PTC Organics, Inc.

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Phase-Transfer Catalysis Process Consulting
by Marc Halpern, PTC Organics Inc.

PTC Process Consulting enhances outstanding process R&D in two stages after a Project is initiated. After initiating the Project, the first stage of PTC Process Consulting is called the "***Design Report***" and the second stage is follow up consulting during development.

The goals and benefits of PTC Process Consulting are:

- To achieve the best performance for the customer processes using phase-transfer catalysis AND
- To benefit from high R&D efficiency to achieve the low-cost high-performance green chemistry that phase-transfer catalysis delivers, using the minimum precious R&D resources.

PTC Organics' consulting typically reduces R&D development time by 1-6 months PLUS the customer achieves better results due to leveraging PTC Organics' highly specialized expertise in industrial PTC. This is why it is usually a no-brainer for customers to invest in PTC Process Consulting at a cost of just a fraction of a month of the typical cost of process development time and results in performance benefits for both the process and R&D efficiency. In other words, the return on investment on PTC Process Consulting is high to very high.

Initiating a PTC Process Consulting Project

A Project is initiated by the customer by submitting to PTC Organics a ***Project Description Form***, typically under secrecy agreement. The Project Description Form and a completed sample form are shown on the last two pages of the PTC Consulting Agreement and can also be printed from www.phasetransfer.com/projectform.pdf. The Project Description is a simple 2-step form that in Step 1 includes a ***customary structure drawing of the specific reaction*** to be developed. The diagram shows the structures of the specific reactants, products and byproducts (must be specific, no R-groups) and includes, above and below the arrow, the current conditions of time, temperature, solvent and catalyst. Results are also shown such as yield and selectivity. Mole ratios are shown for reactants and catalyst.

In Step 2 of the Project Description Form, the customer defines ***specific performance targets*** for the reaction. The performance targets must be specific and measurable such as "increase yield from 85% to at least 92%, preferably 95% or higher" or "replace NaH/DMF with NaOH and a water-immiscible solvent" or "reduce excess Reactant B from 30 mole% to less than 10 mole%, preferably less than 5 mole%" or "reduce the dialkylated impurity to less than 0.5%." It has been our experience that setting nonspecific goals such as "increase yield as much as possible" is less effective for achieving the project goals, especially if tradeoff decisions need to be made that have multiple performance targets.

Once the specific reaction with well-defined performance targets is disclosed in the Project Description Form, PTC Organics provides an estimate of the probability of success for meeting the defined performance targets using phase-transfer catalysis. This is a ***free service*** provided by PTC Organics and is based on 44 years of PTC experience (including 36 years industrial PTC) and participation in dozens of commercial PTC development projects. There is no obligation by the customer to proceed with PTC Consulting after receiving the estimate of the probability of success.

It should also be noted that a Project relates to one reaction step. A second PTC reaction in a sequence has its own requirements and constitutes a second Project.

Stage 1: The "Design Report"

The purpose of the Design Report is to provide the expertise, background and recommendations to execute the Project. This includes an in-depth discussion of the underlying fundamentals, novel PTC concepts and practical guidelines for the specific Project reaction, the design of an experimental program to screen the PTC concepts and process chemistry ramifications (catalyst separation, stability, waste minimization, etc). The Design Report is typically delivered within 2-3 weeks of signing the PTC Consulting Agreement (maximum 4 weeks as per the contract).

The Design Report is crucial at the outset of the Project for several reasons. There are 14 process parameters that can potentially affect the outcome of a PTC reaction, many of which cannot be evaluated using systematic Design of Experiments techniques. The large number of permutations is often the reason that PTC process and profit opportunities remain unrealized. However, typically ***3-5 parameters govern 80-90% of the behavior of a PTC system and they are different from application to application***. In the first part of the Design Report, we describe in great detail the top 3-5 parameters anticipated to be crucial for success based on the above mentioned Marc Halpern's 37 years of experience in PTC. This portion of the Design Report includes the underlying fundamentals for the chosen process parameters, ranges for the parameters, interactions between the parameters, plus critique of relevant PTC patents & literature. The Design Report concludes with the ***design of a resource-efficient experimental program to evaluate the PTC process option***, including highly specialized PTC techniques ("tricks").

Often, a teleconference or face-to-face meeting will be conducted before or during the composition of the Design Report to assure shared understanding of the technical details of the Project, process constraints and sometimes further clarification of the goals. It is not uncommon for these discussions to result in enhanced ideas for a higher quality Design Report.

From an administrative standpoint, the Design Report is submitted after the first payment for PTC Consulting is received. Again, this is typically 2-3 weeks after signing the PTC Consulting Agreement, but no later than 4 weeks.

After the Design Report is submitted, the customers often prefer to study and absorb the content for about a week or so and then a teleconference is conducted to further develop and refine the thoughts and plans for the experimental program.

Stage 2: Follow Up Consulting

In the second stage of PTC Process Consulting, the customer performs scouting experiments and development in the laboratory. PTC Organics provides up to 20 hours of analysis of results generated by the customer for the specific reaction of the Project and additional input for the design, redesign, rationale, ramifications and recommendations for the experimental programs to assure the best process performance in the shortest time during development and scale up.

Results are shared in spreadsheets, chromatograms, E-mails and teleconferences. The frequency of communication is up to the customer and usually more communication of results leads to higher process performance as well as shorter development time. The discussions are very synergistic due to highly cooperative interactions and effective integration of PTC Organics highly specialized expertise in PTC with the expertise of the customer's technical staff with the existing chemistry. ***The merging of thought processes and highly specialized expertise creates a result greater than either party alone***. Free communication and sharing creativity greatly enhances Project performance.