INTELLIGENT NANO-ENGINEERING OF FLUID-SOLID INTERFACE

This project is devoted to development of a novel fundamental methodology for manipulation of the structure and composition of fluid-solid interfaces on molecular/atomic level (i.e., nano-engineering) to ensure desired properties and flow characteristics of the processed nanofluids (i.e., interfacial fluids in thin films and clusters, fluids confined in narrow capillary pores/caves/spaces of several molecular diameters in width, etc.).

The **principle aims** of the project are:

- **to develop new engineering models of nanofluid rheology based on the Pozhar-Gubbins (PG) statistical mechanical theory of non-equilibrium processes in spatially inhomogeneous fluids;**
- **to develop a novel methodology for application of these new engineering models to manipulation of the structure, composition and chemistry of solid surfaces to supply desired properties and flow characteristics of the processed nanofluids.**

The **primary objectives** of the project are:

- to use a rigorous, fundamental physical theory (PG-theory) to evaluate physical mechanisms responsible for non-Newtonian (in particular, rheological) properties of nanofluids, so as to identify those supplying the major contributions to such properties;
- to use the above results and equilibrium molecular dynamic (EMD) simulations for development of practical simplifications of the PG-theory in the case of rheological properties of nanofluids 1) in thin films on solid surfaces and 2) in narrow capillary pores of several molecular diameters in width; to develop engineering models of nanofluid rheology (or ER-models) based upon the above theoretical evaluations and existing experimental data;
- to develop non-equilibrium molecular dynamic (NEMD) codes for simulation of nanofluid flows in thin films and narrow capillary pores; to develop finite element codes to solve the conservation equations of the ER-models of nanofluid flows; to compare predictions of the ER-models and the NEMD simulations in the above particular cases of nanofluids;
- to use the ER-models for development of a novel fundamental methodology for nano-engineering of fluid-solid interfaces possessing desired properties with regard to CO_2, N_2 and CH_4-nanofluid flows 1) in narrow capillary pores of silica-based catalysts and 2) in thin films on doped silica surfaces.

Relevance to Beneficiaries

The **principle benefits** of this work for developers of structural materials will include 1) reduced energy costs; 2) reduced time-to-market, 3) increased scope for innovation and development of new materials and processes, and 4) reduced laboratory overheads. **Immediate beneficiaries** will be industries concerned with fluid processing on the fluid element length scales (e.g., nanocasting, catalysis, etc.). This includes developers of 1) modified and new porous materials and packed beds for gas and liquid processing (porous catalysts, adsorbents, molecular sieves, etc.); 2) well-defined nanotubes; 3) heavy-duty (i.e., anti-corrosive or anti-fouling) surface coatings; 4) lubricants; 5) self-monitoring structural materials, etc. The outcome of this project shall also be relevant to problems of petrochemical industry (e.g., the natural gas processing, gasoline purification, increase of oil sands output), pharmaceutical and food industries (e.g., pill coating, creams and food layering), recycling and water treatment, etc. The project will supply advanced scientific knowledge to furnish fundamentals of a novel methodology for *materials and chemical engineers*. Concerned *scientific community* will benefit from experience gained from this targeted attempt at application of a fundamental physical theory and computational methods to enlighten new technological horizons for materials and process engineering.