LISTING OF ACTIVE PROJECTS (2005/2006)

Projects active during the period June 1, 2005 through May 31, 2006 are classified into categories of the current active projects on multiphase reactors and processes, and the past active project on the preparation of new materials, and process monitoring and control. The results of research contracts funded by individual sponsors and the results of the High Pressure Slurry Bubble Column Consortium (HPSBCC) are reported only to related sponsors. The working titles of all active projects and the names of graduate students or researchers involved are listed below:

Name		Title: key words

AREA I. MULTIPHASE REACTORS AND PROCESSES: EXPERIMENTS AND MODELS

BUBBLE AND SLURRY BUBBLE COLUMNS

A. Shaikh, L. Han, C. Wu (graduate students)	**I-1.**	**Hydrodynamics of Slurry Bubble Columns Using Computer Automated Radioactive Particle Tracking (CARPT) and Computed Tomography:** The details of the hydrodynamics of slurry bubble column have been investigated using CARPT and CT.
L. Han (graduate student)	**I-2.**	**Phase Distribution, Solids/Liquid Velocity, and Solids/Liquid Turbulence in a High Pressure Slurry Bubble Column Reactor Operated at Mimic Fischer-Tropsch Conditions:** This work has been performed for the consortium and the results have been reported to them.
A. Shaikh (graduate student)	**I-3.**	**Scale-up of Bubble Column Reactors:** A new methodology for scale-up bubble column has been proposed and validated for hydrodynamic similarity. Advanced measurement techniques (CT and CARPT) have been used to validate and illustrate the developed approach.
A. Shaikh (graduate student)	**I-4.**	**Characterization of Hydrodynamic Flow Regime in Bubble Column Reactors via Computed Tomography**: CT technique has been implemented to characterize and identify flow regime in bubble column reactors.
L. Han (graduate student)	**I-5.**	**A New Methodology to Measure the Solids Axial Dispersion in High Pressure Slurry Bubble Column Reactor:** CARPT results have been used to simulate tracer response of the solids to characterize and quantify the solids dispersion using a newly developed method.
L. Han (graduate student)	**I-6.**	**Gas-Liquid Mass Transfer in a High Pressure Bubble Column Reactor With Different Gas Sparger Designs:** Both volumetric mass transfer coefficient (k_la) and liquid side mass transfer coefficient (k_l) estimated based on the bubble dynamic results (interfacial area) obtained by 4-poing optical probe have been studied in high pressure bubble column reactors. The effect of sparger design on mass transfer coefficient has been characterized.

C. Wu
(graduate student)

I-7. Heat Transfer Coefficients in a High Pressure Bubble Column: Heat transfer coefficients have been studied in a high pressure bubble column using the modified version of a rode type of heat transfer probe.

A. Akhtar
(visiting graduate student – Curtin University - Australia)

I-8. Modeling of Gas Distributor for 3D Simulation of Bubble Columns: CFD has been used to account for the gas sparger configuration to simulate the flow dynamics in bubble columns.

M. Vesvikar
(graduate student)

I-9. Multiple Particle Tracking (MP-CARPT) Implementation: Low L/D Slurry Bubble Column Reactor: The newly developed MP-CARPT has been implemented to characterize the flow field of low L/D slurry bubble column with low solids loading.

FLUIDIZED BEDS

M. Capitaine
(research associate)

J. Albert
(graduate student – University of Twente)

I-10. Investigation of Catalytic Gas-Phase Olefin Polymerization Reactors - Radioactive Particle Tracking and CFD Studies RPT-CFD: CARPT has been implemented to investigate the flow dynamics of fluidized bed reactors and to provide bench mark data for the development and validation of CFD code and closures to simulate the reactors for catalytic gas-phase olefin polymerization.

W. Jalil
(graduate student)

I-11. Experimental Investigation of the Hydrodynamics of Fluidized Bed Reactors: A study has been initiated to investigate the flow dynamics of fluidized bed reactors for amoxidation of propylene. Advanced measurement techniques will be implemented in this study.

TRICKLE BEDS

P.-Y. Lanfrey
(visiting research associate - France)

I-12. Flow Distribution in a High Pressure Trickle Bed Reactor: A high pressure trickle bed reactor facility has been designed and is currently under development that is equipped with high pressure collecting tray system that measures both the liquid and gas fluxes distribution at the bottom of the reactor. In addition CT technique can be applied to measure voidage and phases cross-sectional distribution.

J. Guo, R.C. Ramaswamy
(graduate students)

I-13. Multiphase Kinetic and Reactor Models: 1D and 2D kinetic and reactor scale model and computer programs has been developed and used for trickle bed reactor processes.

STRUCTURED BEDS

S. Roy
(graduate student)

I-14. Effect of Flow Maldistribution on Monolith Reactor Performance: A Modeling Approach: A new model has been developed that integrate hydrodynamics with kinetics to predict the performance of monolith reactors.

PACKED BEDS

R. C. Ramaswamy (graduate student)

I-15. Steady State and Dynamic Reactor Models for Coupling Exothermic and Endothermic Reactions: A summary of the key findings of this thesis is presented.

R. C. Ramaswamy (graduate student)

I-16. Exergy Analysis and the Reactor Performance: The exergy (which is defined as useful energy, thermodynamically available, to perform work) analysis has been used to compare thermal losses in different modes of coupling exothermic and endothermic reactions.

STIRRED REACTORS

D. Guha (graduate student)

I-17. Quantification of Solids Distribution and Solids Flow Field in Solid-Liquid Stirred Tank Reactors: CARPT has been applied to map the flow dynamics of the solids in a solid-liquid stirred tank reactor.

D. Guha (graduate student)

I-18. Compartmental Model for Stirred Tank Reactors: Evaluation of Turbulence Model: The effect of turbulence model used in CFD has been evaluated on the performance prediction of the CFD-based compartmental model for single phase stirred tank reactors.

PROCESSES and MINI and MICRO-REACTORS

R. Jevtic (graduate student)

I-19. Mini Reactors for Characterization of Hydrocarbon Oxidations: Cyclohexane oxidation was performed in two capillary reactors at different temperatures with and without catalyst. The results were compared with plug flow based reactor model.

K. Ruthyia (research associate)

R. Jevtic (graduate student)

I-20. Modeling the Effects of Temperature, Pressure, and Oxygen Solubility on Liquid Phase Oxidation of Cyclohexane: A model for liquid phase oxidation of cyclohexane that includes kinetics, transport and hydrodynamic parameters is being developed.

N. Subramanya (graduate student)

I-21. Experiments and Mathematical Modeling to Evaluate Solid Acid Alkylation Processes: 5 and 50 ml mini-packed bed reactors set-ups made from titanium have been developed, tested and utilized to estimate the transport and equilibrium parameters for solid acid alkylation processes using B-zeolite catalyst.

C. Tunca (research associate)

I-22. Molecular Simulation Studies of Adsorption Isotherms for Solid Acid Alkylation Catalysts: Molecular simulations are being used to study the important transport properties of solid acid catalyst for alkylation processes.

D. Guha
(graduate student)

I-23. Kinetic modeling and mass transfer effects in Homogeneous Catalytic Hydroformylation of 1-Octene in CO_2 – Expanded Solvent: A detailed batch reactor scale model has been developed to study the effect of mass transfer and catalyst activation on the induction period in 1-ocatene hydroformylation in expanded solvent (CXLs) (a mixture of supercritical CO_2 and solvent.

Z. Kuzeljevic
(graduate student)

I-24. Membrane Steam Reforming Reactor for Pure Hydrogen Production: 2D CFD based simulation has been developed to model the membrane steam reforming reactor for hydrogen production.

AEROSOL / PARTICULATE REACTORS

P. Kumar
(graduate student)

I-25. Aerosol Routes for Synthesis of Nanostructured Magnetic Oxides: Characterization and Transport Behavior: The effects of flame temperature profile and residence time on the shape, size and crystallinity of synthesized γ-Fe_2O_3 have been investigated. The mechanism of the formation of the magnetic oxide has been studied.

MEASUREMENT TECHNIQUES

Z. Zuzeljevic
(graduate student)

I-26. Reduced Tomography For Industrial Application: Using a packed bed with various phantom objects, reduced tomography is evaluated for industrial application and its results are compared with CT results.

R. Varma
(graduate student)

I-27. Development of Dual Source Computed Tomography for Imaging Three Phase Systems: Dual modality CT is being developed to visualize flow distribution of moving three phases systems.

M. Vesvikar
(graduate student)

I-28. Development and Validation of Multiple Particle Tracking (MP-CARPT): Multiple particle CARPT has been developed and validated to track more than one radioactive particles simultaneously to visualize the various phases and/or flow of group of particles in multiphase reactors.

S. Meuller
(graduate student)

I-29. Volumetric Expansion and Phase Transition of Expanded Solvents Using an Optical Fiber Probe: A technique has been developed and validated to measure on-line volumetric expansion and phase transition in expanded beds (CXLs) (a mixture of supercritical CO_2 and solvent).

BIOREACTORS AND BIOPROCESSES ENGINEERING LABORATORY (BBEL)

A. Henriques
(graduate student)
In collaboration with USDA

I-30. Enzymetric Dewatering of Distiller Dried Grains (DDGs): A new process and approach is being developed to enhance energy efficiency in production of bioethanol from corn by using enzymatic dewatering of DDGs.

H. Luo
(graduate student)

I-31. Analyzing and Modeling of Photobioreactors for Microalgal and Cyanobacteria Cultures: A novel modeling approach has been developed that combines cells' movement, hydrodynamic parameters, dynamic photosynthesis and irradiance field to predict and investigate the photobioreactor performance for the growth of high value products microalgae and cynobacteria.

M. Vesvikar
(graduate student)

I-32. Effect of Scale and Mixing on the Performance of Anaerobic Digesters: The effects of mixing and scale-up on the performance of anaerobic digesters have been investigated using laboratory (3.75 lit) and pilot plant (97 lit) digesters.

R. Varma
(graduate student)

I-33. Effect of Sparger Design on Hydrodynamics of a Gas Recirculation Anaerobic Bioreactor: The effect of a single orifice and multi-orifice ring spargers on the hydrodynamic of a gas recirculation anaerobic digester has been studied using CARPT and CT.

USER FRIENDLY MODULES FOR MULTIPHASE REACTORS MODELING

C. Tunca
(research associate)

I-34. Developing User Friendly Modules for Modeling Multiphase Reactors: User friendly software-based simulations are being modulated for multiphase reactor performance, evaluation, design and scale-up.

AREA II. PREPARATION OF NEW MATERIALS

M.P. Dudukovic, P.A. Ramachandran
(faculty)

II-1. Semiconductor Grade Silicon: CREL know-how reviewed.

P. Gunjal
(research associate)

II-2. Melt Dynamics in Czochralski Crystal Growth of Silicon: CFD based model to simulate the hydrodynamics of the Czochralski crystal growth process is being developed to study the influence of the applied forces such as rotational speed and magnetic field in the interface shape and oxygen content in the melt.

AREA III. PROCESS MONITORING AND CONTROL

G. McMillan
(adjunct faculty)

III-1. Process Monitoring and Control: A HYSIS plant dynamic model is available together with the newest Delta-V Pro control system.