	f3	28.847	289	332	107	332	372.51	438.25	491.718	
Power island	Gas turbine	output power,M	266		0.75	73.2	81.984	included	27	p1	682.77	1	166	166	166	166	211.14	211.144	
	Fuel gas compressor	power, MW	10		0.67	6.31	7.0672	included	32	p2	58.44	1	23	23	23	23	30.445	30.4451	
	Steam cycle (turbine, cond	gross power, M	136		0.67	66.7	74.704	15.5	included	p3	939.91	1	273	273	273	315.08	273	315.081	
	Boiler/steam generator	Boiler duty, MV	355		1	52	58.24	eq4	27	p4	97.4	1	16	16	16	17.929	20.293	22.7692	
Solvent recycle system															1379	1379	1379	1379	
														TOTAL	4020	4334	4338	4671	
									eq4	0.1216					n6				
	The calculation for the solvent recycle																		
			cost from Aspen (2	Direct															
	flash column1		6,629,800	22031942.09															
	flash column2		6,367,300	21159610.38															
	flash column3		4,807,900	15977461.52															
	flash column4		181,600	603487.3878															
	radfrac distillation 1		103,900,000	345277200.4															
	radfrac distillation 2		1,270,700	4222750.131															
	radfrac distillation 3		15,007,800	49873447.24															
	FT synthesis			900,862,833															
	heat exchanger1		901,800	2996833.295															
	heat exchanger2		2,037,800	6771342.743															
	heat exchanger3		229,600	762999.4727															
	heat exchanger4		780,800	2594729.314															
	heat exchanger5		780,800	2594729.314															
	pump		560,000	1860974.324															
	condenser1		272,600	905895.7154															
	condenser2		162,200	539017.9202															
	total			1,379,235,255															

Comparison between the three reactors

Category	Item	unit	unit Price	note	Amount/yr	FT (fixed b total MM$	FT (slurry b total MM$	SCFT total MM$
Chemicals								
	NG	$/1000 SCF N	2.1		600023500	1260	1260	1052
	H2O	$/1000gal	1.2			0.2	0.2	0.1
	Catalyst	slurry	4	n1		0.3294	0.3294	
		fixed bed	4			0.8976		0.8976
	pentane	$/gal	3.7			0		436.05
Annual operation	O&M labor	%FCI/yr	4			445.88	428.36	451.04
	operating labor					357.7	357.7	357.7
	supervision, plant overh	%labor	90			321.93	321.93	321.93
	capital charge, insurance	%FCI/yr	15			1672	1606.35	1691
Other	catalyst replacement	slurry				8.30448	8.30448	
		fixed bed				1		0.6
	waste disposal	$/ton	18		2190000	39	39	39
Utility						1897	1897	2570
GHG emissions	GHG emissions	$/t CO2 eq	100		7530096	753		753
		$/t CO2 eq	100		1671408	167		167
Electricity	Electricity	$/MWh	60	v2	2628000	158	158	158
Porducts sale					**sale**	**7985**	**7985**	**8933**
	diesel	$/bbl	129		44677460	5779	5779	3477
	gasoline	$/bbl	132		4959620	657	657	2573
	H2	$/kg	2		696615109.1	1393	1393	1446
	H2O	$/1000gal	1.2		2103252.92	2.5	2.5	2.4
	C6-C7	$/gal	3.7		41211818.18	152	152	1433.72
Total					**annual operatir**	**6154**	**6077**	**7079**
					annual after cas	1498.594	1551.029	1517.319
					ROI	0.114274	0.123107	0.114377
					Capacity	136000 BPD	136000 BPD	126899 BPD
					FCI	11147	10709	11276
					TCI	13114	12599	13266

	Category	Item	unit	unit Price	note	Amount/yr	with condenser total MM$/yr		with no con		replace radfrac		flash sequence		heavy column
	Chemicals														
4760BTU/LB		syngas	$/GJ	13		59,847,124	778.01	56,220,266	731	56,220,266	731	56,220,265	731	56,220,266	731
		Catalyst	fixed bed	4			1		1	-	1		1		1
		hexane	$/gal	1.15		89,790,385,440	103,258.94	89,790,385,440	103,258.94	89,790,385,440	103,259	89,790,385,440	103,259	89,790,385,440	103,259
							-		-	-	-		-		-
							-		-	-	-		-		-
										-	-				
										-	-				
	annual operating	O&M labo	%FCI/yr	4			54		54	-	56		52		52
		operating labor					131		131	-	131		131		131
		supervisic	%labor	90			118		118	-	118		118		118
		capital ch	%FCI/yr	15			203		202	-	210		196		194
	Energy utility														
							1,715		1,715	-	1,880		1,530		1,592
	after heat integration						1,064		1,064	-	1,110		1,047		945
										-	-				
										-	-				
										-	-				
										-	-				
										-	-				
										-	-				
	Porducts sale					**sale**	**3,619**	**sale**	**3,619**	**sale**	**3,619**	**sale**	**3,621**	**sale**	**3,611**
		diesel	$/bbl	82		43,800,000	3,592	43,800,000	3,592	43,800,000	3,592	43,827,060	3,594	43,709,310	3,584
		gasoline	$/bbl	63			-		-	-	-		-		-
		H2	$/kg	2		-	-	-	-	-	-	-	-	-	-
		H2O	$/1000gal	1.2		1,044,119	1	1,026,183	1	1,026,183	1	1,026,183	1	1,044,119	1
		tailgas	$/bbl	50		517,570	26	525,562	26	525,562	26	525,563	26	517,570	26
		hexane	$/gal	1.15		89,774,303,982	103,240	89,699,200,892	103,154	89,699,200,892	103,154	89,698,503,869	103,153	89,774,303,982	103,240
										-	-				
	Total					**operating cost**	**3,017**		**3,056**	-	**3,231**		**2,863**		**2,836**
										-	-				
	annual after cash profit						**466**		**437**	-	**307**		**583**		**596**
	ROI						**0.29**		**0.28**	-	**0.19**		**0.38**		**0.39**
	after heat integration					operating cost	**2,366**		**2,405**		**2,461**		**2,381**		**2,189**
						annual after cash p	954.68		925.71		884.56		945.18		1,080.92
						ROI	**0.60**		**0.58**		**0.54**		**0.62**		**0.71**