High-Throughput Experimentation and Novel Product Development in Cyber-Infrastructure Environments

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Cyber-infrastructures offer tremendous potential to improve current practices in new product and process development which are severely hampered by a lack of (i) Computing power. Simulation and optimization efforts are computationally expensive. Complex problem solving efforts suffer from a lack of capable tools. Cyber-infrastructures enable the provision of computing power to enable the modification of existing tools for such applications. (ii) Integration of methods. Most development and design activities are performed in isolation, sequentially with limited communication between stages. Cyber-infrastructure platforms are employed to integrate tools required in the design activities and facilitate communication mechanisms between tools to phase and coordinate the design activities and exploit synergies. Such platforms offer major reductions in process development times. (iii) Integration of resources across locations. Design activities are performed by separate or distant R&D groups belonging to different organizations and communication problems negatively impact on the efficiencies of the efforts. Cyber-infrastructure frameworks are employed to enable remote resource access to experimental data, analysis tools, model development tools, and novel process design tools can significantly improve the current situation. Prototype applications are presented across the three application areas and towards increasing complexities with the ultimate goal to speed up the individual tools and activities involved in novel product and process development This enables users to achieve maximum benefits from the quick design of innovative high performance processes. The prototype applications will focus on the development of novel products and processes in the field of heterogeneous catalysis, from High Throughput screening to detailed process validation. Cyber-infrastructures stand as an ideal venue to enable applications that would result in major productivity gains in product and process development. In the long term, radical changes in design practices are anticipated as a result of such an integrated process development grid. Improved design efficiency results in lower investment costs to develop more efficient processes and will improve the competitiveness and economic growth of the industry.

The paper describes cyber-infrastructure prototypes geared towards realising the vision of the integrated catalysis product and process design grid illustrated in Figure 1. Developments focus on: · Experimental data analysis for model development and steering of experiments (communication between tools, integration of resources). Experimental data analysis is the most critical exercise for reliable model development and it is critical to provide venues to enable access to data resources and analysis tools to different researchers during a process design project. Different levels of abstraction in reactor and process design call for different requirements for the kinetic models to be used. Whereas detailed models are necessary for validation of final design propositions, the conceptual and intermediate design efforts aim at the investigation of design trends. A Grid prototype will register the experimental data sources together with tools required to develop accurate kinetic models for design validations as well as conceptual black box kinetic models for conceptual decision making. · Reactor and process design optimisation (computing power / communication between tools). These are highly computationally expensive problems that can only be solved by existing stochastic optimisation tools with access to vast computational power. Parallel computation schemes need to be developed to interface and coordinate the individual optimisations and simulations involved in order to identify optimal solutions to real problems. Initial efforts would focus on prototype cyber-infrastructures to enable large scale reactor design optimisation. Later efforts will focus on the integration of different levels of abstraction through the coordination of these optimisation experiments with - detailed computational fluid dynamic simulation studies for efficient validation of the optimised designs; and -

conceptual process design tools to include conceptual process information in the reactor design optimisation studies in order to identify reaction options with optimal performances in the context of the overall process. Experimental design suggestions from screening tools (integration of methods and resources). HTE studies are set up by robots. These studies need to be coordinated through knowledge generated by conceptual reactor optimisation tools. Development efforts would focus on prototype cyber-infrastructures to enable the steering of the robots by the promising scenarios identified in the optimisations. Similarly, mini plant experiments need to be carried out in coordination with process screening tools to ensure the identification of the appropriate process conditions to be investigated. A prototype cyber-infrastructures would enable the automatic control of the mini plant experiments to run at the conditions revealed in process screening. Integrated prototypes to guide process design and experimental efforts in HTE and mini plant studies. Once the experimental data analysis prototype is functional, conceptual reactor optimization tools will be made available through the platform that receive the black box models generated and screen process design variable spaces and supersets of conceptual process configurations to identify regions of promising performances on which further experimental investigations can be based in the light of the underlying chemistry. Detailed kinetic models will be processed by detailed optimization and 2D/3D simulation tools to enable the evolution of reactor designs alongside kinetic model development and create images of the novel designs.