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![Chemical Elements Image]


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Exploratory Chemistry Research in US Industry:
Case Analysis of DuPont Central Research
Bill Nugent
Formerly of DuPont CR&D, Visiting Scholar, Ohio State University
Alexander Tullo
Senior Editor, Chemical & Engineering News

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The Dow/DuPont Deal at a Glance

Dow ~$53.4 B*

DuPont ~$28.5 B

DowDuPont

Dow Corning ~$6.2 B

“New Dow” ~$56.4 B

New Ag firm ~$18.6 B

“New DuPont” ~$13.2 B

*D & E estimates based on 2014 revenue figures.

Dow/DuPont is no big deal
...it’s many smaller deals

Dow ~$6.2 B

“New Dow” ~$7.3 B

Polymers ~$6.1 B

Ag ~$11.3 B

Electronic Materials ~$2.1 B*

Dow Corning ~$6.2 B

New Ag firm

Dow “New Dow”

DuPont “New DuPont”

* C&EN estimate.
**Effect on R&D**

- **DowDuPont** will cut combined R&D spending by $300M, as part of $3B in cost cutting

- **DuPont** to “reorganize” Central R&D into “Science & Innovation” as part of separate, $700 million restructuring

- ~200 layoffs at CR&D (unofficially)

- **DuPont** to spend $1.6B - $1.7B on R&D in 2016, a decline from $1.9B in 2015

- **Dow** spent $1.6B on R&D in 2015

---

**DuPont Experimental Station**
Prehistory of CRD

- During the 1930’s, Chemicals Dept. had demonstrated the value of exploratory research.
  - neoprene (1930)
  - Teflon® (1938)
  - nylon (1939)

- The tradition waned during WWII.

- In 1957 DuPont formalized commitment to basic research by establishing CRD.

Rationale Behind CRD

Mission:
- Do excellent science in areas of company interest
- “Technology push” vs. “market pull”
- “Discover the next nylon”

Intangibles:
- Stable of “in-house consultants”
- Recruiting tool
- Promote university relations
Contributions to Organic Synthesis

- The Tebbe reagent
- The Simmons-Smith Reagent
- Fluorination of alcohols with DAST (Middleton)
- N-Heterocyclic carbene ligands (Arduengo)
- Crown ethers* (1987 Nobel Prize to Pedersen)

Some Commercial Successes

<table>
<thead>
<tr>
<th>Research</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potassium titanyl phosphate (KTP)</td>
<td>Laser frequency doubling</td>
</tr>
<tr>
<td>Group transfer polymerization</td>
<td>Ink jet inks; automotive finishes</td>
</tr>
<tr>
<td>Hyperbaric crystallization of ultra-high molecular weight polyethylene.</td>
<td>Hylamer* polyethylene for hip and knee replacement</td>
</tr>
<tr>
<td>Catalysts for manufacture of hydrochlorofluorocarbons (HCFCs)</td>
<td>Suva* non-ozone depleting refrigerants</td>
</tr>
<tr>
<td>Novel fluorescent labels for DNA</td>
<td>Qualicon* technology (identifies bacteria for food safety)</td>
</tr>
<tr>
<td>Ureas and uracils with herbicidal activity</td>
<td>Establishment of DuPont agrichemical business (later, sulfonylurea herbicides)</td>
</tr>
</tbody>
</table>

*discovered in Elastomers Dept.
Hydrocyanation of Butadiene

\[ \text{Butadiene} + \text{HCN} \xrightarrow{\text{NiL}_4, 70 \degree C} \text{Propargylcyanide} + \text{Propargylcyanide} \] (ca. 2:1)

NiL\(_4\) = nickel triarylphosphite complex, LA = Lewis acid additive.

Technology is now practiced on 2 billion pound per year scale.

Hydrocyanation: Scientific Advances

- Tolman’s introduction of **ligand cone angles** to quantitate steric effects in catalysis

- Also the systematic understanding of electronic effects

- First cyclic representation of a catalytic process using 16 and 18 electron complexes
Why Did It Work So Well?

• **Serendipity** – the encouragement to pursue unexpected experimental results

• **Critical Mass** – both in terms of business opportunities and breadth of expertise

• **The Scientists** – intentional recruitment of “academic” personality types

---

**The First Alkylidene Complex**

Tantalum alkylidene complex containing Ta=C double bond.

Antecedent to first well defined olefin metathesis catalysts.

Np = neopentyl

This work eventually led to the 2005 Nobel Prize in Chemistry.
Birth of Alkylidene Chemistry

Sent down for mass spec. A sample will be catalysed.

Moos spec shows 464 in the main. Could be

\[
\begin{align*}
\text{C}_8\text{H}_8\text{Ta} &\rightarrow \text{Ta} + \text{CH}_3 \\
\text{C}_8\text{H}_8 &\rightarrow \text{Ta}(\text{CH}_3)_2
\end{align*}
\]

This is consistent with mass 1:371:3

220 MHz (2306 c) very good also.

EPR. 3.282, no EPR signal

(c) Up the scale

1.7 g Li + 5.95 g TaC\(_8\)H\(_8\) in 50 c c acetone.

7.7 molar from 1.06 g LiC\(_8\)H\(_8\) (255 c m mol). Oxide reduction

to a slightly grey powder. Evaporated to 6.71 g filtered (from 45)
and dried at 30 C over silica. A 0 c c acetone was now

1.11 molar. 2.5 g molar acetate [molar 1.89]

4H NMR TMS 5.9 g molar. Acetate should be reduced. No good,

Mol wt (EPR) = 3127.5

\[\begin{align*}
\text{Mol. wt. (UV)} = &\ 3127.5 \quad \text{Mol. wt. (IR)} = \ 3127.5
\end{align*}\]

R. Schwoch

WITNESSED BY: J. B. Burke

DATE: 12-10-73
The Benefits of “Critical Mass”

- Bert Ciganek discovers potential non-addictive pain killer
- T.V. RajanBabu attempts innovative synthesis of Ciganek compound using TASF (discovered by Bill Middleton)
- The reaction fails producing instead oligomers. Owen Webster suspects this involves novel polymerization mechanism
- He encourages Dotsevi Sogah to apply to polymerization under practical conditions

Group Transfer Polymerization

- In some runs the reaction resulted in useful polymerization but results were erratic
- Bill Farnham explains the results in terms of trace hydrolysis and formation of bifluoride anion

GTP was the first completely new polymerization process to be identified in two decades and is now used to manufacture printer inks and automotive finishes.
The Scientists

• CRD employed scientists with an academic bent who would be equally at home in a university chemistry department.

• Publication was encouraged as a useful objective in its own right.

• Visiting scientists from universities spent sabbaticals in CRD.

CRD Alumni in Academia

Material Science
Dotsevi Sogah (Cornell)
Michael Ward (NYU)
Arthur Sleight (Oregon State)
Joel S. Miller (Utah)
Galen Stucky (UC San Diego)
E. Bryan Coughlin (U. Mass.)
Zhibin Guan (UC Irvine)
Stephen Craig (Duke)
Anand Jagota (Lehigh)
Paul Smith (ETH)
Bruce Parkinson (Colorado St.)

Organometallic Chemistry
R. Tom Baker (Ottawa)
Pam Shapiro (Idaho)
Richard Schrock (MIT)
Bo Arduengo (Alabama)
SonBinh Nguyen (Northwestern)
Tracy Hanna (Texas Christian)
Todd Marder (Durham)
William Crowe (LSU)
Giambattista Consiglio (ETH)
David Milstein (Weizmann Inst.)

Physical Chemistry
V. Ramamurthy (Miami)
David Dixon (Alabama)

Analytical Chemistry
Bruce Chase (Delaware)
Charles McEwen (U. of Sciences)

Biochemistry
William DeGrado (Penn)
George Lorimer (Maryland)
Jim Lear (Penn)

Inorganic Chemistry
Mas Subramanian (Oregon State)
James Mayer (Yale)
A Metric for Exploratory Research?

**Hypothesis:** A company’s commitment to exploratory chemical research will be reflected by the number of papers it publishes in JACS in a given year

**Advantages of the metric**
- Easy to measure
- Provides a standard of quality

**Potential limitations**
- Alternative journals continually appear
- Page budgets have increased over time

What the Data Shows

Publication in JACS was common among US companies in the 1950s but gradually diminished.

Six elite companies maintained a commitment to exploratory chemistry research into the 21st Century.

- AT&T/Lucent Technologies
- Exxon
- Eastman Kodak
- IBM
- Merck
- DuPont
JACS Papers from US Companies

Industrial Publications in JACS

1954
n = 346

2004
n = 180

US company, no collaboration
US company, collaboration
Foreign company

*extrapolated from 1Q 2009 data
The 1990s – Changing Business Needs

• Shorter investment timeline

• Diminished opportunities (Perception that the “low hanging fruit” had been harvested)

• Concept of “risk management”

• “Technology push” no longer viable

“Apex Research”

• In 1998, DuPont undertook a transformational change in long-term discovery research.

• All proposals required to contain a technical and business case.

• Proposals were evaluated by a group of senior business leaders.
The End of Exploratory Chemistry

- In 2011 for the first time in the history of the department, no JACS papers were published from CRD

- Although CRD was closed in 2016, its original mission was abandoned years ago

- US industry will be increasingly dependent on the universities for breakthrough science
Audience Survey Question

In the future, what will be the most important source of novel chemistry-based technologies for the US industry:

- Start-up companies funded by venture capital
- Colleges and universities
- In-licensed technology from non-US corporations
- In house discovery in existing US companies

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