Innovation Tools for Commercializing Process Technology

Robert H. Jensen

UOP LLC

CHEMRAWN XV
Ottawa, Canada
August 9, 2003

Agenda

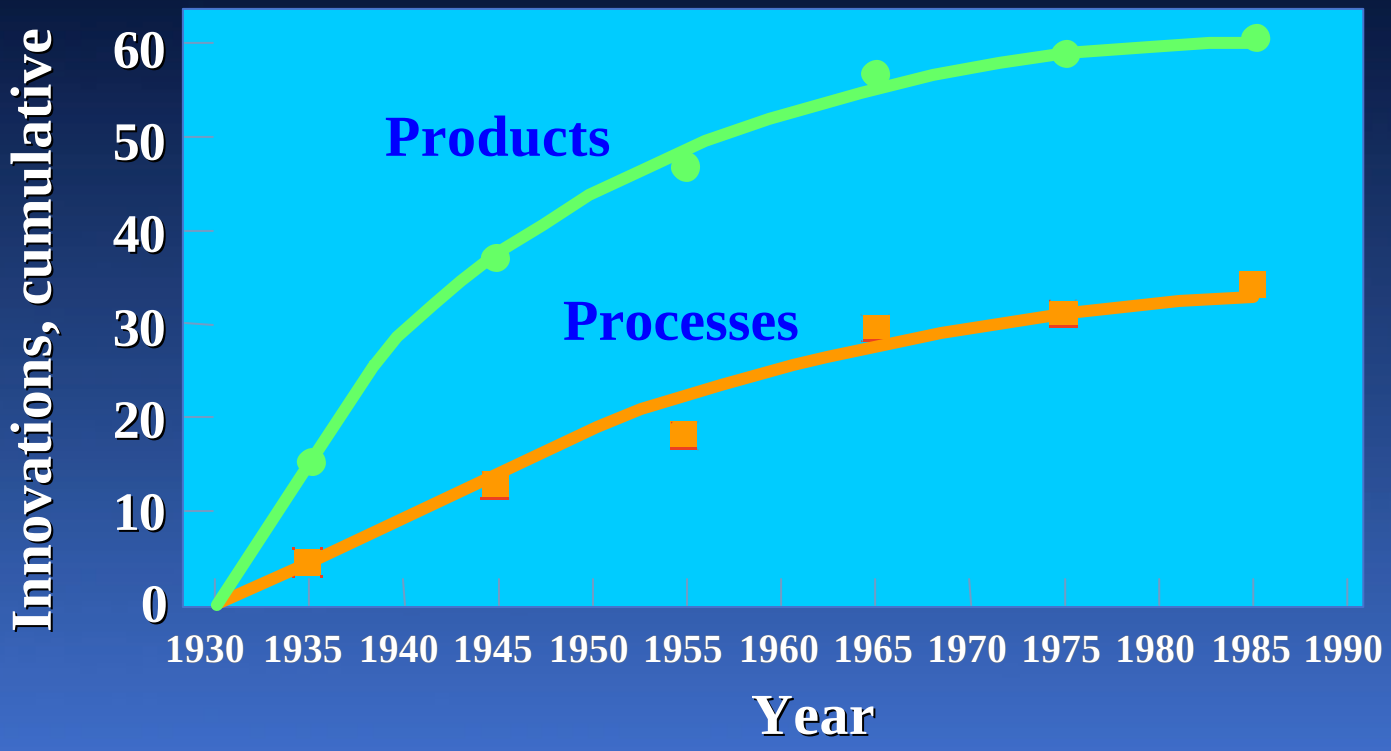
- **Background**
  - **Technology accomplishments in the Process Industry**
  - **UOP's incentive for innovation**
  - **Challenges of the 21st century**
- **Innovation tools**
  - **Gated Technology Delivery Process**
  - **Tools for materials innovation**
  - **Tools for process innovation**

Process Industry Background

The history of the Process Industry is a story of technical accomplishment and innovation.

Achievements during the last century have led to both tremendous growth and a high level of technical sophistication.

Innovations in the Chemical Process Industry are Slowing

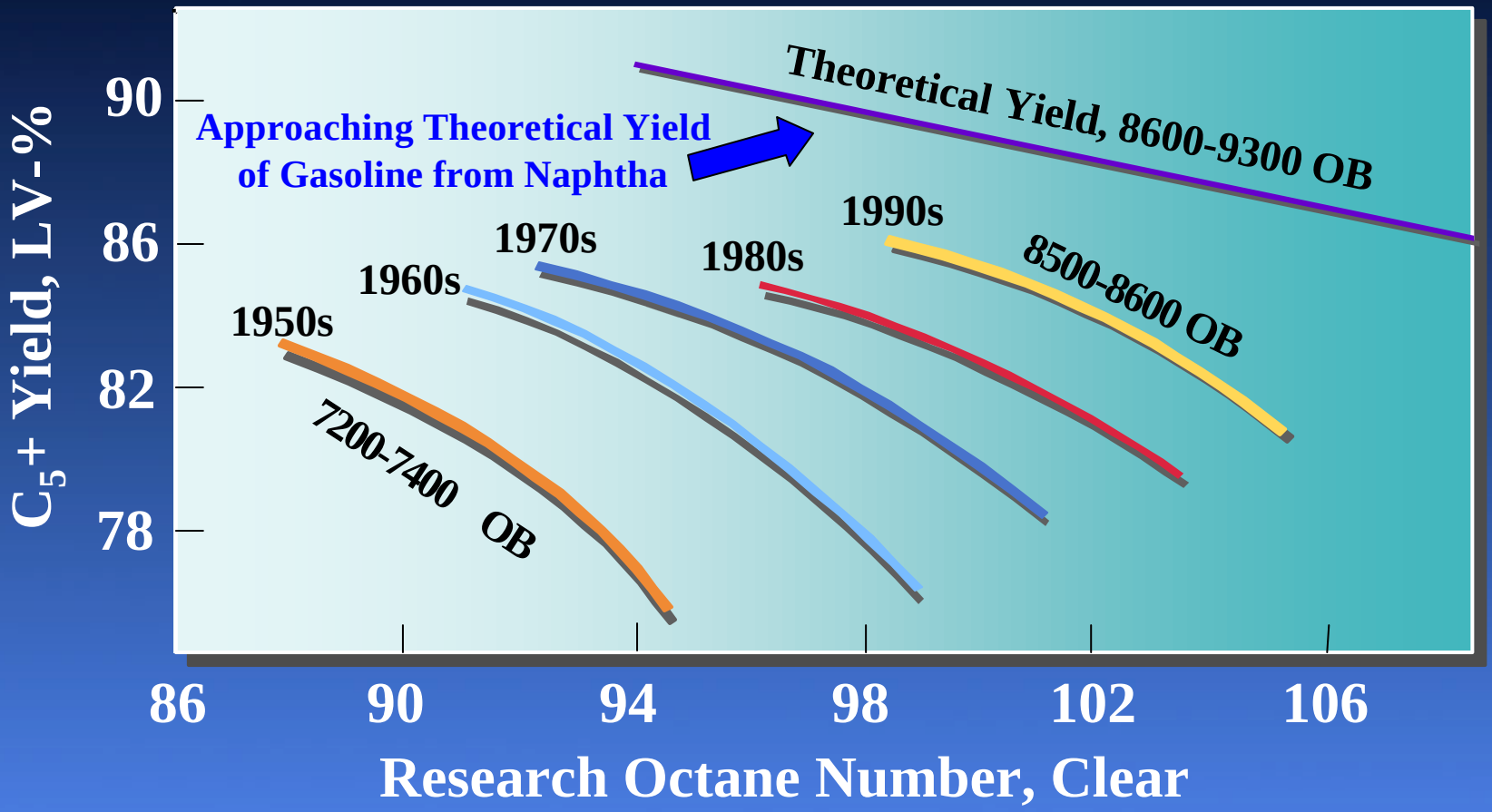


Product and process innovations from 1930 to 1985.

Source: Chemtech 1995, 25(6), 6.

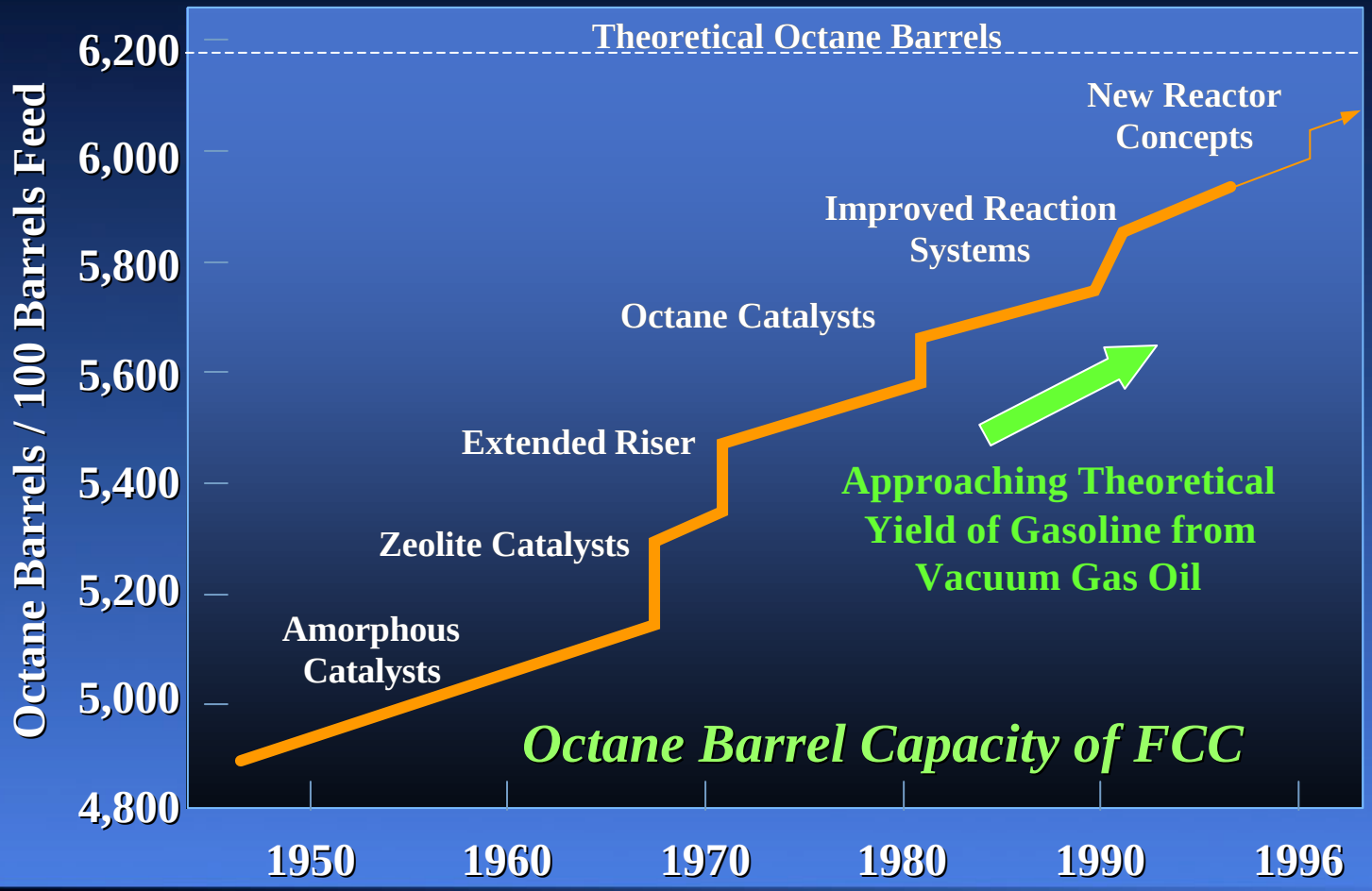
Platforming™ Technology

More Octane Barrels (Yield x RON) via Lower Pressure and More Selective Catalysts



Fluid Catalytic Cracking Technology

More Octane Barrels via Zeolitic Catalysts and Engineering Improvements



Top Ten Refining Processes Licensed by UOP

Process	Description	No. Units
1 Merox™	Mercaptan Oxidation	1650
2. Platforming™	Catalytic Reforming	753
3. Unionfining™ (VGO, Distillate, Naphtha)	Hydrotreating	675
4. Polymerization	Poly Gasoline Production	301
5. FCC	Catalytic Cracking	212
6. Unicracking™	Hydrocracking	126
7. Sulfolane	BTX Extraction	106
8. HF Alkylation	Gasoline Production	105
9. Catalytic Condensation	Higher Olefin Production	101
10. Isomerization	C_5/C_6 Isomerization	99

UOP must continue to focus on innovation to meet the challenges of the 21st century.

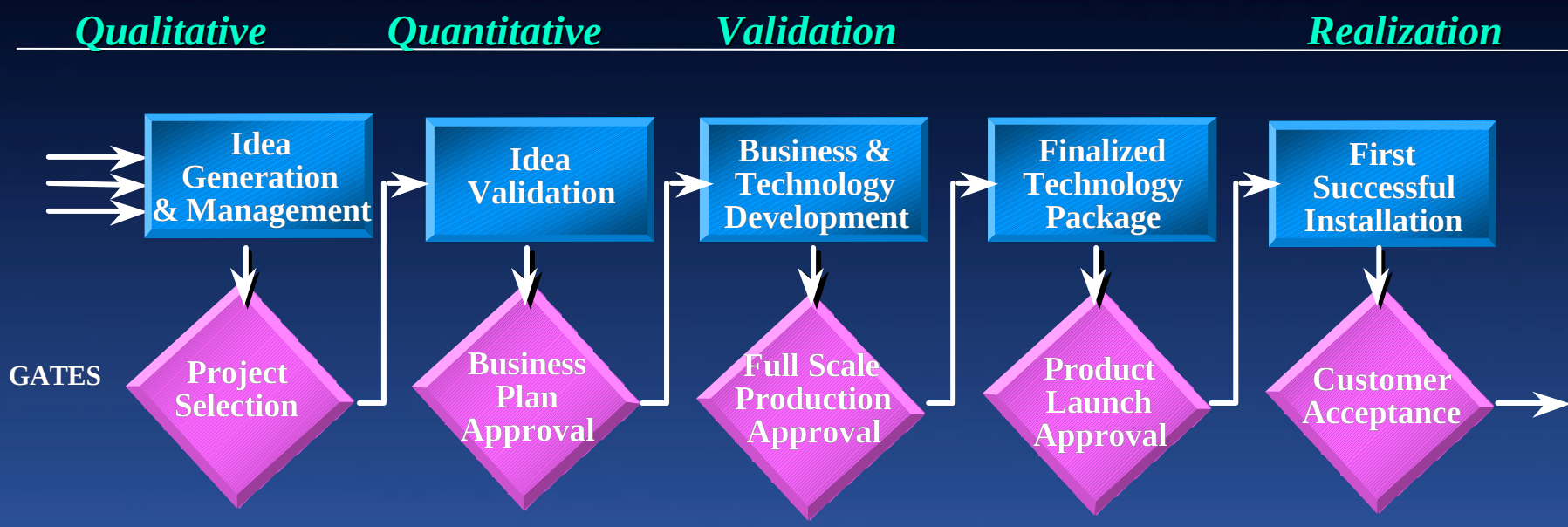
Sustainable Development Challenges of the 21st Century for the Refining and Petrochemical Industry

- **Clean Fuels**
  - Cost-effective ways to produce zero sulfur/low nitrogen transportation fuels
  - Reduction of aromatics and olefins in gasoline while maintaining octane
- **Alternatives to Crude Oil**
  - Natural gas utilization
  - Renewable sources
- **Minimum Environmental Impact**
  - Refinery emissions
  - Spent catalyst handling

Agenda

- **Background**
  - **Technology accomplishments in the Process Industry**
  - **UOP's incentive for innovation**
  - **Challenges of the 21st century**
- **Innovation tools**
  - **Gated Technology Delivery Process**
  - **Tools for materials innovation**
  - **Tools for process innovation**

UOP's Gated Technology Delivery Process



- Designed specifically for new product/process development
- Requires technology goals/economic case
- Requires gate criteria
- Incorporates Six Sigma methodology
- Facilitates collaborations with producer-partners

UOP Processes Developed in Collaboration with Others

Process	UOP Partner	Application
Cyclar™	BP	LPG to Aromatics
Detal™	CEPSA	Fixed Bed Alkylation for Detergent
Ethermax™	Koch	Etherification
MTO	Norsk Hydro	Methanol to Olefins
Sunoco/UOP Phenol Process	Sunoco	Cumene Oxidation
Tatoray™	Toray	Toluene Transalkylation
Thiopaq™ Spent Caustic Treating	Paques Natural Solutions	Biodesulfurization of Caustic

Agenda

- **Background**
  - **Technology accomplishments in the Process Industry**
  - **UOP's incentive for innovation**
  - **Challenges of the 21st century**
- **Innovation tools**
  - **Gated Technology Delivery Process**
  - **Tools for materials innovation**
    - ✓ **New Materials**
    - ✓ **Combinatorial Chemistry**
    - ✓ **Advanced Characterization**
    - ✓ **Manufacturing**
  - **Tools for process innovation**

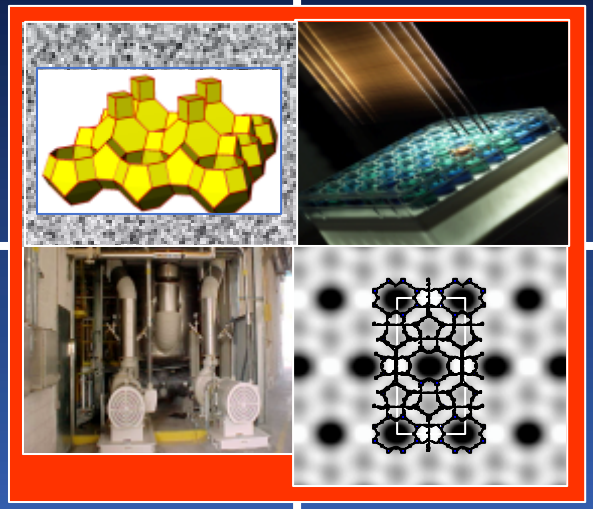
Materials Innovation Tools

Materials

✓*New Materials Invention*
✓*Materials Modification*

Combinatoria Chemistry

✓*End-to-End™ Tool Box*



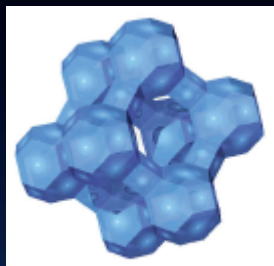
Manufacturing

Rapid Scale-up
Diverse Crystallization Methods
Diverse Portfolio
of Forming Technologies

Advance Characterizatio

Active Site
✓*Structure Solution Tool Bo*
Reaction Mechanism
Adsorption Modelin

Zeolite Discovery and Use By Decade



Decade	Known Structure Types	U.S. Patents (Composition or Use)	Commercialized Structure Types
1950-1969	27	2900	3
1970-1979	11	4900	1
1980-1989	26	7400	2
1990-1999	61	8200	5
Totals	125	23,400	11

Structure Solution Tool Box

Crystals
(>1000nm)

Microcrystals
(10-1000 nm)

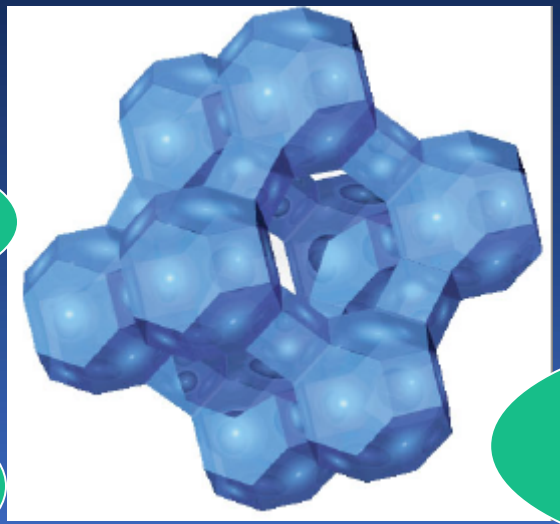
Nanocrystals
(<10nm)

Single

Direct Methods

Molecular Modeling

PD



Structure verification (DLS, Rietveld)

Model building

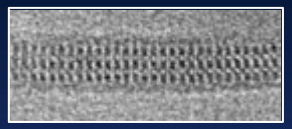
Primary building units (elemental analysis)

Defects (HREM, ED, PD)

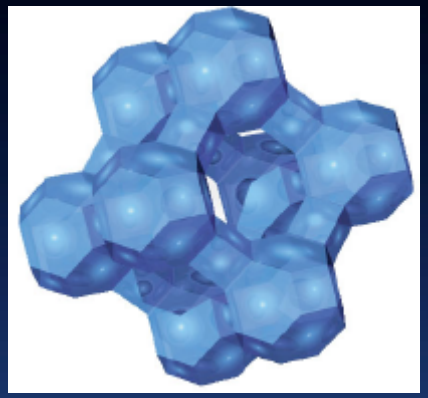
Secondary building units (FTIR, NMR, absorption)

Superstructure (PD, ED, HREM)

Tools Used to Solve the Structure of UFI

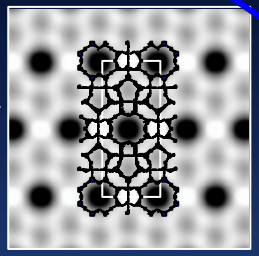


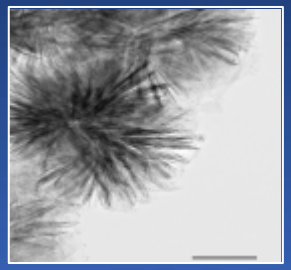
TEM: Unique surface
→ aromatic reactivity



UFI

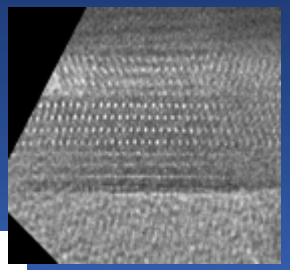
Model
vs.
TEM



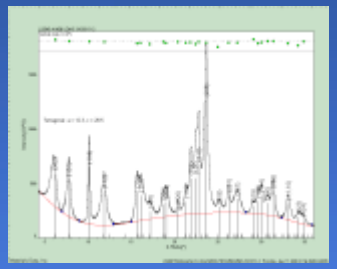


Imaging
TEM

High
Res
TEM

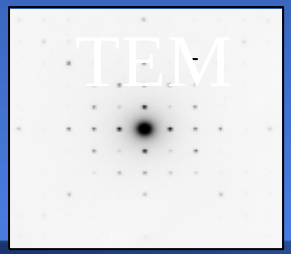


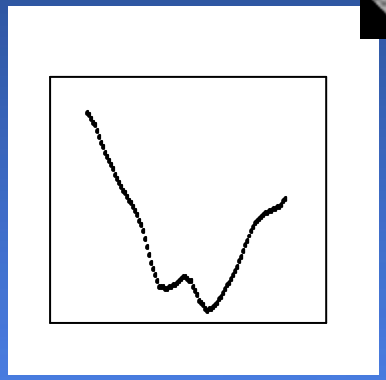
Small
Crystals



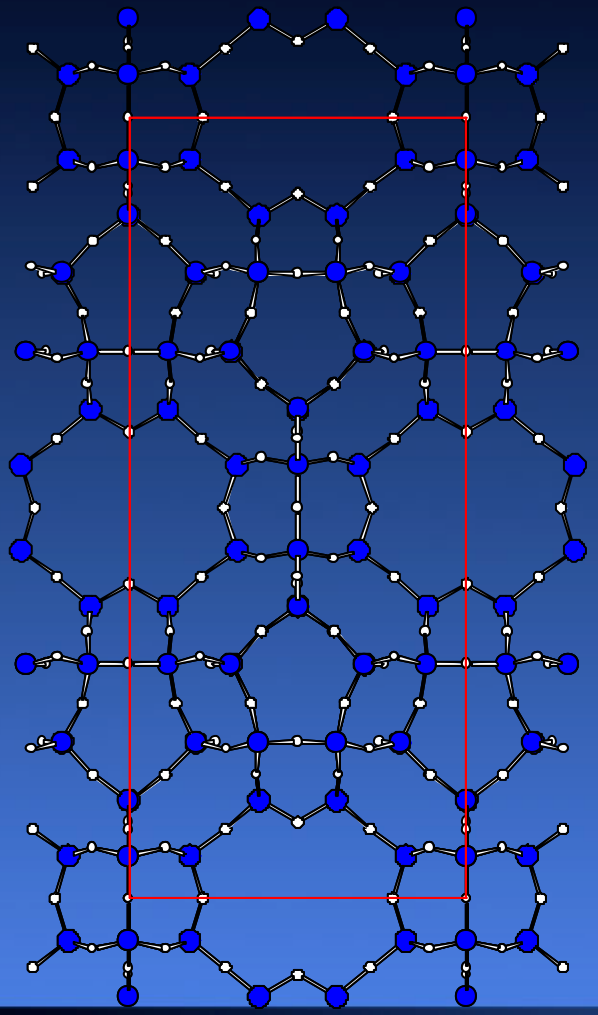
XRD

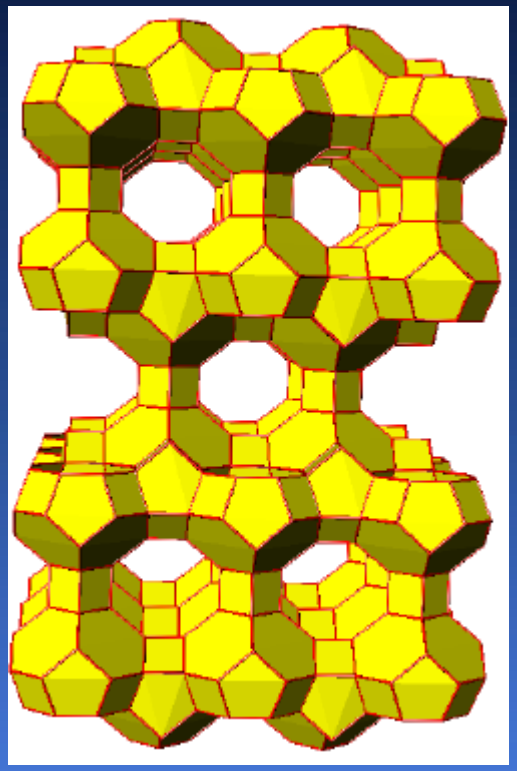
Electron
Diffraction
TEM





Structure Solution of a New Zeolite: UZM-5 (IZA 3-letter code UFI)

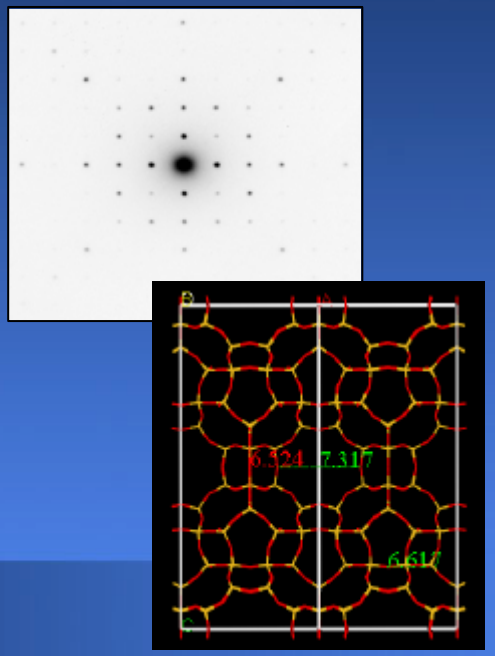




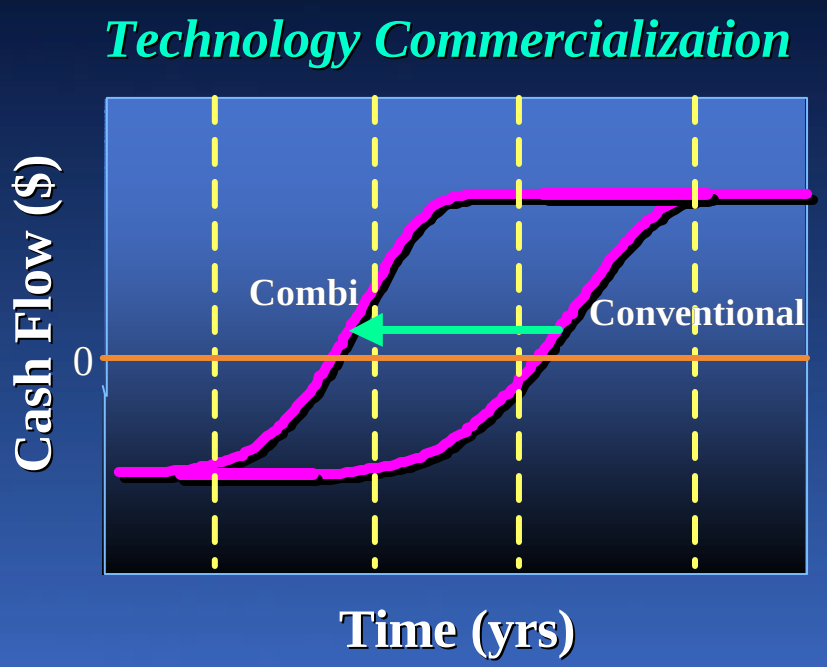
New Tools Accelerate Structure Solution of Nanocrystalline Zeolites

Event	Beta	UZM-5
First Synthesized	1967	1999
Time to Solve Structure	>10 yrs	10 months
Structure Reported	1988	2002

- **Structure provides an understanding of catalytic and adsorptive properties**
- **Zeolites offer high acid site density for catalytic applications (low Si to Al ratio)**
- **Zeolites offer ion-exchange capacity and compositional diversity for separation applications**



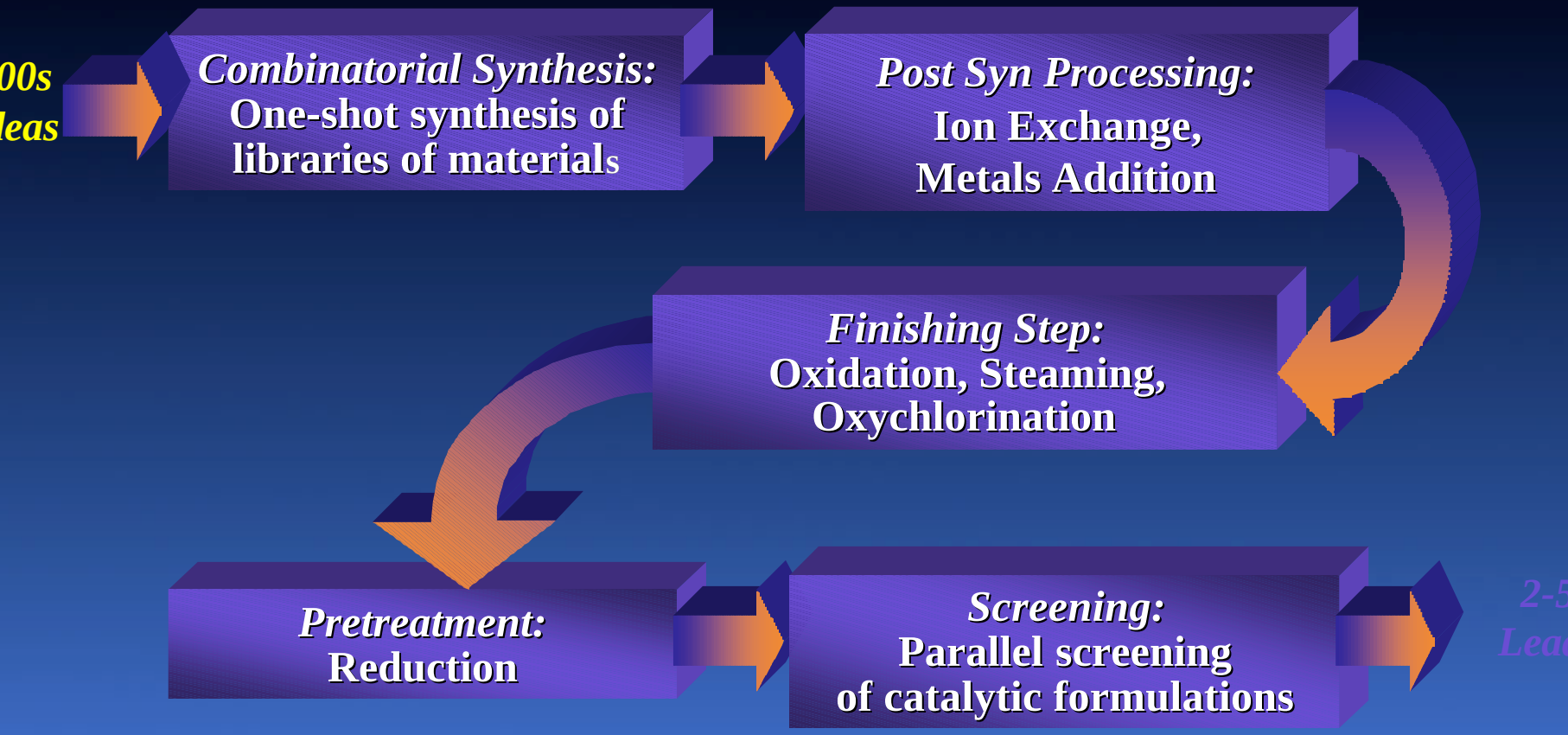
Impact of Combinatorial Chemistry



Reduced Risk for Breakthrough Programs

- **Reduced time for catalyst discovery and process development**
  - **Increased probability of success**
  - **Increased throughput of technology commercializations**
- **Stronger patent position**

End-to-End™ Combinatorial System



- *Fully Integrated Systems*
- *Significant Increase in Throughput*

Combi Target: New Paraffin Isomerization Catalyst

- **C_5 Isomerization**

n-Pentane 61.7 ⇌ *i*-Pentane 93.5

Values are blending RON

- **C_6 Isomerization**

n-Hexane 31.0 ⇌ 2 MP 74.4 or 3 MP 75.5 ⇌ 2, 2 DMB 94 or 2, 3 DMB 105

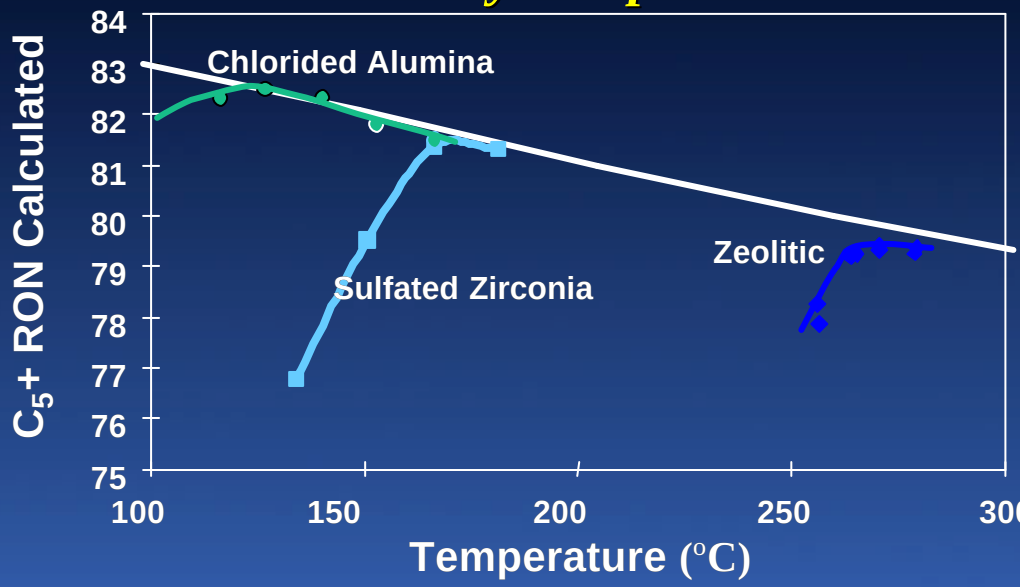
- **Ring Opening**

Benzene 120 $\xrightarrow{H_2}$ Cyclohexane 84 ⇌ Methyl Cyclopentane 96 ⇌ *n*-Hexane 31.0

Commercial Isom Catalysts

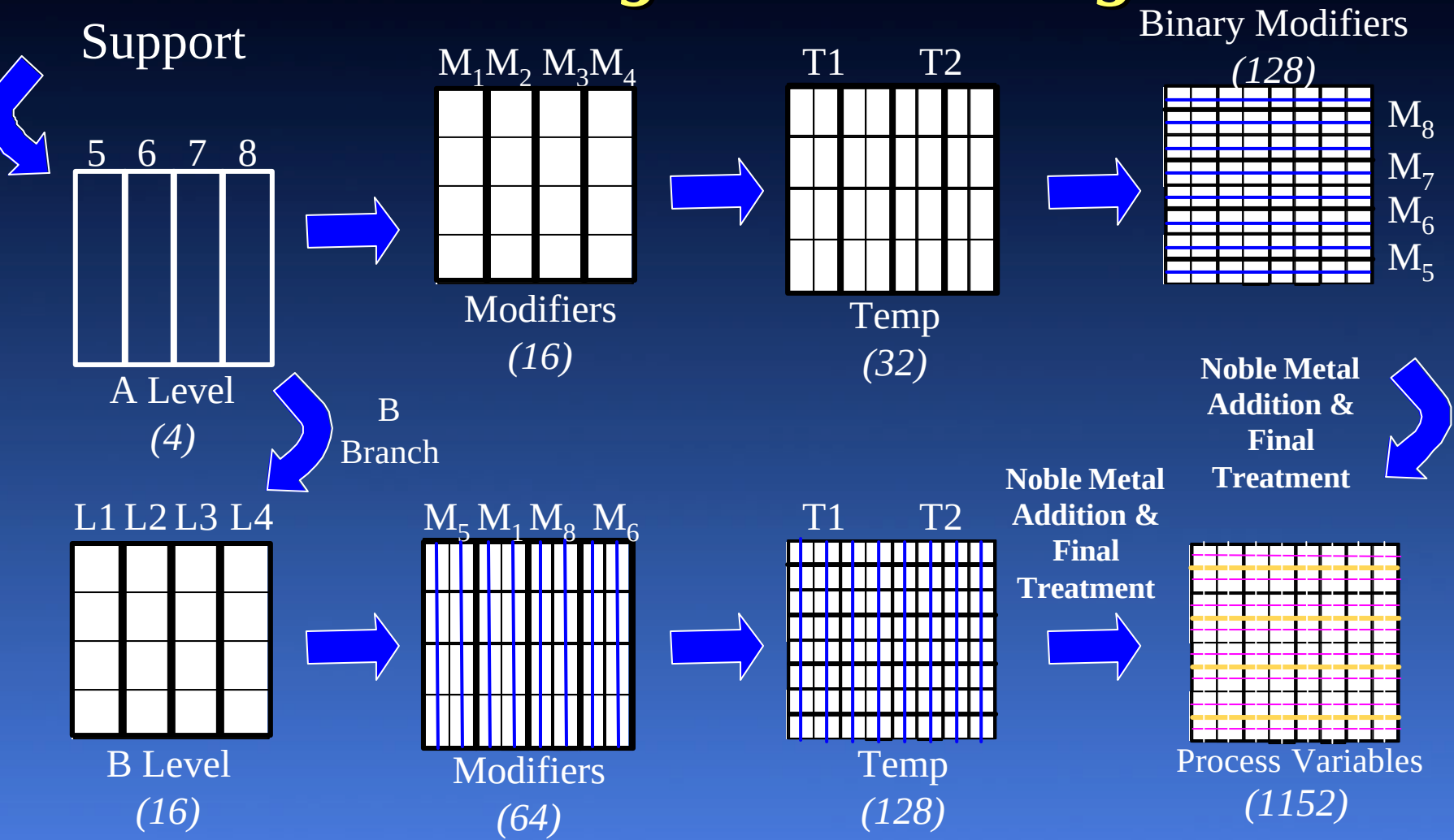
- Formation of high octane products favored by low temperature.
- Two classes of commercial isom catalysts exist:
  - ***Chlorided alumina catalyst:*** most active; reactor system is highest capital investment
  - ***Sulfated zirconia and zeolitic:*** lower activity; reactor system is lower capital cost

C_5/C_6 Isomerization Catalysts Activity Comparison

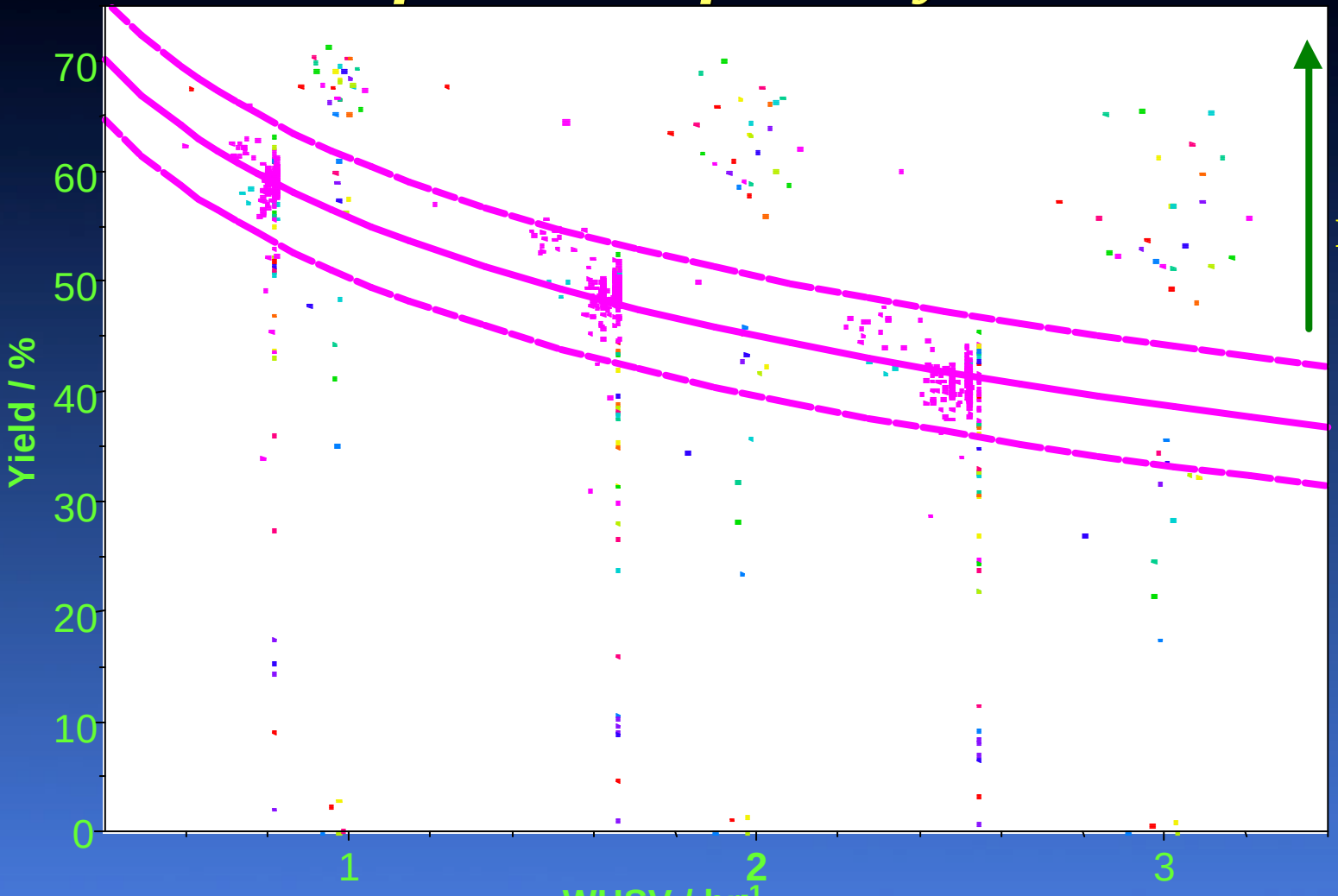


Market Need: higher activity catalyst for use in lower capital reactor system

Post-Synthesis Combi Processing and Finishing



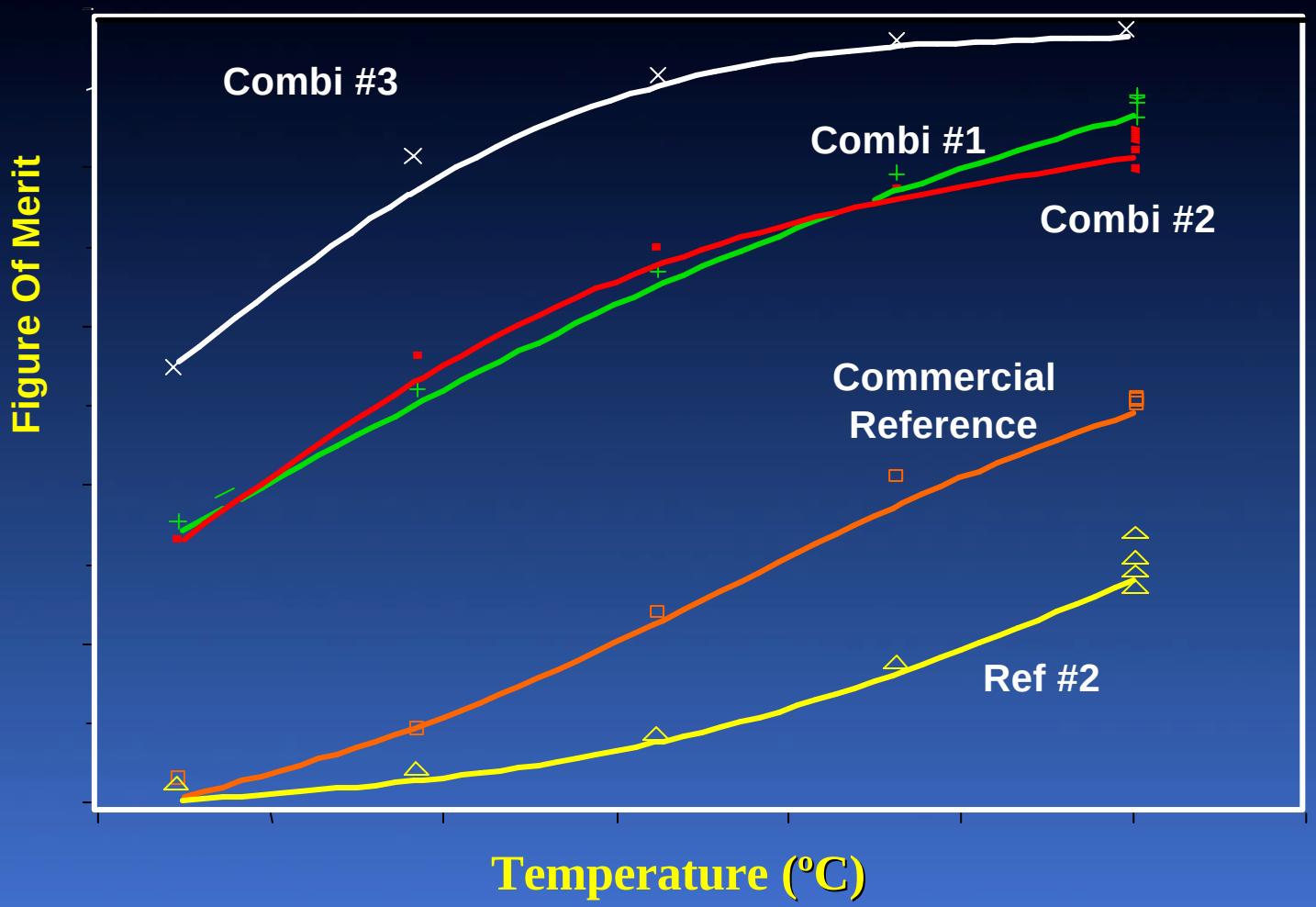
Combi Screening for Rapid Identification of Catalyst Leads



Meets Target > 5% Yield Improvemen

Prototypes are a Significant Improvement to Reference

Pilot Plant Testing Confirms Combi Leads

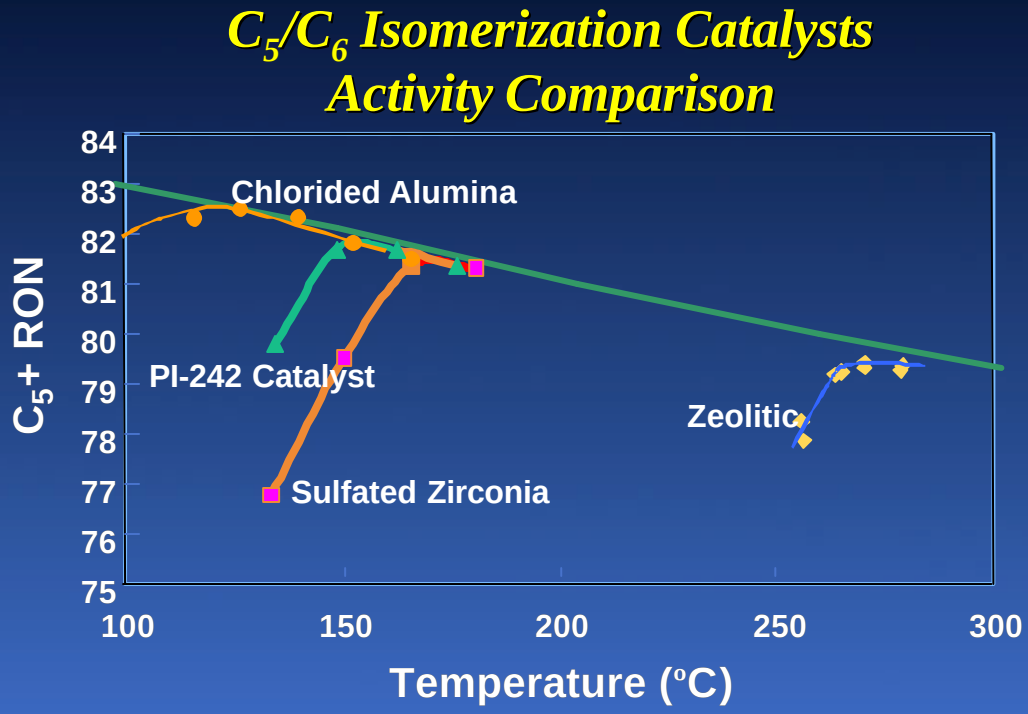


Conventional
271 Catalysts / 3 years

Combinatorial
512 Catalysts / 5 weeks

New, Combi-Developed PI-242™ Catalyst

- **PI-242™ catalyst developed from combi formulation**
- **Higher activity than sulfated zirconia or zeolitic**
- **Simple drop-in into lowest capital reactor system**



Agenda

- **Background**
  - **Technology accomplishments in the Process Industry**
  - **UOP's incentive for innovation**
  - **Challenges of the 21st century**
- **Innovation tools**
  - **Gated Technology Delivery Process**
  - **Tools for materials innovation**
  - **Tools for process innovation**
    - ✓ **Experimental data**
    - ✓ **Engineering technology**
    - ✓ **Separations**
    - ✓ **Modeling**

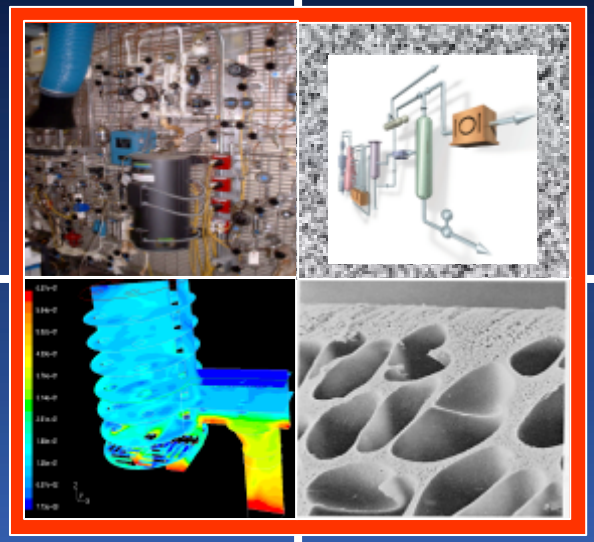
Process Innovation Tools

Experimental Data

✓*Pilot Plants*
Analysis
Informatics

Engineering Technology

Core skill
Instrumentatio
and Contro
Process Flowsheetin
and Desig



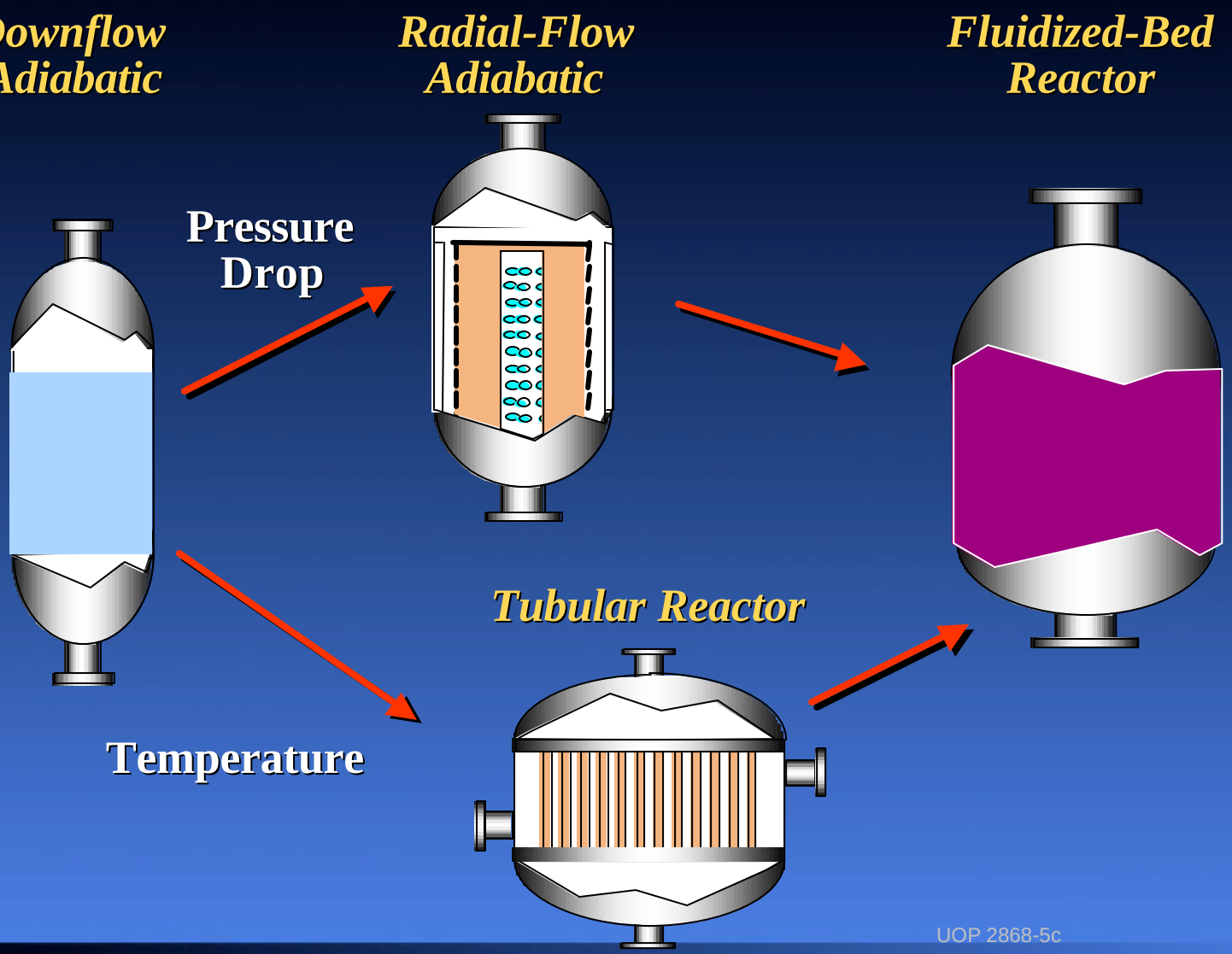
Modeling

✓*Reactor Systems*
✓*Kinetic Modeling*
✓*Cold Flow Modeling*
Computational Fluid Dynamics

Separation

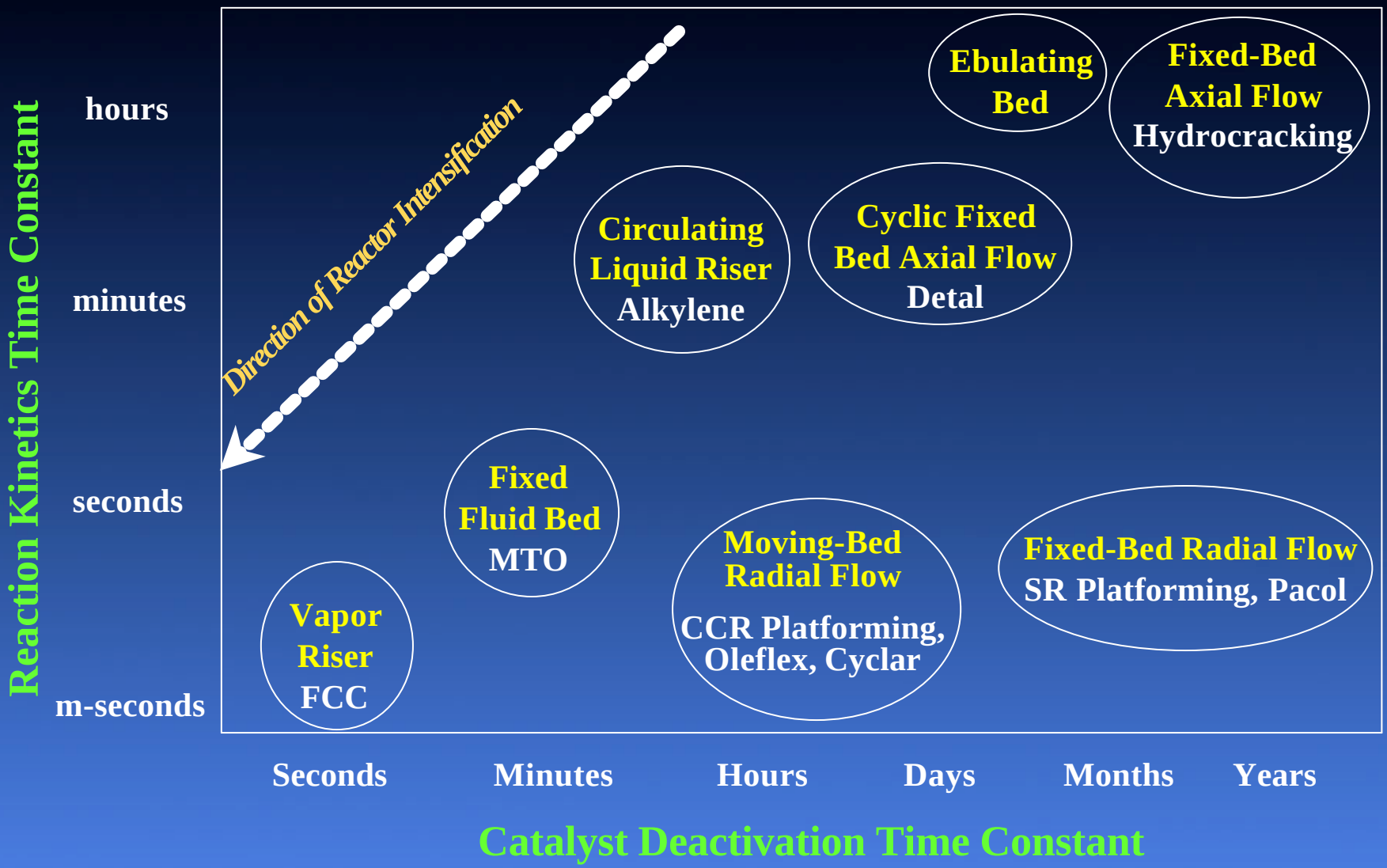
Adsorbents
Adsorption Systems
Membranes

Reactor Design Options

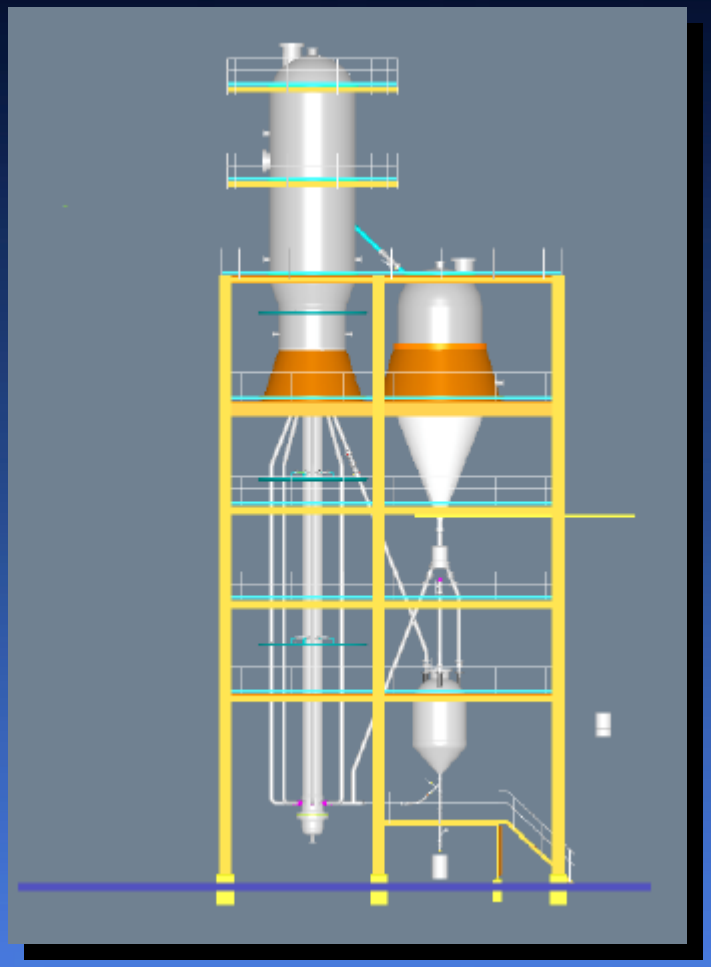


UOP 2868-5c

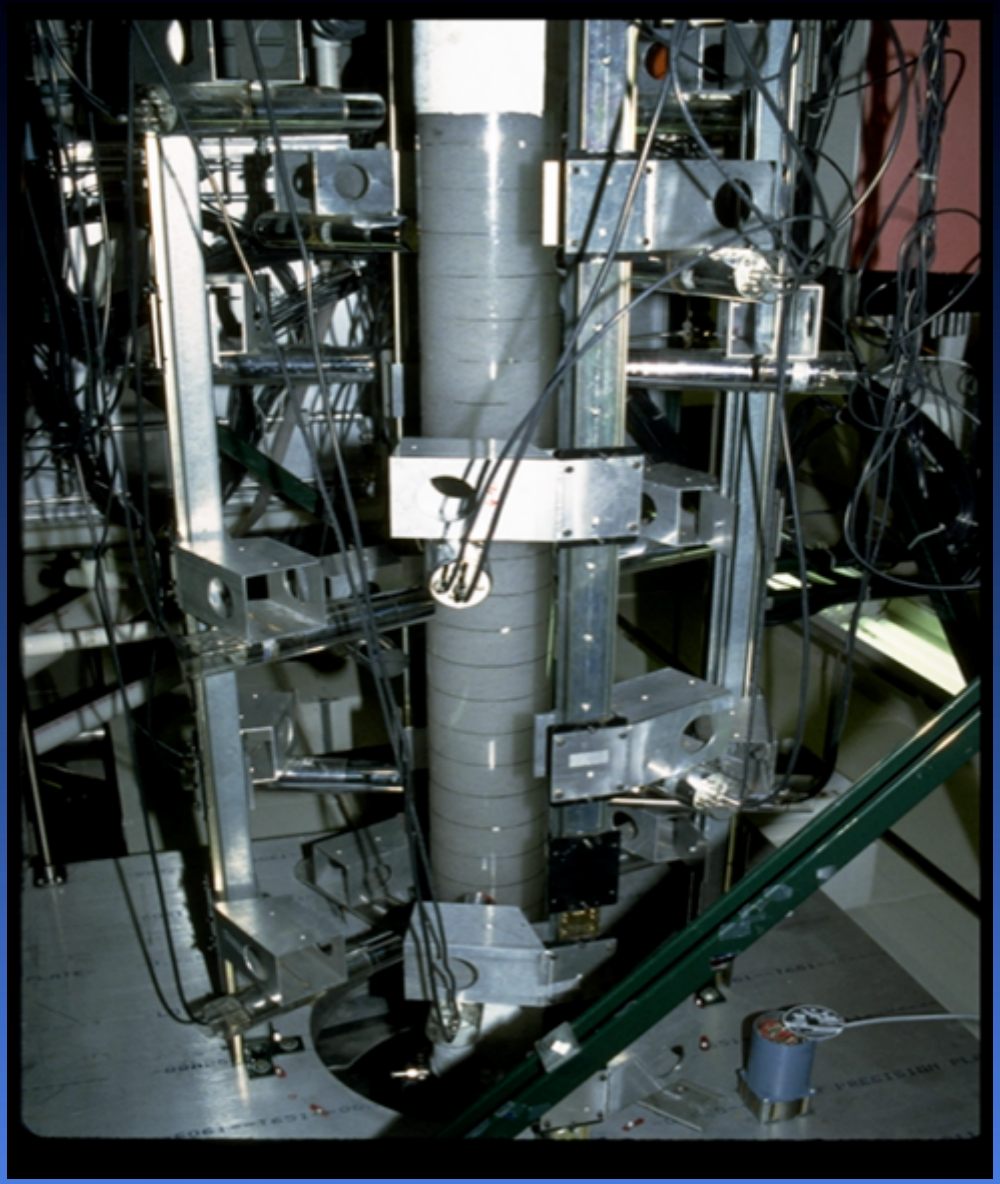
Reactor Design from Kinetic Modeling



Reactor Design for Alkylene Process



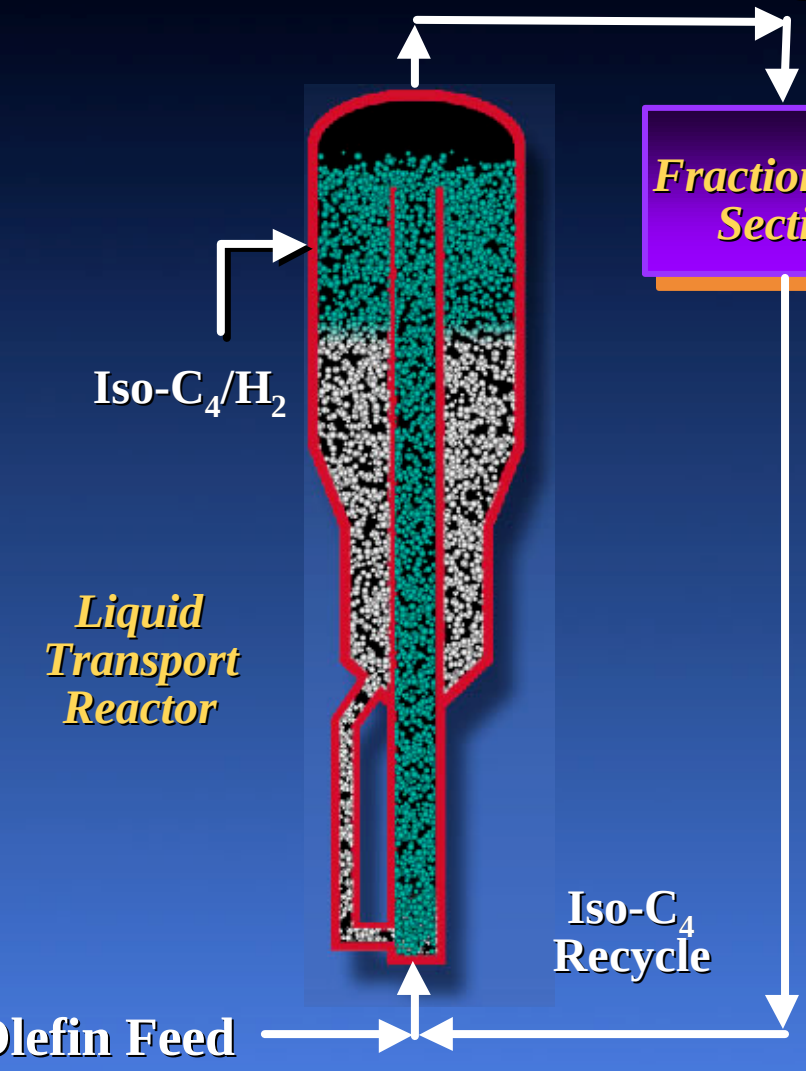
- **Process requirements:**
  - **Short contact time**
  - **Rapid disengagement**
  - **Frequent regeneration**
- **Solution: circulating liquid riser reactor**



Fluidization Testing in Alkylene Cold Flow Model

- *RTD studies*
- *Catalyst density*
- *Catalyst attrition*
- *Distributor design*

Alkylene Process



- Uses solid catalyst
- No acid soluble oil
- No corrosion
- Reduced maintenance
- Higher yields

Innovation Tools:

Novel Catalyst
Unique Reactor Design
Cold Flow Modeling
Computational Fluid Dynamics

Summary

- **The Process Industry must focus on innovation to meet the challenges of the 21st century**
- **Innovation tools can accelerate the delivery of new process technology**
  - **A Gated Technology Delivery Process**
  - **Tools for materials innovation**
    - ✓ **Materials**
    - ✓ **Combinatorial Chemistry**
    - ✓ **Advanced Characterization**
    - ✓ **Manufacturing**
  - **Tools for process innovation**
    - ✓ **Experimental data**
    - ✓ **Engineering technology**
    - ✓ **Separations**
    - ✓ **Modeling**