PTC Organics, Inc.

The Industrial Phase-Transfer Catalysis Experts

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Phase-Transfer Catalysis Process Consulting
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PTC Process Consulting helps industrial process teams achieve better process performance, shorten development time, and increase R&D efficiency for reactions where phase-transfer catalysis may offer a superior solution. Consulting is conducted in **two stages** after a Project is initiated. The first stage is the **Design Report Presentation** 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's process using phase-transfer catalysis
- To increase R&D efficiency and help deliver the low-cost, high-performance green chemistry that phase-transfer catalysis can provide while using the minimum precious R&D resources

PTC Organics' consulting typically reduces R&D development time by **1–6 months** while also improving technical results by leveraging highly specialized expertise in industrial PTC. This is why customers often view PTC Process Consulting as a high-return investment at a cost that is only a fraction of a month of typical process development time. In other words, the return on investment on PTC Process Consulting is often **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 **here**.

The Project Description Form is a simple **2-step form**. In **Step 1**, the customer provides a structure drawing of the **specific reaction** to be developed. The diagram must show the structures of the specific reactants, products and byproducts (**must be specific, no R-groups**) and include, above and below the arrow, the current conditions of **time, temperature, solvent, and catalyst**. Results such as **yield and selectivity** must also be shown as well as mole ratios for reactants and catalyst, when available.

In **Step 2**, the customer must define the **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," "replace NaH/DMF with NaOH and a water-immiscible solvent," "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%." Specific performance targets are required. If the customer provides only nonspecific goals such as "increase yield as much as possible," PTC Organics cannot provide an estimate of the probability of success for the Project. The estimated probability of success may also differ depending on the level of performance requested. For example, the probability of achieving 92% yield may be different from the probability of achieving 95% yield.

Once the customer discloses a **specific reaction** together with **well-defined performance targets**, PTC Organics provides an estimate of the **probability of success** for meeting those targets using phase-transfer catalysis. This is a **free service** provided by PTC Organics and is based on **50 years of PTC experience** (including **42 years of industrial PTC**) and participation in dozens of commercial PTC development projects. There is **no obligation** for the customer to proceed with PTC Consulting after receiving the estimate of 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" Presentation

The purpose of the Design Report Presentation is to provide the expertise, background, and recommendations needed to evaluate proof-of-concept for process conditions that may achieve the performance targets, to be screened in 1-2 weeks by the customer. This includes a systematic discussion of the underlying fundamentals, novel PTC concepts, and practical guidelines for the specific Project reaction, together with the design of an experimental program to screen the PTC concepts and important process chemistry ramifications such as catalyst separation, stability, and waste minimization. The Design Report Presentation is typically conducted by video conference using PowerPoint within **3 weeks** of signing the PTC Consulting Agreement (**maximum 4 weeks** as per the contract).

The Design Report Presentation 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 effectively by systematic Design of Experiments techniques. The large number of permutations is often the reason that PTC process and profit opportunities remain unrealized. However, typically **3–6 parameters govern 80–90%** of the behavior of a given PTC system, and those key parameters differ from one application to another. This is why PTC Organics' highly specialized expertise is crucial.

In the first part of the Design Report Presentation, PTC Organics identifies the **top 3–6 parameters** anticipated to be crucial for success based on Marc Halpern's highly specialized industrial PTC experience. As appropriate, this portion of the Design Report Presentation includes the underlying fundamentals for the selected process parameters, practical ranges for those parameters, and potential interactions between them. The Design Report Presentation concludes with suggestions for a **resource-efficient experimental program** to evaluate the PTC process option, including highly specialized PTC techniques and practical "tricks."

Depending on the Project, a video conference or face-to-face meeting may be conducted before or during preparation of the Design Report Presentation to assure shared understanding of the technical details, process constraints, and project goals. These discussions often lead to additional insights and a higher-quality Design Report Presentation.

After the Design Report Presentation, customers often prefer to study and absorb the content for about a week, after which an additional video conference may be requested to further develop and refine the experimental plan before the customer performs 1-2 weeks of lab screening. The invoice for Stage 1 is submitted for payment concurrently with the Design Report Presentation.

Stage 2: Follow Up Consulting

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

Results are typically shared in spreadsheets, chromatograms, E-mails, and teleconferences. The frequency of communication is up to the customer, although more frequent communication usually leads to both **higher process performance** and **shorter development time**. These discussions are highly synergistic because they combine PTC Organics' highly specialized PTC expertise with the customer's detailed knowledge of the existing chemistry. ***The merging of thought processes and highly specialized expertise creates a result greater than either party alone***. Open communication and sharing creativity greatly enhance Project performance.