ITP Chemicals Subprogram FY2007 Portfolio Review Final Report

Conducted for the
Industrial Technologies Program
Office of Energy Efficiency and Renewable Energy
U.S. Department of Energy
by
Dr. Joseph V. Porcelli, JVP International, Inc.
with support from
BCS, Incorporated

ITP Chemicals Subprogram FY2007

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Contributors

The Fiscal Year 2007 Portfolio Review was organized by a dedicated team supporting the ITP Chemicals program, and the actual review was conducted by a third party, JVP International, Inc.

- Joe Porcelli, JVP International, Inc., Review Chairperson
- Dickson Ozokwelu, Industrial Technologies Program
- Bill Prymak, Industrial Technologies Program, Golden Field Office
- Tim Ramsey, Navarro Research and Engineering, Inc.,
- Sharon Robinson, Oak Ridge National Laboratory
- Leslie Pezzullo, BCS, Inc.
- Ilona Johnson, BCS, Inc.
- Roy Tiley, BCS, Inc.
- Jo Rogers, AIChE

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Executive Summary

The portfolio review process is designed to allow the ITP Chemicals subprogram to monitor the progress of the projects in the portfolio and to judge whether the goals of the program are being adequately met by those projects. The FY 2007 Chemicals subprogram Portfolio Review took place at an AIChE meeting in Houston, Texas in April 2007.

17 projects were reviewed. The projects were evenly distributed between the Reactions and Separations Focus Areas, with one completed project being reviewed that was in the previous Enabling Technologies Focus Area.

Six reviewers and a chairperson (retired industry executives and experts in chemical and petroleum R&D) performed the review, which involved preparation work before the meeting, a number of days at the meeting, and some time after the meeting to complete arriving at consensus opinions.

Each of the reviewers was assigned either eight or nine projects to review, and their comments were captured in a reviewer questionnaire. The highlights of their comments are included in this report, with the full consensus questionnaires for each project in the Appendix.

An overview of the 2007 Portfolio may be seen in Table 1 below:

Table 1: Overview of 2007 Chemicals Portfolio

No. of Projects	17
Total 2030 Annual Energy Benefits (TBtu/yr)	569.2
DOE Spending (Thousands)	$36,014

The projects ranged in projected Energy Savings in 2030 from over 300 Trillion Btu/year to near zero.

A few of the projects in the portfolio have just started while one or two are at or near completion. The aging of the portfolio is shown in Table 2 below:

Table 2: Aging of 2007 Chemicals Portfolio

Project Status	No. of Projects
Total Projects Reviewed	17
Projects Ongoing as of Review	15
Projects Ongoing as of Jan 1, 2008	12
Projects Ongoing as of Jan 1, 2009	4

The projects covered the full range of possible project phases, from Discovery Research to Demonstration. The overall statistics on the number of projects in each phase of research is shown in Table 3 below.

Table 3: 2007 Chemicals Portfolio Phase of Research

Project Phase	No. of Projects
Total No. of Projects Reviewed	17
Discovery Research	1
Applied Research	5
Technology Development	7
Pilot Plant	2
Demonstration	2

The reviewers generally agreed that most of the projects being funded were deserving of that funding; they were working in areas that could yield superior energy savings in future years if they were successful. This is a definite result of the choice of focus areas made by the ITP Chemicals subprogram in past years. A distribution of the projects by sub-focus areas may be seen in Table 4 below.

Table 4: 2007 Chemicals Portfolio Focus Area Distribution of Products

Sub-Focus Area	No. of Projects
Oxidation Reactions	4
Micro Reactors	4
Alternative Processes	3
Distillation & Hybrids	5
Enabling Technologies	1
Total	**17**

With the help of the Chemical subprogram's portfolio management tool, CPMT, the reviewers evaluated the portfolio of projects for each Focus Area as a whole and judged the relative merits of each project in the portfolio. Unfortunately, it was concluded that in some instances, the potential rewards in energy savings did not justify the financial risk and work effort being expended. From their study of the projects, the reviewers concluded which projects were doing very well and which needed attention. Various CPMT graphs (shown in the Appendix) supplemented and confirmed these conclusions. It was recommended that the ITP Chemicals subprogram make a special effort to monitor those projects more closely.

The reviewers were comfortable with the forthcoming changes at ITP from Focus Areas to Technology Platforms, and it appeared that this new structure could successfully address the concerns of the chemical industry going forward.

1. Introduction

The United States Department of Energy, Office of Energy Efficiency and Renewable Energy (DOE/EERE), Industrial Technologies Program (ITP) supports research and development (R&D) aimed at improving the energy efficiency and environmental performance of industrial processes. The program's primary role is to invest in high-risk, high-value R&D projects that will, if successful, reduce industrial energy intensity while stimulating economic productivity and growth in the United States.

The goal of the Chemicals Subprogram is to implement successful strategies that save energy in the chemicals industry and support ITP and national goals for reducing industrial energy intensity. (Other issues addressed include reducing environmental impact of industrial processes). ITP's target is to support the EPAct 2005 goal, which calls for industrial energy intensity to be reduced 25% between 2007 and 2016. The Chemical industry is the largest single energy consumer of all industrial sectors in the U.S. (Figure 1). If the Chemical Industry meets the EPAct 2005 goal, it will achieve annual energy savings of about 1,500 TBtu by 2016.[1] This amount of energy is equivalent to the energy contained in 260 large oil tankers, or about 30% of annual crude oil imports from the Persian Gulf.[2]

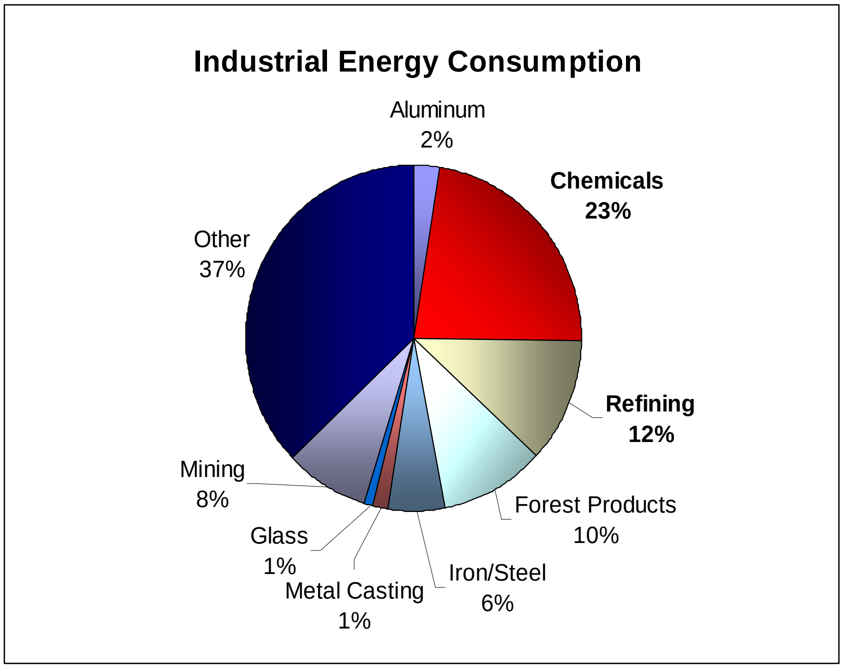

Figure 1: Industrial Energy Consumption by Industrial Sector
(Source: DOE EIA Annual Energy Outlook, 2007)

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[1] Based on EIA, *Annual Energy Outlook 2007*, Supplemental Tables. Projections for the chemicals industry in 2006 include value of shipments equal to $195.5 billion and total energy consumption (including electricity losses) of 7,471 TBtu/year. Energy intensity is calculated at 38.2 kBtu/$ shipments. A reduction of 25% in 10 years would translate to energy intensity of 28.7 kBtu/$ in 2016. When multiplied by EIA projections for value of shipments in 2016 ($213 billion), this would give total energy consumption of 6,113 TBtu/year. Meanwhile, energy consumption in 2016 under the "business as usual" scenario without EPAct 2005 would be 7,603 TBtu/year. Therefore, annual energy savings by 2016 will be 7,603-6,113 ≈1,500 TBtu/year.

[2] Assumes oil tanker carries 1 million bbls of crude oil. US crude oil imports from Persian Gulf equal 2,209 thousand bbls/day or 806,285,000 bbls/year. (EIA *Annual Energy Review 2005* Table 5.4).

ITP's Chemicals subprogram supports R&D relevant to unique challenges in the chemical industry, by:

- supporting collaborative, innovative R&D in chemical process technologies, including novel design tools and methodologies;
- promoting demonstrations of promising technologies;
- promoting the implementation of best practices and emerging technologies.

The ITP Chemicals subprogram carries out annual reviews of its portfolio of on-going R&D projects, for a number of reasons:

- to assess the progress of each R&D project and its likelihood of achieving its technical and commercial objectives;
- to advise the Principal Investigator (PI), who is the lead technical manager of the project, of any modifications to his/her work or commercialization plans;
- to assess the degree of balance on the portfolio and to understand where gaps or over-concentration in certain areas may be;
- to continually improve the processes, methods, and tools utilized by the reviewers and the subprogram staff in the carrying out of these tasks.

1.1 The Review Process

This review was carried out at the Spring 2007 meeting of the American Institute of Chemical Engineers (AIChE), which was held in Houston, Texas in April, 2007. This arrangement allowed chemical and allied industries' AIChE meeting attendees to gain exposure to the R&D projects being supported by the subprogram, and to the PIs and to the representatives of each project's partner organizations.

A team of seven chemical industry R&D experts (see Appendix A, Table A.1), made up of retirees from major companies and independent consultants, participated in the review, which included seventeen projects, organized in several focus areas and in different stages of completion.

Three reviewers were assigned to cover eight projects in the Reactions Focus Area, while three other reviewers covered eight projects in the Separations Focus Area plus a single Enabling Technologies Focus Area project. The seventh reviewer acted as chair of the overall review, with the responsibilities of instructing and aiding the reviewers, leading most of the discussions and writing most of the final report. An outline of the review process follows – details are available in Appendix B.

Starting several months before:

- Selection of Reviewers
- Development and transmission of PI Questionnaire (see Appendix C)
- Development and transmission of Reviewer Questionnaire (see Appendix D) and PI Completed Questionnaire

In Houston:

- Sunday evening, May April 21 – reviewer meeting
    - Introductions
    - Presentation on DOE ITP Program
    - Presentation on review expectations
    - Introduction to CPAT and CPMT
- Monday morning thru Thursday morning
    - Open sessions with PI presentations
    - Closed sessions with PI confidential presentations
    - Reviewers held private "debrief" sessions and reached consensus on project scores
- Tuesday evening – poster session
- Thursday afternoon – meeting of all reviewers
    - Presentations by reviewers on each Focus Area
- Friday morning – Meeting of reviewers, contractors and DOE staff
    - DOE Presentation on ITP background and changes
    - Facilitated discussions on:
        - Opinions on value and shortcomings of CPMT
        - Major concerns of chemical industry
        - Opinions on existing portfolio
        - Opinions on possible future projects
        - Opinions on value and shortcomings of CPAT
        - Lessons learned for future reviews.

1.2 Assessment Tools

Two tools have been developed by DOE to aid in the review process: CPAT (Commercialization Projects Assessment Tool), and CPMT (Chemical and Allied Processes Portfolio Management Tool).

CPAT is used by the PI to evaluate the commercialization potential of his/her proposed technology by comparing its projected economics to that of the conventional technology it would be competing with. Depending upon the favorability of the economics, CPAT projects the rate at which the new technology will be assimilated into industry, in terms of the number of new plants built versus time. The projected market penetration of the new technology allows an assessment of potential energy savings achieved by the project.

CPMT is a software tool used by ITP to visually depict the relative rewards and the risks of each project, taking into account the phase of the research, and the costs of the projects. CPMT develops charts that allow the viewer to quickly judge which projects are indicating appropriate metrics and which are out of line.

Details on these tools appear in Appendices E and F, respectively.

2. Portfolio Issues

An assessment of the ITP Chemicals portfolio was made in consensus meetings held during the latter part of the FY2007 Chemicals Portfolio Review. This assessment included a review of the underlying strategy for assembling the portfolio and a judgment on whether the portfolio was likely to achieve stated goals. One half-day meeting focused on the portfolio at the project level, and a facilitated session on the final day reviewed the program focus areas and portfolio issues. Other items discussed included the impact of the proposed restructuring of the ITP program into Technology Platforms, the issues facing the chemical industry, and ways in which the review process could be improved.

2.1 Current Portfolio Strategy

The Chemicals subprogram strategy has been designed to have the greatest impact on reducing the energy intensity of the chemical industry. Most chemical processes begin with a reaction, followed by separation and recovery of the product from unreacted feedstocks and undesirable byproducts. The feedstocks are recycled back to the reaction section, and the byproducts are removed for disposal. Since many chemical processes have selectivities well below theoretical, and must operate at low conversion/pass to maximize that selectivity, the separation section is usually costly and energy intensive. The equipment sizes are dictated by the size of the recycle streams, also adding to the capital cost of the process. Therefore, the strong focus of the program is finding alternative catalysts or process routes that will allow increased selectivities at the same or lower cost. Figure 2 below graphically illustrates this admittedly simplified model of a chemical process.

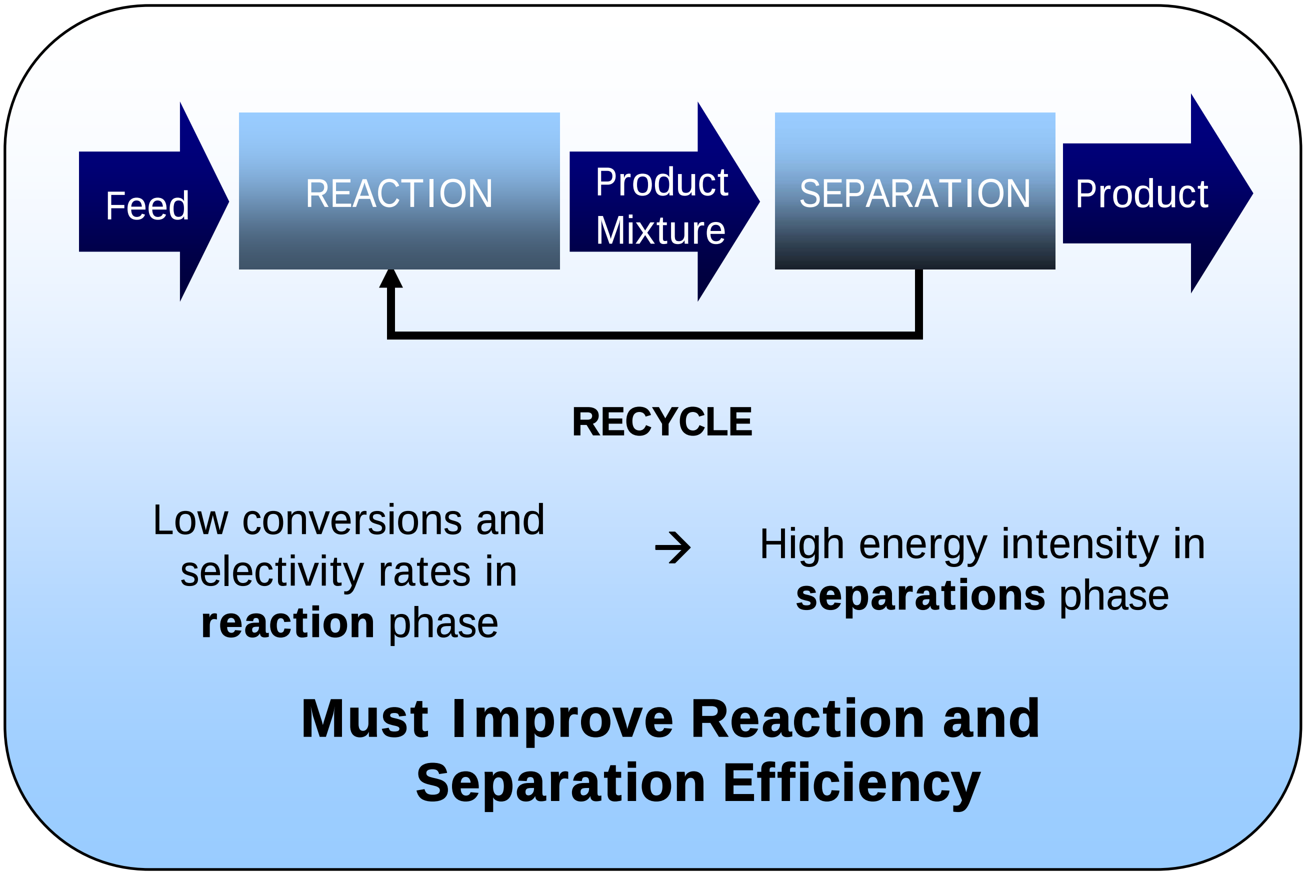

Figure 2: ITP Chemicals Subprogram Chemical Process Model

The current portfolio includes high risk, high return R&D that ranges from discovery research, through applied research, technology development, pilot plant and demonstration projects.

The concerns when reviewing a portfolio are whether the portfolio supports DOE's mission for energy reduction, is appropriately balanced with respect to risk and funding level, and whether gaps exist (i.e. are segments of the target technologies missing?) Questions to be answered include:

- Is the funding being distributed appropriately across the various Focus Areas?
- Are certain areas being over- or under-funded?
- What will be the change in balance as projects are completed?
- Where should be the areas of emphasis in any future solicitations?

The ITP Chemicals portfolio as reviewed in 2007 is summarized in Table 5.

Table 5: Summary of the ITP Portfolio

Focus Areas	Sub Focus Area	Total No. of Projects Reviewed	2030 Annual Energy Benefits* (TBtu/yr)	DOE Spending (Thousands)
Reactions	Oxidation Reactions	4	91.0	$10,378
	Micro Reactors	4	356.0	$8,358
Separations	Alternative Processes	3	79.5	$5,314
	Distillation & Hybrids	5	37.7	$10,493
Enabling Technologies	Enabling Technologies	1	5.0	$1,471
	Total	**17**	**569.2**	**$36,014**

* Energy Savings are the Revised Estimate – please see Table 5 in Section 4.1 below.

Based on the number of projects in each sub-focus area, and the amount of money invested by DOE, the portfolio appears reasonably balanced. Alternative Processes are perhaps a little under-represented, and Enabling Technologies are seriously under. However, given the relatively low "payoff" in energy savings for the one Enabling Technologies project, this focus area may not warrant higher representation.

The question of how the portfolio will change with time (without the addition of new projects) is answered in Table 6.

Table 6: Aging of the ITP Chemicals Portfolio

Sub Focus Area	Total No. of Projects Reviewed	Projects Ongoing as of Review	Projects Ongoing as of Jan 1, 2008	Projects Ongoing as of Jan 1, 2009
Oxidation Reactions	4	4	3	1
Micro Reactors	4	4	3	0
Alternative Processes	3	3	2	1
Distillation & Hybrids	5	4	4	2
Enabling Technologies	1	0	0	0
Total	17	15	12	4

First, Table 5 indicates that two of the 17 projects that were reviewed have been completed. All but two more will extend at least into 2008, but by 2009 only four projects will still be active; 1 in Oxidation Reactions, 1 in Alternative Processes and 2 in Distillations and Hybrids. With the exception that there will be no Micro Reactors projects, the balance does not appear to be harmed through this period.

Information such as that illustrated in Tables 5 and 6 does not guarantee that these results will be achieved. An important factor in the ultimate performance of the ITP Chemicals portfolio is the stage of the research being funded, and what happens at the end of a project. Until a project is commercialized, there cannot be any energy savings. Therefore, it is important to review the information in Table 7 below, in which the stages of the projects in each sub-focus area are noted.

Table 7: Project Phase Statistics

Focus Area	Total No. of Projects Reviewed	Discovery Research	Applied Research	Technology Development	Pilot Plant	Demons-tration
Oxidation Reactions	4	1	2	0	0	1
Micro Reactors	4	0	0	3	1	0
Alternative Processes	3	0	1	1	1	0
Distillation & Hybrids	5	0	2	3	0	0
Enabling Technologies	1	0	0	0	0	1
Total	17	1	5	7	2	2

CPMT tool output charts can be useful in analyzing and discussing portfolio issues. At the end of this review, after coming to a consensus on the Energy Savings in 2030 for each project, a final set of CPMT charts were prepared, and the results analyzed in Appendix H. This should be illustrative of the value of the tools and part of the lessons learned for future reviews.

As an illustration, two of the CPMT charts that appear in Appendix H are reproduced here as Figures 3 and 4. They both compare one “reward” metric, designated “Value” against a risk metric called Technical Risk. Figure 3 is for the group of projects in the Reactions Focus Area and Figure 4 is for the Separations Focus Area Projects.

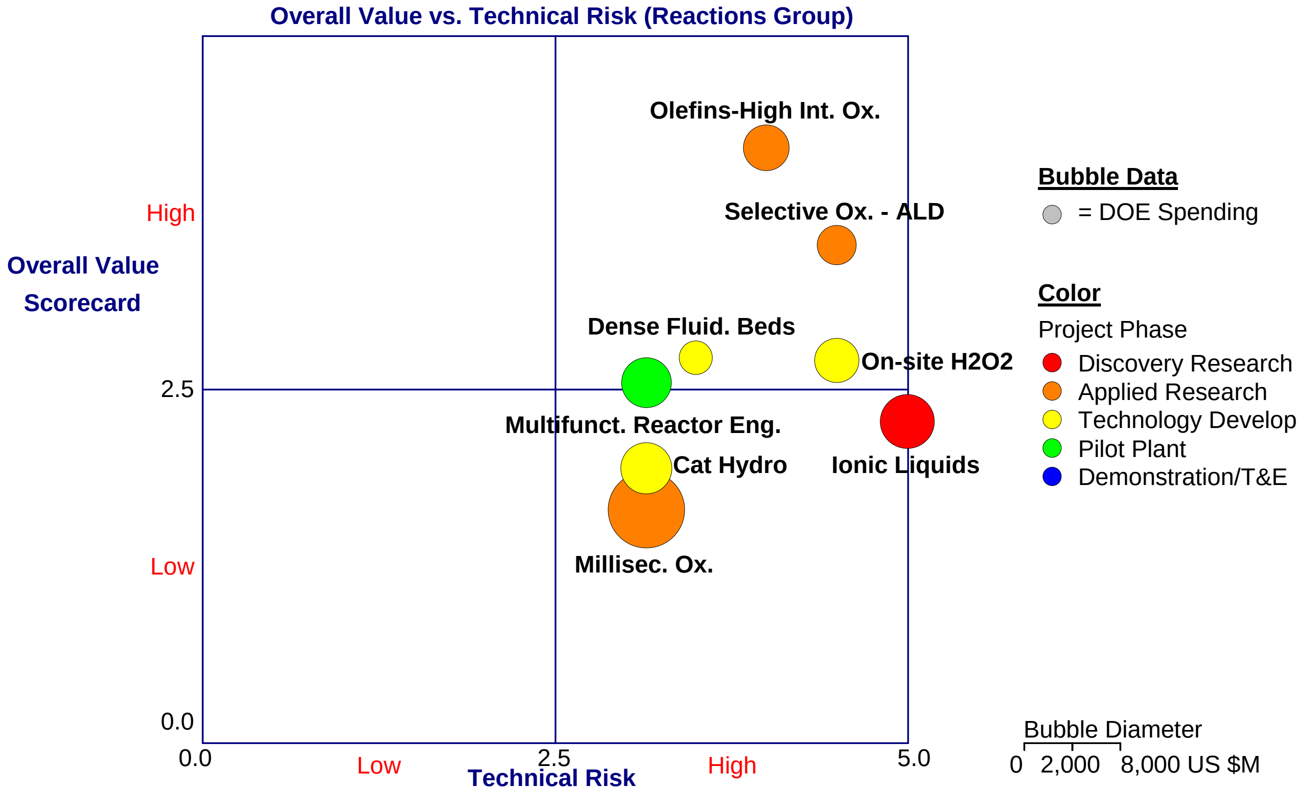

Figure 3: Reactions Focus Area Projects, Overall Value vs. Technical Risk

Overall Value is a composite metric, with a high weight being given to the projected Energy Savings in 2030, but with some contribution from the degree of innovation of the project, the degree of interest shown by industry, the environmental benefits of the new technology as compared to conventional, the effect on society such as job formation, and how well it fits the ITP goals.

Technical Risk is a composite metric also, taking into account the technical challenge, the technical experience of the team, and the program management experience of the PI.

Generally, in a risk-reward diagram such as this, ideal projects should line up on the diagonal line – the higher the reward that is promised, the high the risk one is willing to take. This is complicated because of the various research phases of the projects being compared (indicated by color in the graph) and the degree of completion of the time line of the project. A project near completion should have low technical risk, and a project in Discovery Research ought to have a high technical risk.

The two highest value projects are those promising high selectivities for the oxydehydrogation of ethane to ethylene, so that the endothermic cracking reaction is replaced by an exothermic (or at least neutral) reaction, saving the energy required to fire the cracking furnaces. In addition, those by-products produced are different from the hydrocarbon by-products formed in cracking and presumably can be more easily and less-energetically separated. Both projects are ranked high in Technical Risk, based on their high degree of innovation and technical challenge.

A similar analysis may be made for the Separations Focus Area Projects displayed in Figure 4.

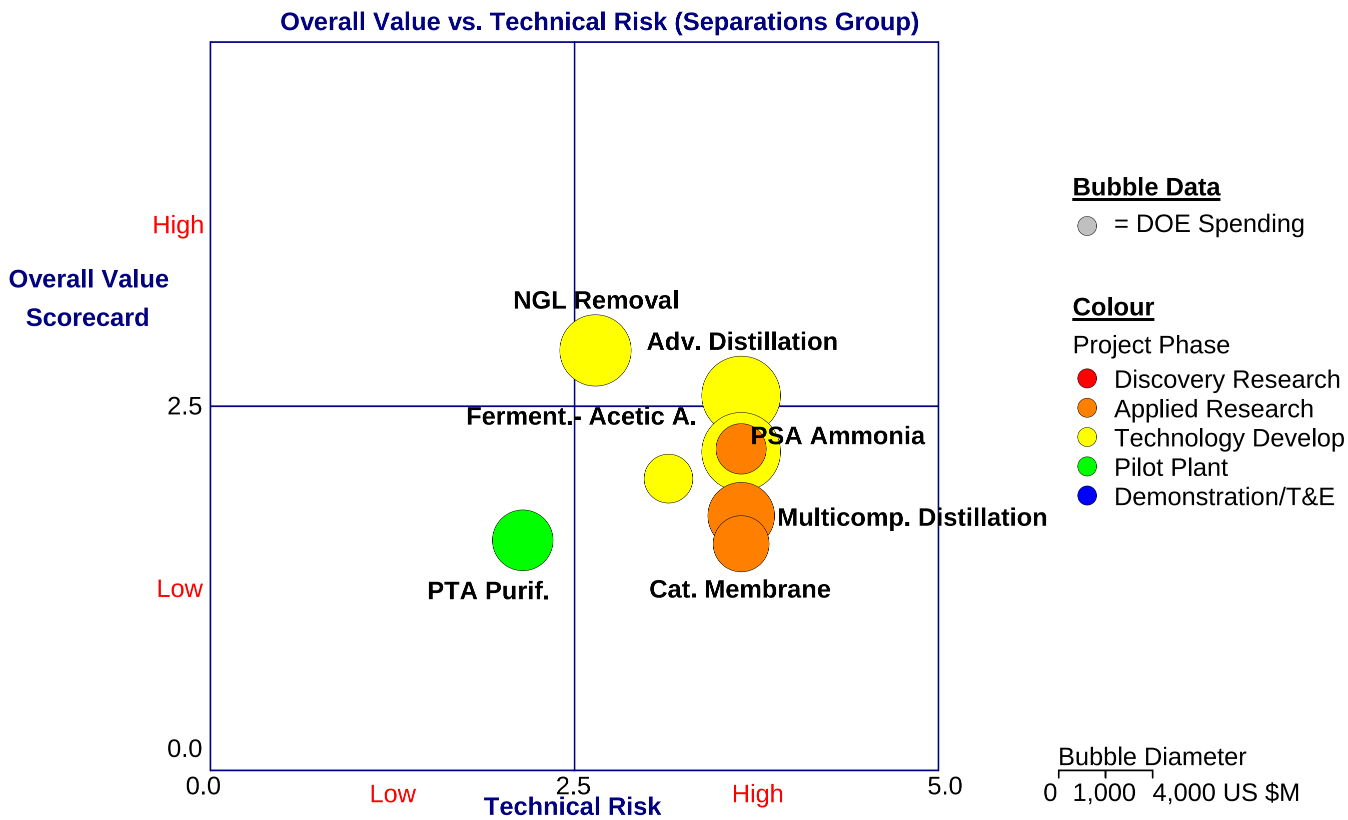

Figure 4: Separations Focus Area Projects, Overall Value vs. Technical Risk

In this case, most of the projects line up nicely along the imagined diagonal. The bottom two projects, Multicomponent Distillation and Catalytic Membranes seem somewhat out of line in a negative direction compared to all of the others. Their technical risks are moderately high, reflecting that these projects have only recently started. On the other hand, they have lower value than many of the other projects with comparable risk, making them less desirable than the others. Unfortunately, it is not easy to influence a project to make adjustments to increase its value, but presumably one can work towards reducing the technical risk.

2.2 Industry Issues

As mentioned earlier, the chemical industry is the largest single energy consumer of all industrial sectors in the U.S. Over half of that consumed energy is in the form of feedstocks, as illustrated in Figure 5 below.

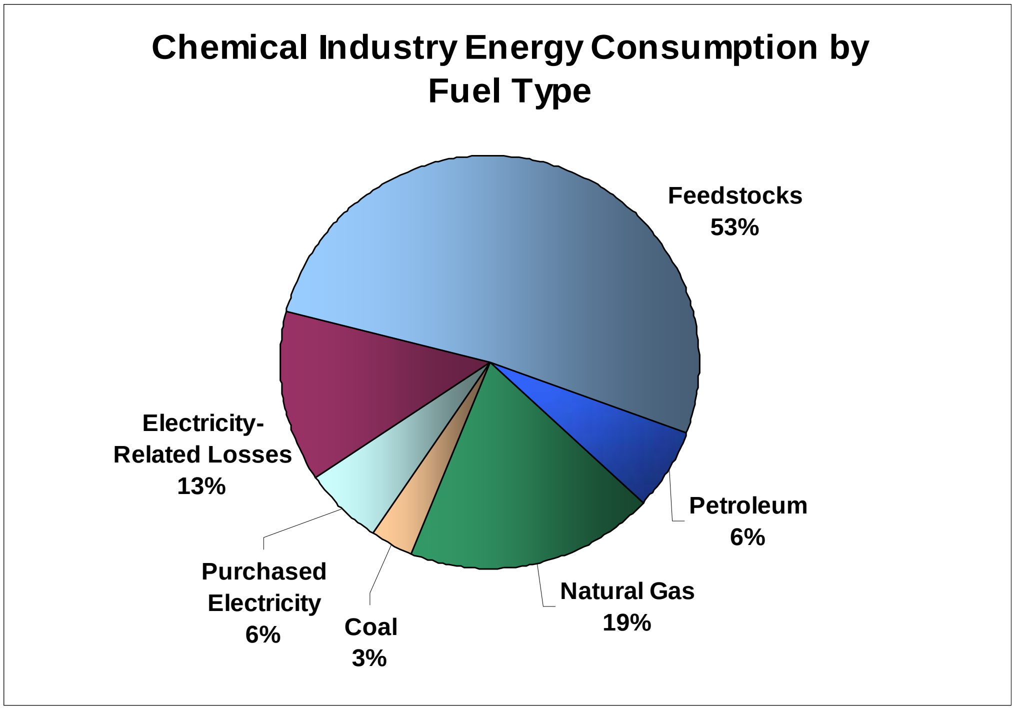

Figure 5: Forms of Energy Consumption in the U.S. Chemical Industry
(Source: DOE EIA, Annual Energy Outlook 2007)

The industry achieved substantial improvements in energy efficiency during the 1970s, as a result of the Middle East oil crises, which resulted in temporary high prices and shortages in certain energy supplies. Since the 1990s, little further improvement in energy efficiency has been noted. It is likely that the last few years, with the step-up in crude oil prices to a higher level and several periods of high natural gas prices and shortages, have prompted industry to make investments in energy-savings equipment and process modifications, but it is too early to discern the magnitude of any energy-saving trend.

Most recently, political as well as economic considerations have prompted the beginning of a move towards alternative and non-fossil energy and feedstock sources, mostly in the automotive fuels and electricity generation areas. However, the largest impact thus far is the substitution of biomass (corn) derived ethanol for gasoline, but the high energy requirement for recovering and purifying ethanol, and its lower efficiency as a motor fuel have called any real overall energy savings into question.

2.3 Reviewers' Views on Industry Issues and their Possible Impact on the Portfolio

The reviewers agreed that industry is concerned about the costs and availabilities of natural gas and petroleum, and their impact on the movement of the basic chemical industry off-shore. Also, the pressures of environmental regulations, concerns about global warming and the security of the U.S. chemical facilities and transportation systems all influence the direction of future R&D.

In the opinions of the reviewers, the current portfolio with its emphasis on major energy-saving technologies is in line with the pressures facing the industry and the events of the last few years. However, the trend for major U.S. producers being bought by investment companies suggests less funding of R&D. Therefore it is imperative that the ITP chemicals subprogram carefully manage its resources to ensure adequate R&D efforts in the most critical areas that could lead to improved energy efficiency and competitiveness of the industry. Given the limited funding available to the sub-program, there is a great need to manage the portfolio tightly, with a mechanism to close down programs early that have no chance to achieve its goals.

Another item of importance to the U.S. chemical industry in the future will be increased utilization of process intensification concepts to aid in the development of economically viable smaller – scale distributed production of hazardous chemicals. The threats of terrorism and the all-too-real risks of industrial accidents with major damage or release of hazardous chemicals are issues that will only grow stronger as time passes. There is pressure to eliminate the manufacture, storage and transportation of hazardous chemicals, but some of them are key intermediates to many major products. Ideally, one would seek to develop alternative processes that did not require these hazardous chemicals, but that is a very long and difficult task, and if successful would disrupt the overall chain of feedstocks and products that were dependent on that feedstock. A more likely achievable solution would be to produce the hazardous chemical at its point of use, to avoid transportation of that chemical, arguably the most vulnerable link in the supply chain. These "distributed" production facilities would have lost the economics of scale, so that innovative engineering, simplifying these plants is required to regain favorable economics, and that is where process intensification and its "relative", microchannel systems, comes in.

A related issue that is required is the acceleration of the rate of innovation and of research and development itself. The industry needs these solutions today, under the threats mentioned above and those imposed by global competition from low feedstock cost and low labor cost regions. High throughput experimentation is a reality, thanks in part to support from DOE and NSF, so that the earliest phases of R&D have been accelerated successfully. Flexible pilot plants, that can quickly move from one project to another, have been a long-term goal, with some progress being made. But every phase in an R&D project from concept to commercialization needs to be accelerated.

2.4 Portfolio Actions in Response

The reviewers agreed that ITP funding of key energy-saving technologies in the chemicals industry is helping address major industry concerns regarding the cost and availability of natural gas. Moreover, given that fewer resources are currently being directed to R & D efforts by industry, ITP's role in reducing chemicals industry energy consumption is particularly important. Therefore, no redirection of the general ITP chemicals portfolio strategy is needed. The reviewers also suggested that since R & D funds within the chemicals program are limited, ITP should tightly manage its portfolio and quickly end projects that are unlikely to succeed. This is in agreement with current portfolio management practices, which include regular portfolio reviews in order to ensure that all projects meet their stated goals. The reviewers also discussed industry trends towards process intensification and distributed production; this trend is currently being addressed by the Microreactors focus area included in the chemicals portfolio. Additionally, reviewers mentioned the need to accelerate all phases of R & D, including the construction of pilot plants. Unfortunately, pilot plant development is very costly, and would require significant resources. The current strategy followed by ITP is to fund high-risk, high-value research. As projects enter later phases of development, which entail less uncertainty, ITP funding is less critical to ensuring the success of projects. Given the resources currently available to the chemicals subprogram, ITP is pursuing the most fruitful avenues for reducing energy intensity in the chemicals industry. Based on reviewer feedback, it was determined that the chemicals subprogram is meeting critical industry needs for R & D in energy saving technologies; no adjustments to the overall portfolio strategy are needed at this time.

3. Focus Area Issues

3.1 Current Strategy and Content of Focus Areas

The Chemicals portfolio strategy is continually changing as industry needs change and as R&D projects are added to the portfolio while others are completed. The focus area concept is intended to guide R&D solicitations and help in the choice of projects to fund. Currently, the portfolio is divided into three Focus Areas (Reactions, Separations, and Enabling Technologies) with a number of sub-focus areas (Micro Reactors, Oxidation Reactions, Distillation & Hybrids, Alternative Processes) as shown in Table 8.

Table 8: ITP Chemicals Projects Organized by Current Focus and Sub-focus Areas

<table>
<tr><th>Focus Area</th><th>Sub Focus Area</th><th>CPS#</th><th>Project Title</th></tr>
<tr><td rowspan="10">Reactions</td><td rowspan="4">Micro Reactors</td><td>14209</td><td>Microchannel Reactor System Design & Demonstration for On-Site H2O2 Production</td></tr>
<tr><td>16375</td><td>Microchannel Reactor system for Catalytic Hydrogenation</td></tr>
<tr><td>16636</td><td>Olefins by High-Intensity Oxidation</td></tr>
<tr><td>16637</td><td>Advances in Process intensification through Multifunctional Reactor Engineering: Novel Flow Regimes, Supports, Catalysts and Processes</td></tr>
<tr><td colspan="3">Total Number of Projects: 4</td></tr>
<tr><td rowspan="4">Oxidation Reactions</td><td>15987</td><td>Enhanced Productivity of Chemical Processes using Dense Fluidized Beds</td></tr>
<tr><td>17606</td><td>Using Ionic Liquids in Selective Hydrocarbon Conversion Processes</td></tr>
<tr><td>17619</td><td>Millisecond oxidation of Alkanes</td></tr>
<tr><td>17784</td><td>Development of High Selective Oxidation Catalysts by Atomic Layer Deposition</td></tr>
<tr><td colspan="3">Total Number of Projects: 4</td></tr>
<tr><td rowspan="10">Separations</td><td rowspan="5">Distillation & Hybrids</td><td>14202</td><td>Scalable Production and Separation of Fermentation -Derived Acetic Acid</td></tr>
<tr><td>15857</td><td>Catalytic Membrane Reactors</td></tr>
<tr><td>15858</td><td>Optimal Configuration for Multicomponent Multi-Column Distillation Processes</td></tr>
<tr><td>15986</td><td>Development of Advanced Membranes Technology Platform for Hydrocarbon Separations</td></tr>
<tr><td>17664</td><td>Advanced Distillation</td></tr>
<tr><td colspan="3">Total Number of Projects: 5</td></tr>
<tr><td rowspan="3">Alternative Processes</td><td>1623</td><td>PTA Purification Process</td></tr>
<tr><td>15898</td><td>New PSA Process for Production of Ammonia</td></tr>
<tr><td>16634</td><td>Low Cost Chemical Feedstocks Using Energy Efficient Natural Gas Liquid (NGL) Removal Process</td></tr>
<tr><td colspan="3">Total Number of Projects: 3</td></tr>
<tr><td rowspan="2">Enabling Technologies</td><td>Enabling Technologies</td><td>14211</td><td>Development of In-Situ Analysis for the Chemical Industry</td></tr>
<tr><td colspan="3">Total Number of Projects: 1</td></tr>
<tr><td></td><td colspan="3">Grand Total Number of Projects: 17</td></tr>
</table>

3.2 Changes at ITP and Future Technology Platform Structure

There is a possible re-organization of the ITP program at DOE, and the new concept was presented to the reviewers. A few questions were posed by the moderator to stimulate discussion on how the current portfolio might fit into the new structure. The contemplated new structure would divide the entire ITP portfolio into Technology Platforms as follows:

- Reactions and Separations
- Energy Conversion Systems
- High Temperature Processes
- Fabrication and Infrastructure

The reviewers were asked to consider how the current portfolio would fit, and which platforms might be most important to the chemical industry going forward; Table 5 in the Appendix contains the questions and answers on this topic.

The reviewers agreed that all of the current projects would fit into the Reactions and Separations platform, and that most future projects should also fit under that umbrella. Other ITP programs, such as Forest Products, for instance, might also have projects in this platform, and some of the Chemical projects could be cross-cutting over other industries, the dense fluidized bed project being noted as one.

3.3 Recommendations for Focus Areas and their Contents

The reviewers made the following comments and recommendations regarding the focus areas pursued by ITP Chemicals portfolio:

- The current focus areas capture the important issues of the day
- Use of alternative feedstocks such as biomass and coal will be increasingly important for the future; efficient reactions, separations and creative use of by-products will be issues.
- Stranded methane to methanol appears very important given the possible impact on transportation fuels.
- Consider more emphasis on inorganic chemistry, given the future importance of economic solar energy and other alternative energy sources. The reviewers recognized that production of inorganic materials such as silicon will likely grow as a result of increased solar panel production, and ITP could potentially pursue opportunities that reduce energy intensity in this growing industry.

3.4 Focus Area and Content Actions in Response

The reviewers confirmed that the chemicals subprogram focus areas encompass the most promising technologies for reducing energy consumption in chemicals manufacturing. They also highlighted the increasing role of alternative feedstocks such as biomass and coal. This issue has been raised in a number of committees, including the Fiscal Year 2005 chemical review team, and the Chemicals Industry Vision2020 Technology Partnership. ITP is currently funding a few projects in this area, such as the project "Scalable Production and Separation of Fermentation -Derived Acetic Acid." Additionally, ITP recently conducted a study of alternative feedstocks in conjunction with Vision2020 and Oak Ridge National Laboratory[3]. ITP will consider new project funding opportunities based on the results of this report. Additionally, reviewers discussed potential for ITP to become involved in reducing energy intensity of inorganic chemicals manufacturing, especially in growing industries affiliated with solar panels or other alternative energy technologies. ITP is already funding research in the manufacture of inorganic chemicals under its "alternative processes" focus area (e.g. the project "New PSA Process for Production of Ammonia"). Additionally, as the reviewers suggested, there are developing opportunities for ITP to fund inorganic chemicals that will experience increased production due to solar panel manufacture. In addition to silicon manufacture, there may be opportunities in other chemicals, such as cadmium telluride, which is produced in an energy-intensive manufacturing process requiring vacuum distillation. ITP Chemicals, which has substantial experience funding research in process engineering to promote energy efficiency, would be well-positioned to address this area. Based on reviewer feedback, ITP will continue in pursuing the projects in its current focus area structure, as well as consider new opportunities in both alternative feedstocks and inorganic chemicals manufacturing.

[3] Chemicals Industry Vision2020 Technology Partnership *Alternative, Renewable, and Novel Feedstocks for Producing Chemicals*, July 2007

4. Project Issues

The projects in the Chemicals portfolio were reviewed over 3-1/2 days of the portfolio review. Each reviewer was responsible for reviewing all of the projects in his assigned Focus Area, and his review was based on the material submitted in advance by the PIs, and the material presented (and questions answered) at the open and closed sessions. The main document that contains the reviewers' opinions is the Reviewer's Questionnaire, and each Focus Area group of reviewers worked with the DOE staff and support contractors to develop a consensus of their opinions. The resulting filled-in consensus questionnaires are attached in Appendix G.

4.1 Review of Project Energy Savings Estimates

An important part of the review was the Energy Savings projected for 2030, by the PIs' use of CPAT. There were some difficulties experienced by some of the PIs in running CPAT, so that some of the results available to the reviewers in Houston were revised after the review. The figures as developed by the PIs and the revised figures, agreed upon after discussion with the reviewers, appear in Table 9 below.

Table 9: CPAT Energy Savings Estimates -- Original and Revised

CPS #	Project Title	PI Estimate: Energy Savings in 2030 (TBtu/year)	Reviewers' Comments	Revised Estimate: Energy Savings in 2030 (TBtu/year)
Reactions Focus Area				
14209	Microchannel Reactor System Design & Demonstration for On-Site H2O2 Production	78.0	Energy savings numbers are not based on the market that they can penetrate at this concentration of H2O2 (not addressing market as they defined)	29.0
16375	Microchannel Reactor system for Catalytic Hydrogenation	14.7	Energy savings assumptions are extremely aggressive	7.0
16636	Olefins by High-Intensity Oxidation	357.0	The market penetration is aggressive	300.0
16637	Advances in Process intensification through Multifunctional Reactor Engineering: Novel Flow Regimes, Supports, Catalysts and Processes	120.0	Because of high risk, refining industry is reluctant to move rapidly Potential is huge if they can get one running in a refinery - close to initial commercialization	20.0
17606	Using Ionic Liquids in Selective Hydrocarbon Conversion Processes	14.0	discovery program - with very aggressive estimates	5.0
17619	Millisecond oxidation of Alkanes	36.6	The market impact and energy savings numbers are going to be heavily dependent on the marketplace.	0.0
17784	Development of High Selective Oxidation Catalysts by Atomic Layer Deposition	Ethylene = 157.7 Propylene =295.5 Total = 453.2	Extremely Aggressive	Ethylene = 86.0 Propylene = 0.0 Total = 86.0
15987	Enhanced Productivity of Chemical Processes using Dense Fluidized Beds	Acrylo = 0.12 TiO2 = 0.13 Styrene = 5.99 Propylene = 4.08 Felxicoking =0.48 Total = 10.80	Estimates seem appropriate and in line w/ potential	Acrylo = 0.12 TiO2 = 0.03 Styrene = 0.20 Propylene = 20 Felxicoking = 0.05 Total = 0.60

Table 9: CPAT Energy Savings Estimates – Original and Revised (Continued)

CPS #	Project Title	PI Estimate: Energy Savings in 2030 (TBtu/year)	Reviewers' Comments	Revised Estimate: Energy Savings in 2030 (TBtu/year)
Separations Focus Area				
1623	PTA Purification Process	11.6	Energy savings assumptions are reasonable	5.0
16634	Low Cost Chemical Feedstocks Using Energy Efficient Natural Gas Liquid (NGL) Removal Process	48.9	Energy savings assumptions are reasonable	48.9
15898	New PSA Process for Production of Ammonia	95.2	Aggressive estimates	25.0
17664	Advanced Distillation	77.5	Optimistic market penetration	31.0
15986	Development of Advanced Membranes Technology Platform for Hydrocarbon Separations	27.9	Did not include utilities in energy savings estimates	27.9
14202	Scalable Production and Separation of Fermentation -Derived Acetic Acid	31.2	Energy savings assumptions are aggressive	10.0
15858	Optimal Configuration for Multicomponent Multi-Column Distillation Processes	NA	NA	6.7
15857	Catalytic Membrane Reactors	14.6	Aggressive market penetration. Assumes technology will extend to entire ester business	3.0
Enabling Technologies Focus Area				
14211	Development of In-Situ Analysis for the Chemical Industry	NA	NA	5.0

4.2 Project Ranking

As part of the review process, presentations were made by each group of reviewers to the other. In these presentations, the reviewers described the projects and then ranked them, discussing their reasons for positive and negative opinions on each project.

For each Focus Area, the list is in order from those judged the "best" to those judged the "poorest", but it should be recognized that there are relatively few projects in each group, and the projects differ in their degree of completion of their timelines. Further, it must be emphasized that there was relatively little difference between the top and bottom projects on each of the lists.

4.2.1 Reactions Focus Area Project Rankings

For this Focus Area, the projects were listed by the reviewers in three tiers as follows in Table 10 below.

Table 10: Reactions Focus Area Project Rankings

CPS #	Project Title	Ranking	Pros	Cons
16637	Advances in Process intensification through Multifunctional Reactor Engineering	Top Tier	Comments omitted to protect confidential information.	
15987	Enhanced Productivity of Chemical Processes using Dense Fluidized Beds	Top Tier		
16636	Olefins by High-Intensity Oxidation	Top Tier		
17619	Millisecond Oxidation of Alkanes	Middle Tier		
17784	Development of High Selective Oxidation Catalysts by Atomic Layer Deposition	Middle Tier		
14209	Microchannel Reactor System Design & Demonstration for On-Site H2O2 Production	Bottom Tier		
17606	Using Ionic Liquids in Selective Hydrocarbon Conversion Processes	Bottom Tier		
16375	Microchannel Reactor system for Catalytic Hydrogenation	Bottom Tier		

4.2.2 Separations Focus Area Project Rankings

In this focus area, the reviewer team split the projects into "Active" and "New" Projects. The order within each of the two groups is an indication of relative merit, from best to poorest. The project ranking appears in Table 11 below.

Table 11: Separations (and Enabling Technologies) Focus Area Project Rankings

CPS #	Project Title		Pros	Cons
Active Projects				
17664	Advanced Distillation	1	Comments omitted to protect confidential information.	
16634	Low Cost Chemical Feedstocks Using Energy Efficient Natural Gas Liquid (NGL) Removal Process	2		
1623	PTA Purification Process	3		
14211	Development of In-Situ Analysis for the Chemical Industry	4		
15986	Development of Advanced Membranes Technology Platform for Hydrocarbon Separations	5		
14202	Scalable Production and Separation of Fermentation -Derived Acetic Acid	6		
New Projects				
15858	Optimal Configuration for Multicomponent Multi-Column Distillation Processes	1		
15898	New PSA Process for Production of Ammonia	2		
15857	Catalytic Membrane Reactors	3		

4.3 Project Synergies

The following are project commonalities observed by the portfolio reviewers:

- A number of projects involved proposed innovations in the ethylene and propylene production processes – as these are among the highest energy consumers in the industry, this emphasis is proper.
- Microreactors were also involved in a number of projects, although for most the projected energy savings were disappointingly modest.
- More work is needed to educate PIs about proper use of CPAT.

Key differences among the projects included:

- The range of development phases was broad, with one Discovery Research (Ionic Liquids) and several Demonstration phase projects (In situ Analysis and Dense Fluidized Beds.
- Some project teams were working well together (Olefins by High-Intensity Oxidation, Dense Fluidized Beds) while other projects suffered from ineffective teamwork (New PSA Process, Membranes for HC Separation, Scalable Acetic Acid, Compact Membrane Systems).
- Some projects had just started (Compact Membrane Systems, Multi-column Distillation and New PSA Process), others were stretched out due to inadequate funding (Multi-functional Reactors, ALD Catalysts), and several were completed (Scalable Acetic Acid and In situ Analysis).

Detailed project information is included in the Appendix.

4.4 Project Recommendations

The reviewers were asked to provide overall improvement recommendations for the projects reviewed and the review process itself.

Regarding the projects themselves, the following comments are made to encourage the PIs -

- The microchannel hydrogen peroxide project would benefit from more rigorous market information and by developing plans for commercialization with their industrial partner.
- The Microchannel hydrogenation project needs a more active industrial partner.
- The Ionic Liquid Catalyzed Methane to Methanol project needs to engage an industrial partner.
- The scalable Acetic Acid team needs to update economics to confirm competitiveness against large plants, and needs to find an serious industrial partner.
- The Multicomponent Multi-column Modeling team needs to develop a marketing plan
- The Catalytic Membrane Reactor team needs to more narrowly focus future efforts.

Regarding the review process -

- Reviewers recommended more education of the PIs and the future reviewers on the proper use of CPAT.
- Some questioned the usefulness of this tool for specialty chemicals such as hydrogen peroxide, not recognizing that new process could always be added to software.

- The Reviewer Questionnaire ought to be more focused on helping the reviewers uncover the progress of the projects toward achieving their milestones and overall goals.
- A stronger monitoring on milestones and go/no go decisions by DOE is needed to stop or re-organize poor performing projects.
- Future projects should be limited to those with high energy-saving potential. This comment brings up the need for cross-cutting innovations that have the potential for high energy savings in the aggregate over time. Examples would be process intensification, where learnings on one technology may well extend across the chemical industry and beyond.

4.5 Project Actions in Response

The reviewers provided helpful feedback on the value and progress of each project in the portfolio. They helped evaluate the projected energy savings from each project, provided DOE with a ranking of each project in its portfolio, and provided suggestions for improving each project. The reviewers' feedback will be shared with project teams in order to guide future efforts. ITP will also use reviewer feedback to evaluate the distribution of funding for its projects in future years. Since the Chemicals Subprogram currently has sufficient funds for each of its projects, it will only discontinue those projects that are clearly not meeting their stated objectives. In response to reviewer feedback, the program's first course of action will be to evaluate projects of concern. If the evaluation confirms that adequate progress is not being made, ITP will provide recommendations and try to redirect the project. If the progress is still not being made in the following months, appropriate actions will be taken which may include withdrawing funding from that project. In this case, the funding will be redirected to other identified priorities.

The reviewers' rankings of different projects in the portfolio highlighted those "bottom tier" projects that may warrant additional attention and/or site visits to confirm project performance. These projects are discussed below.

Microchannel Reactor System Design & Demonstration for On-Site H_2O_2 Production

Reviewers raised concerns that the low concentration of H_2O_2 manufactured via this process would limit the technology's commercialization potential. ITP staff recently visited the pilot plant in order to assess its progress. It appears that the reviewers failed to acknowledge that the team has in fact met its stated goal, which is to use its michrochannel reactor system to produce H_2O_2 with a 1% wt concentration. Since the portfolio review in April, FMC has achieved a 2% wt concentration, and is currently working towards achieving a 5% wt concentration. The H_2O_2 could successfully be used to produce propylene oxide and has potential for a substantial market impact. Based on ITP's evaluation, this project is meeting its objectives and has the potential to successfully reduce energy consumption in the chemicals industry.

Using Ionic Liquids in Selective Hydrocarbon Conversion Processes

The reviewers raised questions about the progress achieved by this project. While the reviewers acknowledged that the team is ahead of others in the field, significant challenges will still need to be overcome. In response, ITP staff will work with the project team in order to further assess project progress.

Microchannel Reactor system for Catalytic Hydrogenation

The reviewers commented that this project should be further along at this time, and that it needs a more active corporate partner. ITP accepts reviewer comments and will further evaluate this project's progress.

Development of Advanced Membranes Technology Platform for Hydrocarbon Separations

At the time of the review, the project team had stalled its work on the project. ITP will need to determine whether the team plans to continue its work. If not, the funds will be redirected to other high priority activities.

Scalable Production and Separation of Fermentation -Derived Acetic Acid

The reviewers expressed concern about the difficulty experienced by the team in working with an industrial partner. ITP acknowledges that the team has not thoroughly pursued commercialization, despite the fact that the project achieved its technical goals. ITP looks forward to potentially including this project among other projects that can compete for validation funding from DOE.

New PSA Process for Production of Ammonia

The review team gave mixed feedback on this project. The reviewers agreed that if successful, this project may achieve significant energy savings. However, 2 of the 3 reviewers conveyed skepticism about the feasibility of overcoming major technical challenges (e.g. high temperature adsorption). ITP notes these comments, but will take no action at this time. This is a new project; therefore it is too early to assess the team's progress. Its progress will be evaluated again at the next portfolio review.

Catalytic Membrane Reactors

As with the project "PSA Process for Production of Ammonia," reviewers were concerned about the significant technical challenges associated with this project. They also suggested that the team's efforts be more narrowly targeted. ITP notes these comments, but since this is a new project, it is difficult to make any judgment at this time. Project progress will be evaluated again at the next portfolio review.

5. Conclusions

Key achievements of the portfolio review included:

- Most PIs successfully used the improved web-based Commercialization Project Assessment Tool (CPAT) to estimate the degree of superiority of process economics for the New Technology over the Conventional Technology, leading to a forecast of Energy Savings in 2020 and 2030.

- Reviewers used a project evaluation form with anchored scales, and arrived at consensus scores and comments for all of the projects reviewed.

- The Portfolio Review took place at a large technical chemical industry meeting, offering chemical industry exposure to ongoing R&D projects, and exposure of the PIs to industry representatives.

- Reviewers offered candid comments and valuable technical and marketing insights to the project PIs to help guide the projects in progress.

- The portfolio management tool, Chemical and Allied Processes Portfolio Management Tool (CPMT) was implemented. This tool illustrated the relative ranking of all of the projects in each focus area, for a number of useful metrics. This helped highlight those projects that required special attention.

- Comments were received from the reviewers regarding the forthcoming change from Focus Areas to Technology Platforms, and chemical industry issues that require addressing in the future.

- The reviewers made recommendations on improvements to the review process.

In response to the valuable feedback provided by reviewers, the ITP Chemicals subprogram will:

- maintain its current overall portfolio strategy, designed to accelerate R & D in high-risk, high-reward energy-saving technologies for chemicals manufacturing.

- continue its current portfolio organization with sub-focus areas in Micro Reactors, Oxidation Reactions, Distillation & Hybrids, and Alternative Processes.

- provide feedback to each project team based on reviewer comments intended to improve project performance.

- continue its current practice of carefully monitoring projects to ensure that teams are meeting their stated goals. ITP staff will give particular attention to those items of concern highlighted by the review team. For projects that are not performing adequately, ITP will provide feedback and suggestions for improvement. If the project team fails to display progress in the future, funding will be redirected to other high priority activities.

- investigate new potential projects in both alternative feedstocks and in inorganic chemicals with high potentials for market growth.

Appendix

Appendix A: Reviewer Backgrounds

Table A 1: Reviewer Groups and Expertise Organized by Focus Areas

Reviewer	Expertise
Reactions Focus Area	
Don Johnson	Carbohydrate Chemistry, Biotechnology, Polymers, Adhesives and Surface Active Materials
Jim Stevens	Catalyst and Reaction Engineering, Multi-phase Reactor Systems, Mixing, Batch Reactors and Bio-reactor Design
Francis Via	Catalysts, Separations, Petrochemicals, Process Development and Advanced Materials
Separations and Enabling Technologies Focus Areas	
Doug Bouck	Refinery Separations Processes
Ron Chance	Separations Technologies
Godwin Igwe	Filtration and Separation Process Techniques, Extraction, Distillation, Fuel Cell Technology

Appendix B: Description of Review Process

The review process started with the selection of the reviewers and the development of the overall program to be followed. A questionnaire was developed and sent to each PI, to be filled out and returned to headquarters in advance of the meeting (See Appendix C). Also included in this mailing was a list of other documents to be submitted in advance by each PI, and instructions for two presentations to be made by each PI at the review; one a public (Open) presentation, at which AIChE meeting attendees were allowed to attend, and a second private, confidential (Closed) presentation, to be made to the reviewers. Included in the package were instructions to the PIs to utilize the improved CPAT (Capital Projects Assessment Tool) software to estimate the economic benefits and projected energy savings for their projects. A Reviewer Questionnaire was sent to each reviewer (see Appendix D for Reviewer Evaluation Guide), along with the package of documents submitted by each PI for those projects (including the CPAT results) to be reviewed by the particular reviewer, and the Reviewers were required to submit their first draft responses to the questionnaire to headquarters the week before the meeting.

The five-day review started on Sunday evening, April 21, with a meeting of the reviewers, Chemical subprogram staff members and support contractors. A DOE presentation described the organizational and focus area changes taking place at DOE, and a second presentation discussed the schedule and expectations for the review itself. A quick description of CPAT and CPMT (Chemical and Allied Processes Portfolio Management Tool) was given to the reviewers, as these tools are fundamental to the analysis of the portfolio.

Open sessions (integrated with AIChE meeting sessions) started on Monday morning, April 22 and continued through Wednesday, April 24, with each reviewer attending those in his respective Focus Area. Closed sessions began Monday afternoon and were finished on Thursday morning, April 25. In these sessions, a fixed period of time was given to each PI for a presentation, followed by questioning by reviewers. A second time period was set aside for the reviewers to discuss their opinions of each project, and to allow them to modify and complete their questionnaires for the project just reviewed.

A “poster session” was organized for Tuesday evening, to allow the public another chance to see the presentations and talk with the PIs, and to give the reviewers a chance to see those projects in the other Focus Area.

On Thursday afternoon, April 25, a joint meeting was held with all reviewers present, with the Reaction Focus Area reviewers presenting their conclusions on the projects to the others, and then the Separations Focus Areas reviewers presenting their conclusions.

On Friday morning, April 26, a first presentation was made for background, covering the Chemicals Bandwidth Project results and including a discussion of the changing Focus Areas of the ITP, and the new approach that will be integrating the various Industry-related Focus Areas into four new technology platforms. It was reiterated that current on-going projects would be completed as planned, but that new solicitations would be based on the new structure.

For the rest of Friday morning, a facilitated discussion took place among the reviewers, contractors and staff on:

- the reviewers' evaluation of the results developed with the CPMT tool
- the reviewers' opinions regarding the major concerns of the chemical industry and the likely changes relating to energy use and feedstocks, and their impacts on the current portfolio
- the reviewers' opinions on the existing portfolio; its gaps, the needs for the future
- the reviewers' views on the directions chemical-related projects might take under the restructured ITP
- the reviewers' opinions of the value and shortcomings of CPAT
- the reviewers' advice on possible improvements to the review process (lessons learned) for the next Chemicals Portfolio Review.

Appendix C: PI Questionnaire

FY07 ITP CHEMICALS SUBPROGRAM PORTFOLIO REVIEW
Principal Investigator Questionnaire

Project Title:

Principal Investigator: Name, organization, address, phone, fax, email

Project Partners: Name, organization, and form of contribution (in-cash or in-kind).

Project Description: Please provide a brief summary of your project, including the problem it addresses, the project objectives, and a short description of how your project is unique from other ongoing work in your field

The questions below are intended to help DOE and the Chemicals Review Team gain insight into developments in your project since your project initiation. In addition to this questionnaire, the Peer Review Team will read your DOE solicitation response that lead to this award. Therefore, you do not need to repeat information already submitted to DOE as part of the solicitation response, but rather expand upon it based on the work you have completed to date. If you have already had a review of your project, address how you have implemented any review suggestions into you project work, or if you have not, why.

YOUR ANSWERS TO QUESTIONS 1-10 SHOULD NOT EXCEED 8 PAGES.

1. **Project Schedule:**
   a. Initiation date
   b. Original expected completion date
   c. Describe and explain any variances from original anticipated schedule and whether these will impact completion date. Or, if your project has already been completed, state the completion date.
2. **Project Objectives:** Have there been any changes in project objectives and scope? If so, please explain.
3. **Technical Approach:** Describe the technical concept and how this project is addressing the problem, including technical performance goals and the applicability across the industry Please highlight any modifications in your approach since your project start date.
4. **Technical Barriers:** Describe technical barriers (including technical hurdles, performance requirements for economic competitiveness, theoretical limits, regulatory requirements for commercialization/implementation, etc.) and how they are being addressed. Discuss new barriers that may have arisen as part of work since your project initiation.
5. **Technical Work Plan:** Please discuss any changes in your work plan, including schedules, contributions of each participating organization, experimental design, techniques used, approach to data analysis, key equipment and facilities, etc.

6. **Project Output and Status of Milestones:** Discuss progress in achieving each technical milestone as scheduled in the proposal plan. Attach your original schedule of milestones and discuss any variances from the original plan and how they are being addressed. How do your technical achievements support the project's technical goals as outlined in your proposal? Have these goals been met on the original project schedule? If not, why and what is the implication for the remaining project schedule? Discuss how the results support the commercialization plan, or if not, what is being proposed to overcome the problems? Also provide a bibliography of publications emanating from this project.

7. **Commercialization Plans:** Please discuss your progress towards commercialization, including intellectual property agreements or formal commercialization agreements. To what extent are potential end-users committed to this project? Also describe any new developments that may influence your commercialization plan, such as competing technologies, regulations, market changes, changes in team partners who were key in commercialization plans, or changes in your economic evaluation. When do you estimate the first commercialization is likely to occur?

8. **Efficiency Improvement Merits:** Describe your original proposal's estimates and revised estimates for improving energy efficiency, reducing emissions, enhancing productivity, reducing costs, and/or reducing materials usage. Use the web-based energy assessment tool (CPAT) provided by DOE ITP for energy efficiency estimates (https://cpat.chemicals.govtools.us/CPAT/login.asp).

   Note: Some projects may not conform to the CPAT model. If you have this difficulty, or if you have any other questions about using CPAT, please contact Ilona Johnson at ijohnson@bcs-hq.com or 410-997-7778 x236. Additionally, DOE will soon be beta testing a new desktop version of CPAT. The principal investigators for all R&D projects funded by the Chemicals Subprogram will be asked to enter data into the CPAT desktop version at a later point in time. We suggest that as you use the web-based version of CPAT for the Chemicals Review, you keep a record of your data, as it will make it easier for you to use the new version in the future. You will receive more information about this later on.

9. **Environment, Health and Safety Issues:**

   a. Describe the environmental impact of your project (beyond emissions reduction from energy savings).

   b. How will your project impact industrial water use?

   c. What are the health and safety concerns associated with your project (aside from combustion-related emissions), and how do they relate to applicable rules and regulations?

10. **Budget**

   a. Complete the following budget tables showing the original planned (approved) spending for the project and also the actual spending for the project by project year. You may match your budget periods to calendar quarters to match your submitted quarterly reports. Please describe the reasons for variances between planned and actual spending (e.g., changes in project staffing; equipment procurement delays; DOE funding delays; etc). How has the project plan been modified to address these variances?

			Planned (Approved) Spending				
Budget Period			**DOE Amount**[a]	**Cost Share 1**[b]	**Cost Share 2**[b]	**Cost Share 3**[b]	**TOTAL**
	From	To					
Year 1	xx/xx/xxxx	xx/xx/xxxx					
Year 2							
Year 3							
Year 4							

a Provide any comments on DOE funding here.
b. Provide the name of cost share provider (organization) and nature of cost share (cash or in-kind – if both, please indicate split between cash and in-kind) here.

			Actual Spending				
Budget Period			**DOE Amount**[1]	**Cost Share 1**[2]	**Cost Share 2**[c]	**Cost Share 3**[d]	**TOTAL**
	From	To					
Year 1	X/X/XXXX	X/X/XXXX					
Year 2							
Year 3							
Year 4							

a Provide any comments on DOE funding here.
b Provide the name of cost share provider (organization) and nature of cost share (cash or in-kind – if both, please indicate split between cash and in-kind) here.

b. List the approximate level of effort in person-months by the PI and key personnel
c. Approximate level of effort by consultants and sub awardees
d. Major materials and significant permanent equipment leased or purchased

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Principal Project Personnel: (note that your responses below are in addition to the 8 page maximum set for previous questions).

If there have been any changes in project personal, including the principal investigator, please provide the following information for <u>each new participant</u>:

a. Role in the project.
b. Principal areas of research and expertise.
c. An indication of the percentage of time, or annual hours, each devotes to the project.
d. Education.

e. Relevant professional employment history, including a list of the institutions, dates employed, and positions held.
f. Relevant professional activities and honors.
g. Relevant publications not emanating from this project. (Do not include extensive lists of publications of little relevance to the project being evaluated.)

Appendix D: Reviewer Questionnaire

Reviewer Evaluation Guide

Evaluation Questions

The questions below will guide you in completing the Reviewer Evaluation Form contained on your CD. Your responses will help DOE evaluate how well its Chemicals Subprogram portfolio meets its objectives of funding high risk, high value projects. You will also help gauge the success of projects since their start date. Use the descriptions to guide your interpretation of the meaning of each number/anchor point. When rating each question, try to be objective and select the score for which the words most closely fit your personal assessment of the project.

I. Project Overview

A. Project Phase
In your opinion, which phase best describes the project?

Selections are:

1. Discovery Research	Organized scientific investigation to solve problems by creating new knowledge; fundamental, theoretical or experimental investigation to advance scientific knowledge, the immediate practical application of which is not a direct objective.
2. Applied Research	Early phase of development that is very exploratory and unproven; research directed toward using knowledge gained by basic research to make things or to create situations that will serve a practical or utilitarian purpose. The technology being developed has the potential to create significant change and innovation for the industry but carries high risk. Includes proof-of-concept work.
3. Technology Development	Bench scale technology development.
4. Pilot Plant	Latter phases of development of a promising technology, possibly involving scale-up to pilot level; or adaptation of a technology that may be practiced in other industries but not fully developed for the target industry.
5. Demonstration	Significant scale-up and demonstration of the technology, usually in an operating environment at a commercial site. May involve a part or full-scale installation at a manufacturing site and subsequent full-scale commercial applications.

Chemical Chain

Which chemical chain(s) would this project fall under?

Please select all that apply.

Ethylene
Propylene
BTX
Agricultural Chemicals
Chlor-Alkali
Butadiene
Methane
Oxygenates

Other ____________________________________

C. Product/Process Development

ITP is charged with the responsibility of encouraging the development of energy efficient process technologies. Rather than funding research for end products that only benefit a single company, the Chemicals Subprogram is interested in funding R&D of ***process technologies*** *with applicability to multiple manufacturers. It promotes R& D related to reaction kinetics, separations techniques, and other opportunities that will result in improved or alternative manufacturing processes.*

Given the research target and commercialization plan of the project in question, do you think that this project meets the program goals for focusing on ***process*** *technologies with broad industry applicability? If not, why?*

II. CPAT Assumptions

Your reviewer package includes summary reports from the Chemicals Project Assessment Tool (CPAT). CPAT was developed to enhance DOE's ability to evaluate the national energy savings potential of its collaborative research projects. CPAT's estimates are based on the potential for commercial deployment, stemming from the magnitude of economic incentive calculated from operating cost savings and capital requirements over extant or current technology.

The CPAT software includes a large database of chemical products' production rates, manufacturing costs, projected market growth rates, and energy consumption. The principal investigators have entered estimates for how their new technology will influence capital costs, energy consumption, etc. In some cases, they may have also changed input data describing current technologies. These changes will be highlighted in orange on the CPAT Summary.

Please evaluate a) the assumptions made on the Chemicals Project Assessment Tool summary report (for both conventional and new technologies) and b) the output from the summary report. Suggest and justify alternative assumptions.

Please comment on the assumptions for:

Market Growth Rate
Capacity and Capital Requirements
Current and New Technology Energy Use (feedstock, fuel/steam, & electricity)

Please comment on whether you think the CPAT outputs in the following areas are reasonable:

Year of Technology Introduction
Market Penetration
Market Impacts

Energy Savings by Project's Technology (feedstock, fuel/steam, & electricity):

Waste Reduction
Non-combustion Air Pollutant Reduction

III. Energy Savings

A. Conservatism of Estimates

How conservative are the assumptions used by the PI in CPAT?

Selections are:

0.Extremely Aggressive	The PI uses extremely aggressive assumptions in the Project Evaluation Tool. The date of commercialization and/or degree of 2020 market impact is unreasonable.
1.Aggressive	The PI uses aggressive assumptions in the Project Evaluation Tool. The date of commercialization is likely to slip significantly and the degree of 2020 market impact is likely to be much less than the scenario proposed by the PI.
2.Reasonable	The PI uses reasonable assumptions in the Project Evaluation Tool. The date of commercialization or the degree of 2020 market impact is likely to slip modestly from the scenario proposed by the PI.
3.Conservative	The PI uses conservative assumptions in the Project Evaluation Tool. The date of commercialization and the degree of market impact in 2020 is likely to be met.
4.Extremely Conservative	The PI uses extremely conservative assumptions in the Project Evaluation Tool. The technology would likely to be commercialized faster or have greater

2020 market impact than the scenario proposed by the PI.

B. Cross Industry Leveragability

How many other industries will have interest in this technology once it has been proven? Please choose from aluminum, forest products, food, agriculture, glass, metal casting, mining, petroleum refining, and steel. List applicable industries in the "Comments" Section of the Reviewer Evaluation Form.

Selections are:

0.One Industry Only	This technology is applicable only to one industry.
1.One Industry; No Stated Interest	This technology should be applicable to 1 other industry. However, there has been no stated interest by this other industry
2.One Industry; With Stated Interest	This technology should be applicable to 1 other industry and there has been stated interest by this industry.
3.Two Industries; With Stated Interest	This technology should be applicable to 2 other industries with stated interest.
4.Three Industries; With Stated Interest	This technology should be applicable to 3 or more other industries with stated interest.

IV. Innovation

A. Innovation Level

How innovative is this project/ product to the world? To what extent does it change industry structure?

Selections are:

0.None	No innovation or equal to current technologies.
1.Incremental	Improves existing product or process. Typically a result of continuous improvement efforts or competitive activity.
2.Substantial	Significantly improves product or process. May change the basis of competition between the company and its national competitors.
3.Transformational	Creates new markets, businesses or fundamentally changes industry structure.

V. Programmatic Merit

A. Health and Safety

To what degree are there significant health and safety issues (including damage to public health resulting from a terrorist attack) associated with the proposed technology (aside from combustion-related emissions)? Have potentially applicable rules and regulations been adequately considered? (Refer to question 9c in the PI Questionnaire.)

Selections are:

0.Significant Issues Not Considered	The project's technology has significant health and safety issues. The project team has not considered these issues and has not addressed the applicable rules and regulations.
1.Significant Issues Considered Not Addressed	The project's technology has significant health and safety issues. The project team has considered these issues but has not addressed the applicable rules and regulations.
2.Minimal Issues Not Considered	The project's technology has minimal health and safety issues. The project team has not considered these issues and therefore has not addressed the applicable rules and regulations.
3.Minimal Issues Considered, Not Addressed	The project's technology has minimal health and safety issues. The project team has considered these issues but has not addressed the applicable rules and regulations.
4.Significant Issues Considered and Addressed	The project's technology has significant health and safety issues and the project team has considered theses issues and has addressed the applicable rules and regulations.
5.Insignificant or Minimal Issues Considered and Addressed	The project's technology has insignificant or minimal health and safety issues. For technologies with minimal issues, the project team has considered the issues and has addressed the applicable rules and regulations.

VI. Risk Variables

A. Technical Challenge

Assuming concepts are based on sound scientific principles, how challenging is the conceptual plan for this project? In other words, what level of technical risk is apparent in the proposed project?

Selections are:

0.None	There is no scientific challenge left in the work of the project; all technical hurdles have already been overcome. Only industrial scale demonstration must be completed to fully prove the project.

1.Very Low	Data have already shown that the proposed approach has a high probability of technical success.
2.Low	There is a reasonable amount of data showing that the proposed approach has the potential for success. However, the process needs to be scaled-up to obtain initial design data and evaluate parameters.
3.Moderate	A small amount of data has been obtained showing that the proposed approach has the potential for success. However, the ability to reproduce the results and optimize variables still needs to be shown.
4.High	Proof of concept has occurred, but more experimentation is required to provide data to ***validate*** proof of concept.
5.Very High	This project poses high technical risk with multiple scientific hurdles that must be overcome to prove the concept. There is currently no data available that can predict the potential success of the proposed approach.

B. Technical Experience

To what degree does the project team possess the technical expertise/strength required to achieve the project objectives? This should be profiled based upon the technical objectives and technical challenge of the project.

Selections are:

0.None	This is a new scientific knowledge area requiring substantial development of new principles. There is no known source for this expertise.
1.Weak	Knowledge would have to be acquired. – The project team does not possess the expertise required to meet the technical objectives of the project. While some knowledge can be acquired from outside sources, important expertise would still have to be developed.
2.Challenged	There will be a significant learning curve. – This is not a technical strength for the project team or any outside sources, but some know-how exists.
3.Moderate	Learning curve will be moderate. - Good technical expertise within outside resources available to the project team, but not within the project team.
4.Strong	Learning curve will be small. - Good level of expertise resident within the project team.
5.Dominant	Learning curve minor to none. - Very high level of project team-resident technical expertise.

C. **Project Management Expertise**
To what degree is the project plan (budget, milestones, timing, etc.) appropriate to delivering the project objectives and to what extent does the project team possess the project management expertise to deliver the project objectives?

Selections are:

0.Poor Plan	The project plan (budget, milestones, timing, etc.) is not realistic for delivering the project objectives.
1.Poor Project Team	Regardless of the appropriateness of the project plan, the project team is incapable of executing it.
2.Plan and Team Marginal	The project plan is marginal for delivering the objectives and the team's project management capabilities are also marginal.
3. Plan Marginal, Team Good	The project plan is marginal for delivering the objectives but the team's project management capabilities are good so there is a reasonable expectation the team will overcome the inadequacies of the plan.
4. Plan Good, Team Marginal	The project plan is a good one for delivering the objectives but the team's project management capabilities are marginal.
5.Plan Good, Team Good	The project plan is a good one for delivering the objectives and the team's project management capabilities are good.

D. **Technical Progress**
Are the technology performance goals adequately being pursued and technical milestones being met? Has the team achieved its technical milestones, and has it done so according to schedule? (Refer to question 6 in the PI Questionnaire).

Selections are:

0.No Credible Plan	Some milestones are not met, and there is no credible plan for remedying the deficiency.
1.Key Milestones Not Met	All milestones are addressed; most are met and documented. One or more key milestones are not met. A credible plan is in place to remedy the deficiency(ies), with clear action items for the project team and clear monitoring points for DOE.

2.Milestones Not Met	All key milestones are met and documented, but one or two milestones are not fully met and documented. A credible plan is in place to bring the project back onto schedule within 30 days.
3.Meet Requirements	All scheduled milestones are met technically, and documented. The results meet, but do not significantly exceed, requirements. A credible plan keeping the project on schedule is in place for the next reporting period.
4.Exceed Requirements	All scheduled milestones are fully met technically, and documented as required. Results more than meet requirements. A credible plan keeping the project on schedule is in place for the next reporting period.

E. Project Team Functionality

How well is the project team functioning as it relates to meeting its technical objectives as currently budgeted and scheduled?

Selections are:

0.Dysfunctional	This project team is dysfunctional. Planning is not realistic, and seams between the various contributions are evident weak spots where team members do not agree on the goal and/or approach. Execution also suffers – in part as a result of these planning deficiencies. Mileposts have not been met, and no credible plan is in place to remedy the deficiency.
1.Not Functioning Well	The project team is functioning, but not well. Input from all participants is not evident in planning, and the participants have not allocated resources as needed to meet their milestones. The project team has identified unforeseen problems, but has no credible plan in place to deal with them. Project team members seem committed to the goals of their parent firm, but not to the goals of this project. Changes will be needed if this team is to effectively meet its stated goals and planned mileposts.
2.Not Functioning Seamlessly	The project team is functioning, but not seamlessly. Input from all participants is evident in planning, and the participants have allocated resources as needed to meet most milestones. The project team has identified some unforeseen problems that they have not yet dealt with.

3.Functioning Well	The project team is functioning well. Input from all participants is evident in planning, and each party is carrying their load in execution. The project team has identified some unforeseen problems, and devised plans to deal with them within the schedule.
4.Functioning Exceptionally	The project team function is exceptional. Input from all participants is evident in the planning, and each party is carrying their load in execution. Moreover, the project team has dealt effectively with unforeseen problems, with minimal disruption of schedule.

F. External Uncertainty

To what degree will competing technologies, patents, and other external factors (e.g., policy, regulations, social, competitive, market, economic, etc.) affect this project's ability to meet its objectives?

Selections are:

0.Very High	Major issues are present of which the project team is unaware.
1.High	Known issues are present over which there is no control by the project team. These issues may include other competing technologies being developed that will definitely be of greater commercial value.
2.Moderate	Known issues are present over which there is a limited amount of control by the project team. Other competing technologies may be being developed that appear to be of equal or greater commercial value.
3.Low	Known issues over which there is a high level of control by the project team. Actions have not as of yet been taken to address these issues.
4.Very Low	Known issues over which there is a high level of control by the project team. If other competing technologies are being developed, they appear to be of lesser commercial value. Actions have already been undertaken to address the issues and the prognosis is very favorable.
5.None	Straight forward situation in which no issues exist. There are no competing technologies being developed.

G. Probability of Commercial Success

What is the likelihood that the project will yield a commercial success? Factors influencing commercialization include technical feasibility, business conditions, and commercial expertise of the project team. Estimate the overall probability of commercial success (POS).

Selections are:

0.Commercial POS < 30%	Commercial success is not likely. Potential reasons include: - The business climate and/or forecasts make it unlikely that this project will be able to attract a timely commitment from key end users. - The team has little to no commercial expertise, - There is currently no commercialization partner.
1.Commercial POS > 30%	Commercial success is in jeopardy. Potential reasons include: - Technical feasibility is questionable. - Business conditions or forecasts do not appear realistic. - The project team does not appear to have a high level of commercial expertise. - Major revisions to the project scope and/or commercialization plan are needed if success is to be achieved.
2.Commercial POS >50%	Commercial success appears likely. - Technical feasibility is reasonable, but revisions to the project scope and/or schedule are needed to keep the commercialization plan realistic. Or, - The project team may not have a high level of internal commercial expertise, but good expertise is available from outside resources.
3.Commercial POS >80%	Commercial success is probable. Reasons may include: - Technical feasibility is good. - Business conditions are favorable for widespread implementation. - The project team has a high level of commercial expertise.
4.Commercial POS >90%	Commercial success is highly probable. - Technical feasibility is high.

- Business conditions are excellent for widespread implementation.
- The project team has a very high level of commercial expertise.

VII. US Industry Interest

A. End User Need and Commitment

***To what extent are potential end-users committed to this project? Will they be involved in developing the detailed plans for the demonstration phase? Will they be involved in the demonstration phase as now envisioned*?**

Selections are:

0.No End User; No Plan — No potential end-user is a participant in this project, and no credible plan to attract an end-user is in place.

1.No End User; Plan in Place — No potential end-user is a participant in this project. The project plan recognizes the need to attract an interested end-user before demonstration phase planning begins, and includes this as a key milepost. (Rating should never apply to any but startup projects.)

2.One End User Committed through Demonstration — At least one potential-end user is a participant in this project, and committed to being involved through planning and execution of the demonstration phase.

3.One End User Committed through Commercialization — A potential end-user is a participant in this project, and has committed to involvement in all phases of the project – including commercialization if the project goals are met.

4.Multiple End Users Committed through Commercialization — Potential end-users are participants in this project, and are committed to involvement in all phases of the project – including commercialization if the project goals are met.

B. Corporate Economic Attractiveness

How economically attractive will this project be to a corporation facing the decision concerning implementing the technology?

Selections are:

0.Not Attractive	This technology does not have economics that will make it attractive for a company to implement it unless required by regulations.
1.Marginally Attractive	This technology offers marginal attractiveness. It will be attractive only to companies with specific circumstances.
2.Attractive	This technology has attractive economics that will make it a better choice than existent alternatives.
3.Significantly Attractive	This technology's economics are extremely attractive and will drive accelerated penetration.

VIII. Environment

A. Environmental Benefits

How significant are the environmental benefits of project's technology beyond the benefits of emission reduction from reduced energy use? (Please refer to the CPAT summary report and questions 8 and 9a in the Principal Investigator Questionnaire.)

Selections are:

0.Increased Pollutants	The proposed technology increases the level of environmental pollutants.
1.No Direct or Indirect Benefits	There are no direct or indirect environmental benefits from the proposed technology.
2.Modest Benefits	The environmental benefits are modest and would allow current facilities to meet environmental requirements without the addition of other pollution control equipment.
3.Significant Benefits	The environmental benefits are significant and would partially offset existing technologies for pollution control equipment.
4.Substantial Benefits	The environmental benefits are substantial and the proposed technology could be used in place of existing pollution control equipment (market transformational).

B. Water Use Impact

By how much will full implementation of this technology impact industrial water use? The project principal investigator should have answered this in question 9b of the PI Questionnaire. Please refer to his/her answer regarding industrial water use, and modify as necessary based on your expert opinion.

Selections are:

0.Increase Use	The proposed technology increases water use.

1.No Change	The proposed technology does not change the amount of water use.
2.<1% Decrease	The proposed technology reduces the amount of water used by all industry by < 1%.
3.<2% Decrease	The proposed technology reduces the amount of water used by all industry by < 2%.
4.<3% Decrease	The proposed technology reduces the amount of water used by all industry by < 3%.
5.>3% Decrease	The proposed technology reduces the amount of water used by all industry by >3%.

IX. Societal Impacts

A. US Competitive Advantage

Is it likely that the technology will be utilized in the US instead of abroad? To what extent will US industry gain competitive advantage in the global economy by using this technology?

Selections are:

0.Less Competitive	U.S. firms may actually become less competitive from use of this technology. U.S. organizations are not the major developers of the technology and U.S. firms will not be the primary targets for deployment.
1.Insignificant Change	U.S. firms will experience insignificant competitive advantage gain through the use of this technology, due to the fact that the technology is deployed worldwide.
2. Some Competitive Gain	U.S. firms will gain some competitive advantage by development of this technology within the U.S.. The US has a large market for the technology.
3.Significant Competitive Gain	U.S. firms will gain significant competitive advantage by the development and primary deployment of this technology within the U.S.

B. Effect on US Jobs

To what extent will this technology affect the number of jobs in the US?

Selections are:

0.	Jobs Exported Implementation of this technology will cause US jobs to be exported to other countries.
1. Fewer Jobs	Implementation of this technology will cause a reduction in US jobs, but will not result in exporting jobs.

2. No Affect Implementation of this technology will not affect the number of US jobs.

3. Gain Implementation of this technology will increase the number of US jobs.

X. Overall Project Assessment

A. What is your overall assessment of this project? Do you think that the team's current scope and plan are on target? Please provide a list of positive and negative project attributes as well as details and explanations of your assessments.

B. What are the key improvement actions that you recommend to the project team and how would you prioritize these actions? Make sure to address each Merit area: Programmatic Merit, Technical Merit, and Commercialization Merit. Include priorities for each of your recommendations and explain the impacts these actions will have on the project's industrial success.

Appendix E: Description of CPAT

Introduction to CPAT (Commercialization Project Assessment Tool)

CPAT was developed to enhance DOE's ability to evaluate proposals that DOE has solicited and received for collaborative research projects aimed at developing energy-efficient processes. CPAT provides meaningful and objective projections of the energy-savings potential of the proposed projects. CPAT also provides realistic projections for commercial deployment for the new concepts based on the magnitude of the economic incentive to implement the new technology if it were to be successfully developed. Without such an economic justification, new technology cannot be expected to displace conventional technology and save energy.

CPAT has been most completely developed for the chemical industry, and contains information in its database on over seventy of the major products and processes utilized today by the U.S. chemical manufacturing sector. For each of those products and processes, information is provided on the current market size and growth rate, present day raw material and utilities consumption and prices, by-product production and prices, etc. In addition, the capacity of a typical conventional plant is contained in the database together with its estimated Inside Battery Limits (ISBL) capital cost and its feedstock and process energy consumption. The user is directed to input the same type of information for the new technology, so that an economic comparison may be made and the rate of market penetration (and resulting energy savings) predicted.

(CPAT is now being populated with a Forest Products industry database, so that similar developments of economics and energy consumptions can be computed for conventional Forest Products processes and proposed novel technologies, equipment, etc. Finally, CPAT will be further enhanced by adding similar databases for some of the other ITP industries, including Aluminum and Steel, and first examples of such are available for demonstration purposes.)

Appendix F: Description of CPMT

Introduction to CPMT (Chemical and Allied Processes Portfolio Management Tool)

CPMT is a proprietary portfolio management tool that has been adapted by the ITP DOE team for use in evaluating the appropriateness of new projects being proposed for funding, and in tracking the progress of ongoing projects. In the present case, the latter function is being applied

CPMT graphically portrays a group of projects indicating their relative positions for a number of useful metrics, to allow some judgment of the relative merit of each project. The placement of each project in each graph is based on a series of responses to the Reviewer's questionnaire, each question relating to one or more important metrics of project quality and performance. Several major metrics depend upon the Energy Saving projected for the year 2030 if a project is successful. That energy saving is computed by use of CPAT, as described above.

When projects are first selected for funding, the selection process focuses on five criteria: Energy Benefits, Environmental Benefits, Economic Benefits, Technical Merit, and a combination of the Project Management Plan, Commercialization Plan, Team Capabilities and Facilities. Each of these criteria are evaluated via a number of questions answered by numerical rankings, and they are combined, with the use of "weighting percentages" to the various CPMT variables. It is possible to plot any of the CPMT variables against any other, and there are some "roll-up" metrics which are weighted combinations of CPMT variables.

In a portfolio review of on-going projects, such as the current one, the same procedure is followed, but weighings may be different based on the stage of R&D of a particular project, and the time yet to go before completion. Appendix G below indicates the consensus responses of the Reviewers to the Reviewer's Questionnaire.

The three most-frequently used "roll-up" metrics are Value, Technical Risk and Non-technical Risk. Value consists of a combination of Energy Savings, Innovation Level, U.S. Industry Interests, Society, and Environmental Benefits, in reducing order of weightings. Technical Risk is based on Technical Understanding, and Non-technical Risk is based on a combination of Technical and Management Expertise, and to a lesser extent Business Risk and Project Plan.

There are other metrics are similarly defined as combinations of segments of the responses to each criteria.

The CPMT plots appear as colored circles of different diameters, placed on a square divided into four quadrants. The colors may indicate the Focus Areas when the entire portfolio is reviewed, or the stage of R&D for a given focus area. The size of the circle indicates the funding for the project. (See Appendix H below).

Appendix G: Reviewer Consensus Evaluation Forms

Appendix G is omitted to protect confidential information.

Appendix H: Supplemental Portfolio Analysis Utilizing CPMT

H.1: Energy Savings vs. Technical Risk

These are plots of the energy savings estimates (determined by CPAT and Review Team) vs. Technical Risk. The technical risk scorecard is based on reviewer scores for “Innovation Level” and “Technical Challenge,” and adjusted according to the project phase.

Figures H 1 and H 2 just following represent the Reactions Focus Area projects. Two plots are utilized because one project is substantially higher than any of the others in terms of Energy Savings projected via CPAT. In Figure H.1, all of the Reactions projects are included, and most of the projects are clustered together at the bottom of the figure. In Figure H.2, the highest Energy Saving project is omitted, giving a more useful graph.

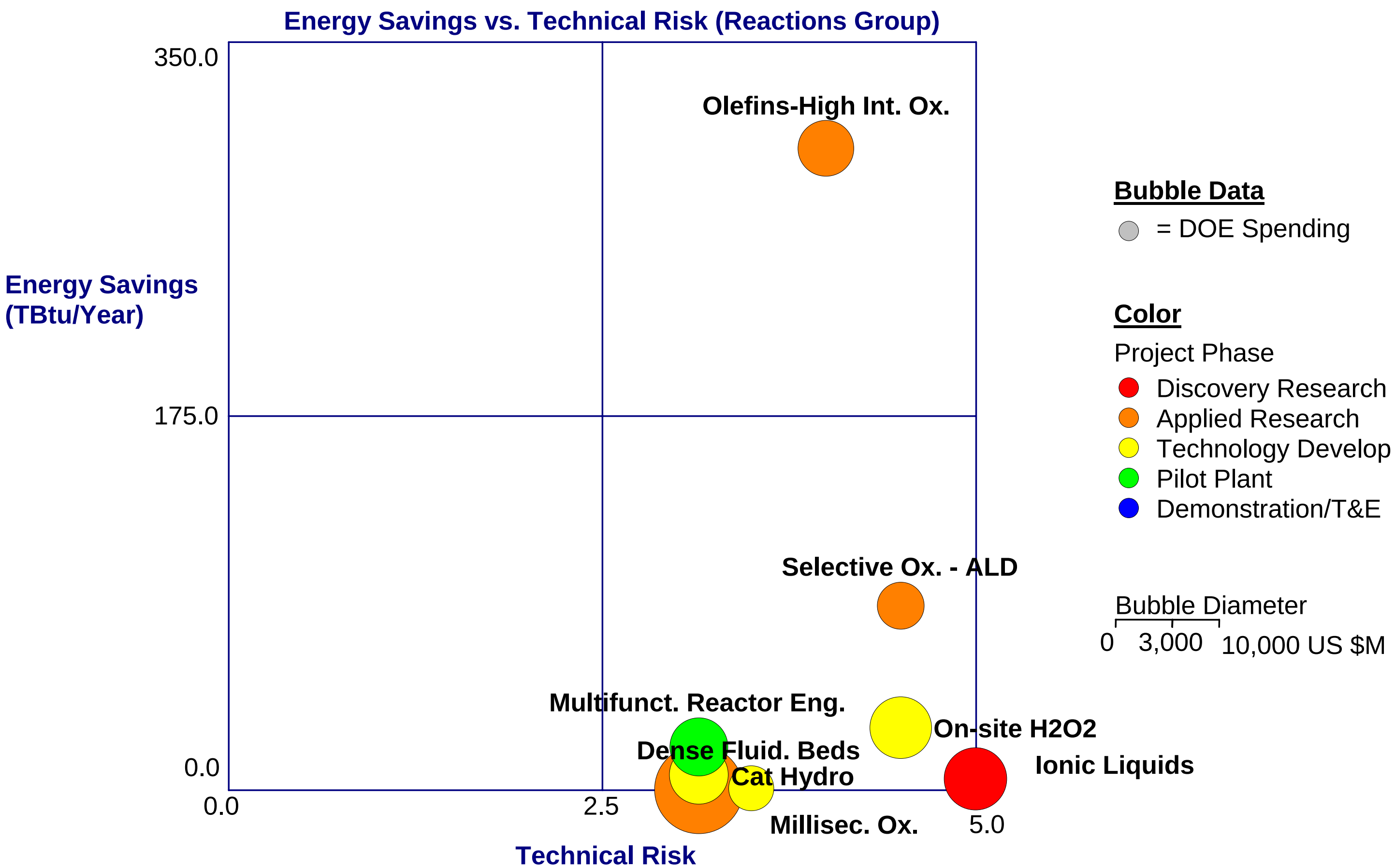

Figure H 1: Reactions Focus Area Projects, Energy Savings vs. Technical Risk -- all Projects

In Figure H 1 above, the two highest energy-savings projects are those promising high selectivities for the oxydehydrogation of ethane to ethylene, so that the endothermic cracking reaction is replaced by an exothermic (or at least neutral) reaction, saving the energy required to fire the cracking furnaces. In addition, those by-products produced are different from the hydrocarbon by-products formed in cracking and presumably can be more easily and less-energetically separated. Both projects are ranked high in Technical Risk, based on their high degree of innovation and technical challenge.

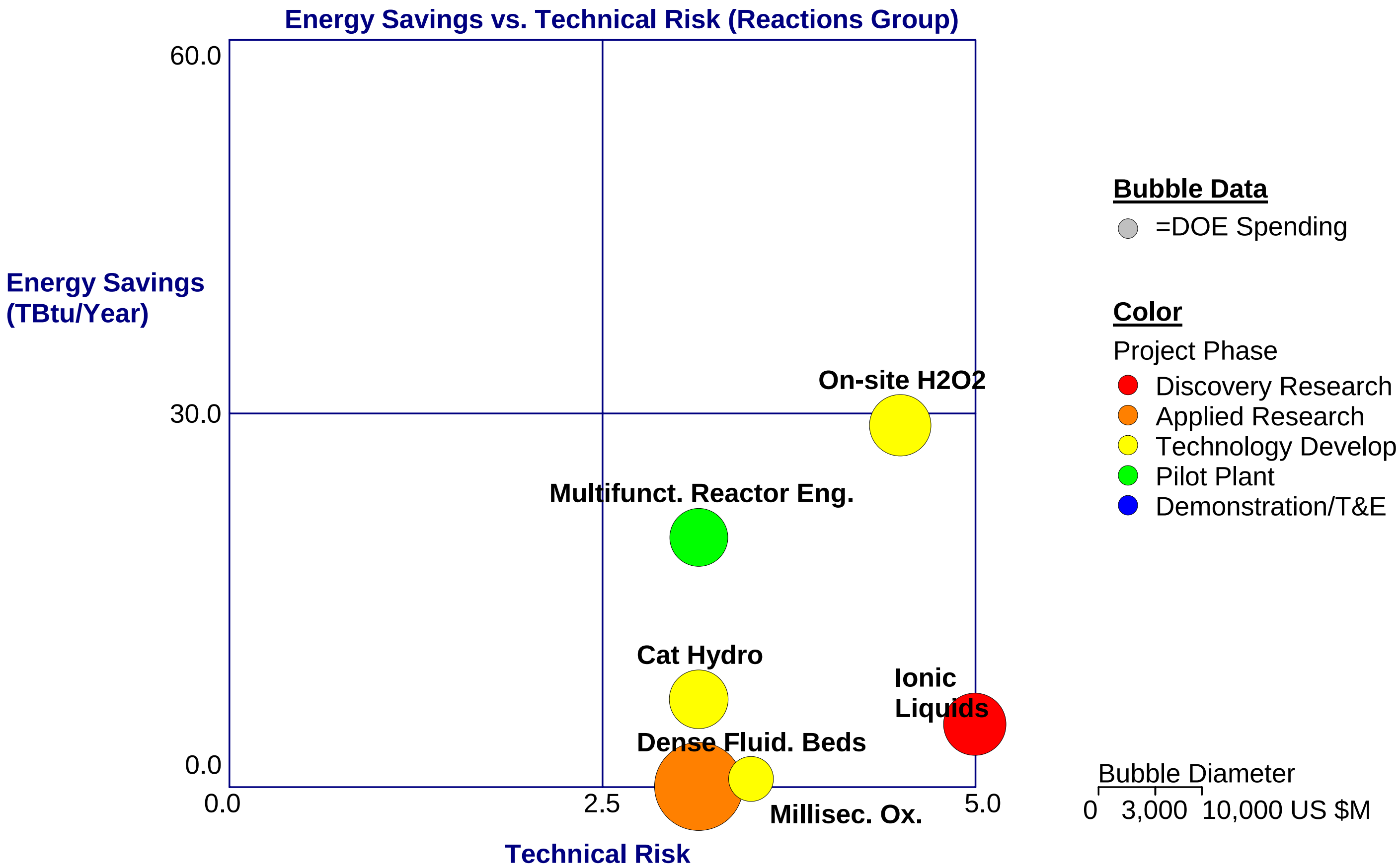

Figure H 2: Reactions Focus Area Projects, Energy Savings vs. Technical Risk (Cutoff at 60 TBtu/yr Energy Savings in 2030)

Figure H 2 above eliminates the two highest energy-saving projects, giving a more informative picture of the remaining Reaction Focus Area projects. It seems appropriate that the On-site H_2O_2 project and the Ionic Liquids project (firect, catalytic oxidation of methane to methanol) have the highest degrees of risk, again based on their innovation level and their technical challenges. It is disappointing that the latter project promises such a low level of energy savings. Interestingly, all of the projects fall into the right two quadrants indicating the higher range of technical risk. The two projects at the bottom call for some review. The Dense Fluid Bed project is a “model development” project, and the potential applications are several, but the promised energy savings are very modest. The Millisecond Oxidation project is the oxidative dehydrogenation of propylene to propane, for acrylic acid, and suffers from the fact that while substitution of propane for propylene may be economic (not a certainty at this time in the U.S.), it does not easily save energy.

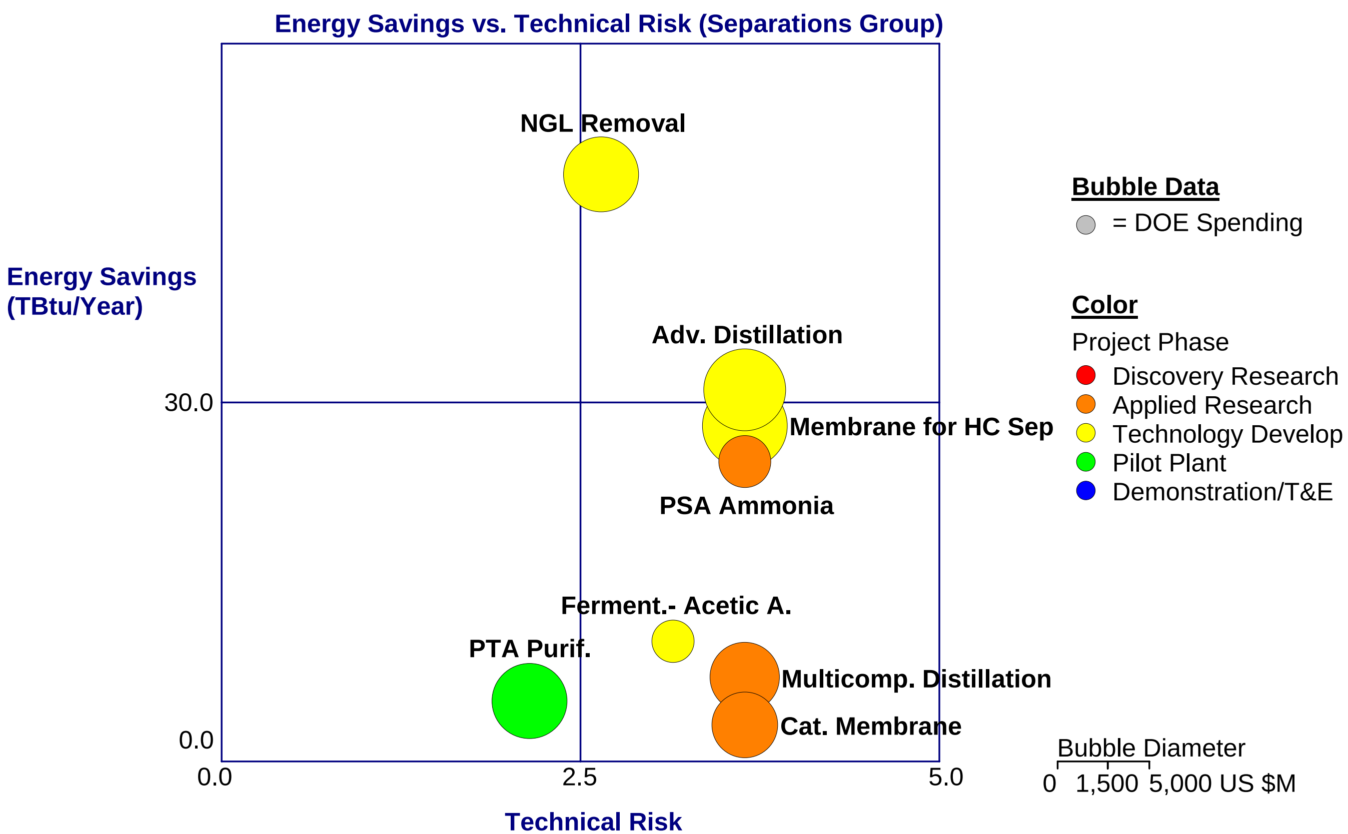

Figure H 3: Separations Focus Area Projects, Energy Savings vs. Technical Risk

Figure H 3 above contains all of the Separations Focus Area projects. It is interesting that the highest energy saving project is one of the lowest risks. That is an encouraging sign, although it make suggest that the project should have (or would have) gone ahead with out DOE support. The next three highest energy saving projects are also the highest risk, which seems an appropriate tradeoff. Likewise, the lowest risk PTA Purification project has a modest energy saving – the low risk is consistent with the late stage of development (pilot plant) of this project. The project that is possibly cause for the most concern is the Catalytic Membrane project, since the potential energy savings is relatively low. However, this project and the Multicomponent Distillation project are early-stage projects, when one would expect the highest risks. The acetic acid project appears to have a reasonable tradeoff between energy savings and technical risk.

H.2: Overall Value vs. Technical Risk

Figures H 4 and H 5 are similar charts for the Reaction and Separation Focus Area projects, respectively, but this time the "y-axis" is Overall Value rather than Energy Saving. The "Overall Value" scorecard is based on return on investment, cross-industry leveragability, end user need and commitment, corporate economic attractiveness, environmental benefits (beyond energy reduction), US competitive advantage, innovation level, and energy savings.

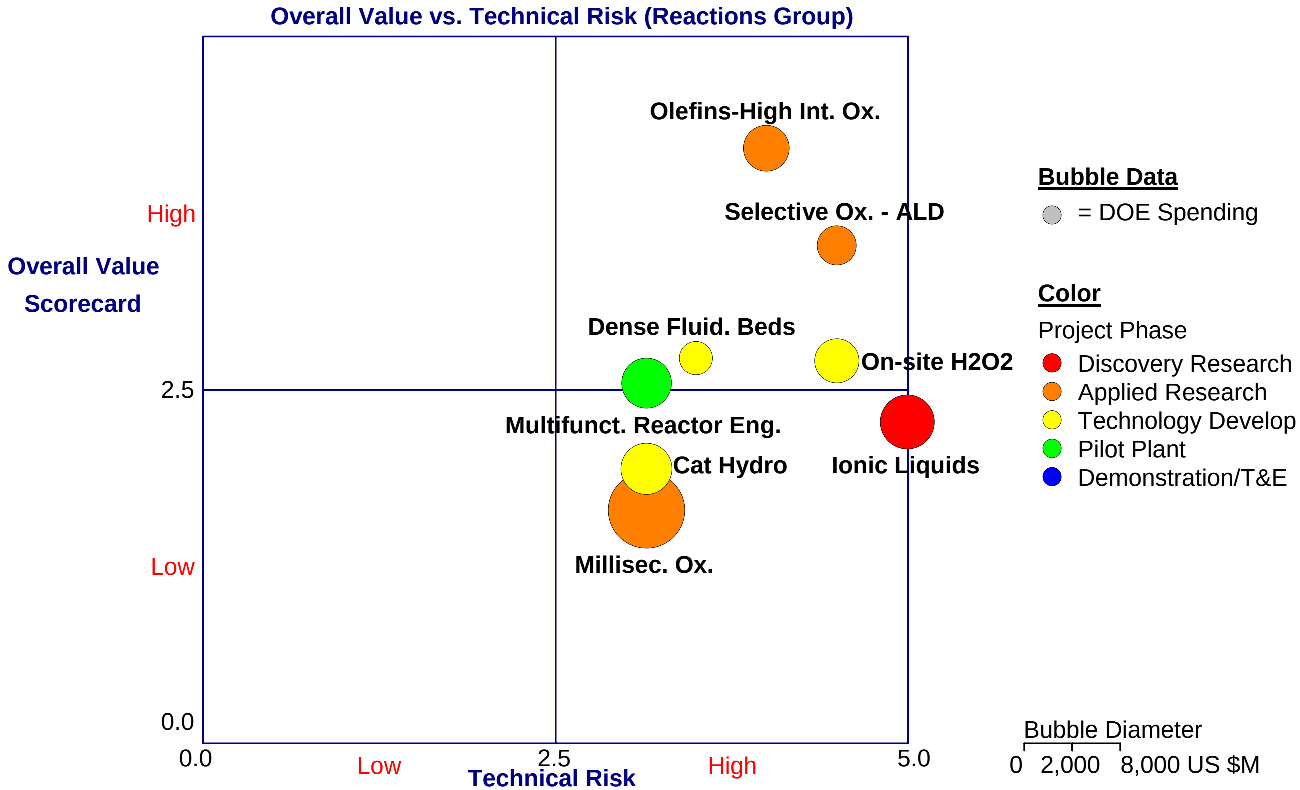

Figure H 4: Reactions Focus Area Projects, Overall Value vs. Technical Risk

It can be seen that utilizing the Overall Value scorecard, the impact of energy savings, while still important, is de-emphasized, bringing the projects closer together. The conclusions drawn in the discussion on Figures H 1 and H 2 still tend to apply.

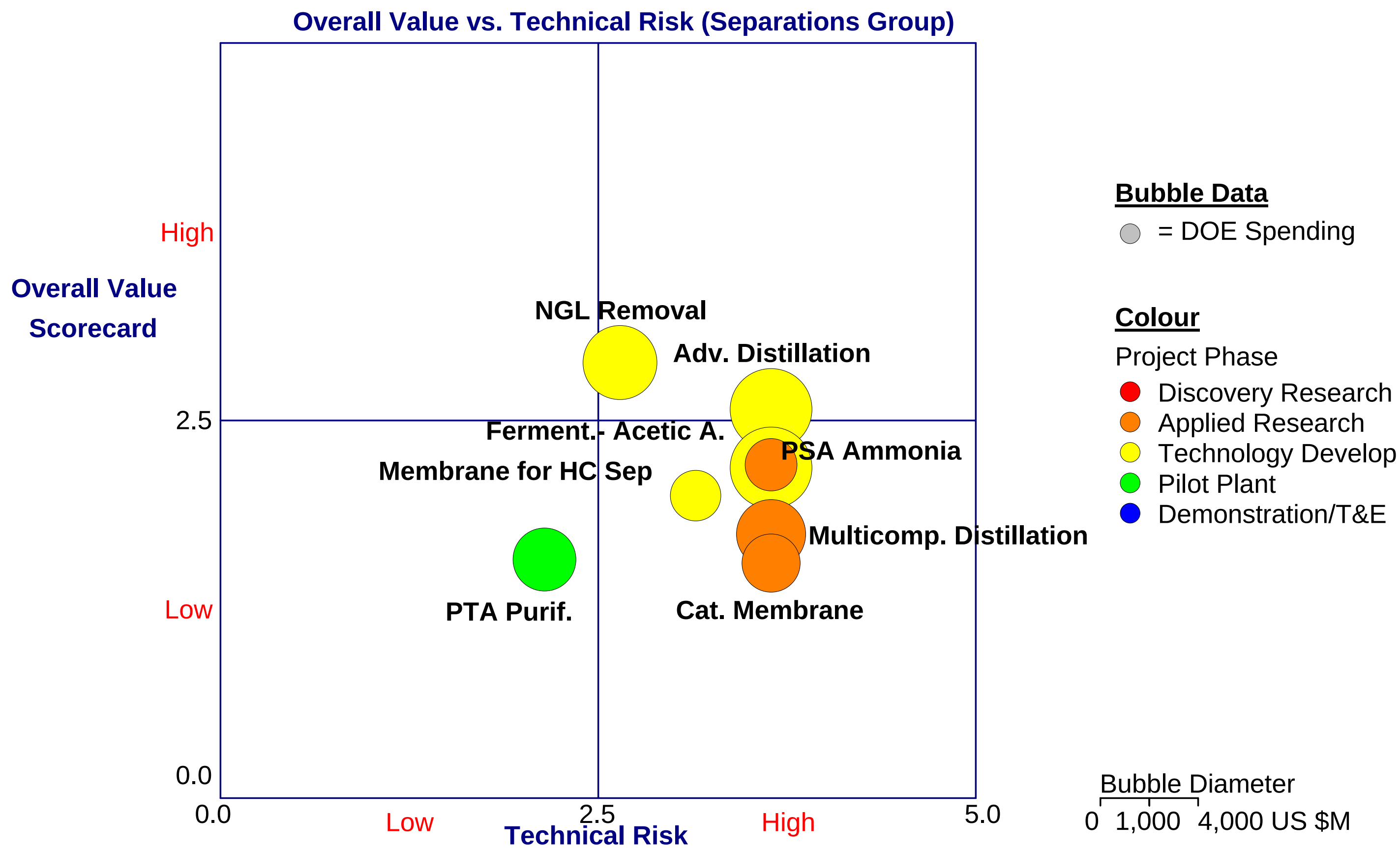

Figure H 5: Separations Focus Area Projects, Overall Value vs. Technical Risk

Likewise, the Overall Value scorecard de-emphasizes the Energy Savings for the Separations projects as well, but again, there is little difference in the conclusions from the discussion of Figure H 3. The bottom two projects, Multicomponent Distillation and Catalystic Membranes seem somewhat out of line in a negative direction compared to all of the others.

H.3: Overall Value vs. Non-Technical Risk

In Figures H 6 and H 7, the same Overall Values are plotted against Non-Technical Risk, for the Reactions and Separations Focus Area projects, respectively. The “Non-Technical Risk” scorecard is based on technical experience, project management expertise, technical progress, project team functionality, external uncertainty, and probability of commercial success. For Non-Technical Risks, four of the six metrics making up that risk can be improved: technical experience, project management expertise, technical progress, and project team functionality. These require attention and possibly action on the part of the DOE representatives following these projects. The last two metrics are to a large extent beyond anyone’s control; external uncertainty and probability of commercial success.

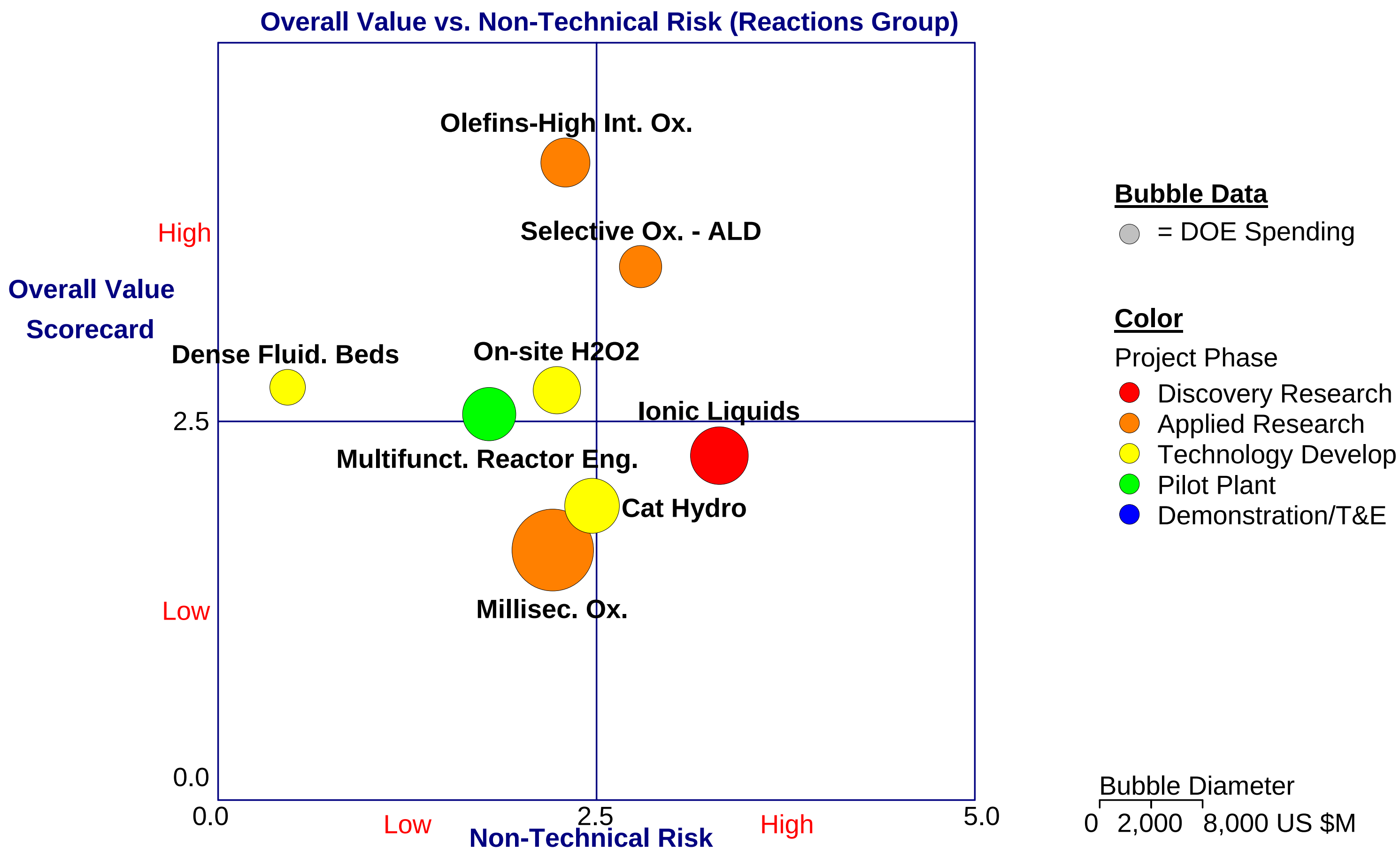

Figure H 6: Reactions Focus Area Projects, Overall Value vs. Non-Technical Risk

The only two projects in the Reactions Focus Area to fall into one of the High Non-Technical Risk quadrants are the project involving Ionic Liquids and the Selective Oxidation using ALD catalysts project. In the case of the former, the causative factor is the the lowest grade in terms of probability of commercial success, based on the difficulty of the task and the early stage of the work. For the latter project, the probability of commercial success was almost as low, and inaddition, the reviewers felt that there were threatening external activities that were not discussed/addressed by the PI.

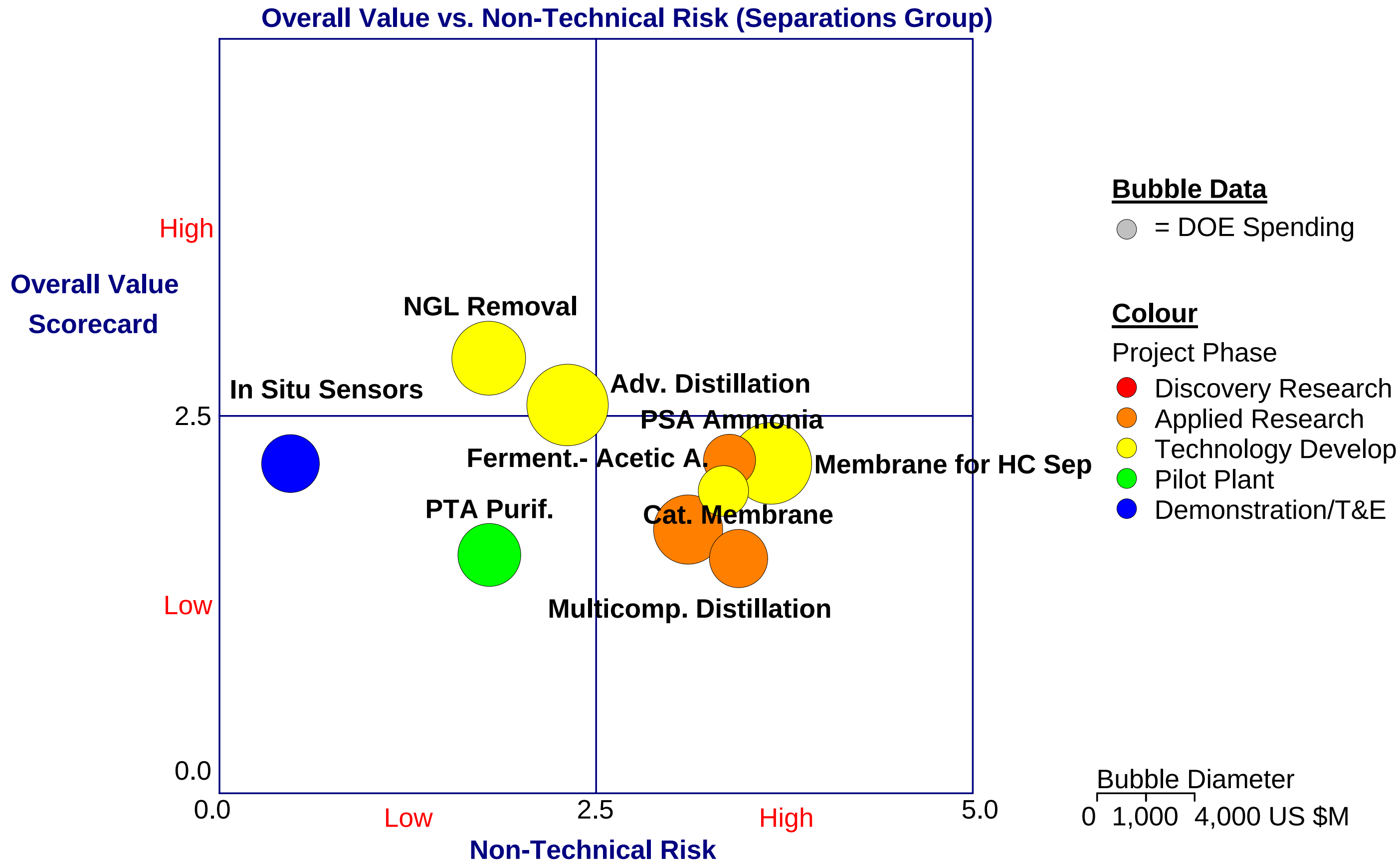

Figure H 7: Separations Focus Area Projects, Overall Value vs. Non-Technical Risk

Interestingly, in the case of the Separations Focus Area projects, five out of eight projects fell into the two High Non-Technical Risk quadrants. The worst score was the Membrane for Hydrocarbon Separations project, which was given the lowest chance of commercial success as well as poor ratings due to little progress and a non-functioning team.
The Multicomponent Distillation project had a lowest rank for chance of commercial success, due to the early stage of the project but also the lack of a commercialization concept. The PSA Ammonia project was ranked lowest in terms of chance of commercial success, but the reason was a concern about achieving technical success – viable high temperature adsorbents. Thus this project is rated unfairly low regarding Non-Technical Risks. The Fermentation Acetic Acid project was given the lowest chance of commercial success ranking also, based on the loss of the industrial partner, other changes in the project staffing, and the lack of information on economics, manufacturing

and scale up. The fifth project, Catalytic Membranes had just started, and was judged too early to give it any chance of commercial success, Here again, the reviewers might have been giving it a poor technical rather than non-technical risk ranking.

Appendix I: FY 2007 Portfolio Review Consensus Meeting Q&A

Table I 1: Portfolio Balance Questions and Answers

Question 1: Is the overall portfolio appropriately balanced and focused on the most fruitful avenues for achieving increased energy efficiency in the chemicals industry?
Well-balanced for the program size
Fully addresses the DOE industrial program objectives associated with energy savings and the more efficient use of feedstocks
Focused upon large energy consumers in the chemicals sub group
Diverse in scope
If commercialized, projects can enables significant energy savings
Consider funding more work in heat management/combustion efficiency.
Question 2: Is the range of projects in the Reactions Group appropriately balanced? Are there any key areas that should be further explored? Are there any areas that are overrepresented?
Well-balanced
Addresses priority developments
Significant energy intensive processes are addressed
Process intensification micro-channel process technology has to show scalability to the huge production areas before its promise can be accurately estimated.
Consider Silicon chemistry because of its impact on future markets and the relationship to potential fuel cell developments
With expanded budget additional areas can be considered.
Several programs are near commercial development stages.
Question 3: Is the range of projects in the Separations Group appropriately balanced? Are there any key areas that should be further explored? Are there any areas that are overrepresented?
All key areas are adequately represented and strategically explored
More areas could be addressed with an expanded budget
Membranes are well represented but also each aimed at a specific, very high energy use process
It is surprising that ionic liquid technology is not represented
There should be some studies on how micro-channel systems with very high numbers of reactor units can be monitored and controlled.
Good alignment with energy savings opportunities indicated in bandwidth study
Recommend more effort on sorption-based separations
Real time analysis that was explored by Dow project still has future potential.

Table I 2: Chemical Industry Issues and their Impact on the Portfolio

Question 1: What are the chemical industry's greatest concerns about energy?
Cost
Availability
Environmental Impacts, global warming
Movement off-shore due to global differential energy costs
Policy impacts
Balance of initiatives— The use of natural gas for power generation was driven by desire for cleaner energy. However, natural gas is very valuable to the chemical industry as a feedstock. Increasing costs are an issue.
Security—Need systematic approach to chemical industry operations for protection from terrorists. Movements to reduce on-site storage and use on-site, just-in-time, production.
Question 2: How do you foresee the chemical industry changing its energy consumption patterns over the coming decade? What efforts are required to reduce the chemical industry's energy consumption
Price certainty
Government policy to encourage conservation
Changes to adapt to alternative fuels and feedstocks—it will take government to help make this happen.
There are also options for the chemical industry to support ongoing efforts for alternative energy sources—ie supporting solar power production.
Question 3: What changes in feedstocks do you anticipate?
In the future, the chemicals industry may become more involved with inorganic-based chemicals rather than organic-based chemicals. Certain products are moving off-shore, while others cannot move off-shore because of transport, etc.
Question 4: What technical, economic, or competitive changes that have occurred during the past year will impact the portfolio? How will the portfolio be impacted?
Continued increase in energy costs will make the chemicals portfolio more valuable
Variability and lack of price stability is an issue. Are energy costs a long term problem?
Chemical companies being bought by investment companies will reduce the amount of research being initiated by industry.
Trend in industry has been to eliminate all research except near-term market research. There is a bigger need for long-term DOE research to address the gap.
New Democratic majority in Congress is increasing emphasis on CO_2 reduction.
Question 5: What parts of the portfolio would be of greatest interest to the chemicals industry?
Top-ranked projects (see report) would be of greatest interest.

Question 6: What are the gaps in the portfolio? What shifts would be of greatest interest to the chemicals industry?
More focus on lignin feedstocks for the industry
On-board reforming of methanol and ethanol as a carrier for hydrogen and fuel cell storage. Chemistry to look at making fuel cells better should be looked at from the chemical industry perspective
Consider switching to C1 chemistry for feedstocks
A large fraction of the portfolio is focused on microreactors, which is not likely to have a major impact on overall energy savings.
Question 7: What would strengthen the portfolio in the coming twelve months?
Obtain more funding to enable R & D to a larger number of projects
Manage limited resources by cutting funding for low performing projects early on.
Balance portfolio for near-term and long-term areas of research.
Consider gaining more academic input.

Table I 3: Technology Platform Questions and Answers

Question 1: Given ITP's new technology platform structure, which R & D topics would be most beneficial to the chemicals industry?
Reviewers ranked platforms in terms of potential for impacting chemical industry energy consumption: 1. Reactions and Separations 2. Energy Conversion Systems 3. High Temperature Processes 4. Fabrication and Infrastructure
Question 2: Which projects in the current chemicals portfolio have the best potential for cross-cutting impacts in multiple industries?
Enhanced Productivity of Chemical Processes using Dense Fluidized Beds
Methane to Methanol (such as Ionic Liquid Project at Cal Tech)
Question 3: What future chemicals R & D projects would you suggest in order to maximize cross-cutting energy savings?
Alternative feedstocks such as biomass and coal

Table I 4: Review Process Questions and Answers

Question 1: What challenges did you face in interpreting the Principal Investigators' CPAT analyses (inputs, results, justification)
CPAT is most meaningful for commodity chemicals with a broad market. For specialty chemicals such as H_2O_2, the CPAT analysis is less meaningful.
Question 2: What suggestions do you have for best integrating CPAT and CPMT into the review process
Need to better educate reviewers about CPAT and CPMT prior to the review.
Revise the questionnaire and evaluation form to improve clarity.
Question 3: Was the time allotted for sessions appropriate?
Overall, the time allotted was appropriate. However, more time could have been allotted for review of the portfolio as a whole.
Question 4: What suggestions would you provide for the portfolio review consensus meeting?
More time should be allotted for discussing the portfolio as a whole and for evaluating CPMT results.
Might want to consider having a group session with the Principal Investigators
Consider holding some of the reviews in a closed forum rather than in conjunction with AIChE. (Save money, time, etc)
Questionnaire should be more focused on progress made by projects, rather than on answering CPMT questions.
Question 5: Would you like to see any changes in CPMT?
Needed better energy numbers to integrate with CPMT.
Multiple questions tend to move final scores to a middle ground—difficult to compare projects.
Consider alternate portfolio management tools.
The range of scores is not high enough. Consider using a 0-10 scale rather than a 0-4 scale.
Question 6: What suggestions do you have for providing you better project information before the review?
The presentations were much more informative than the documents provided before the review.
Questionnaires for PIs should ask for more information about progress and significance of results.
Quarterly reports were not very useful