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The HOWARD P. ISERMANN
DEPARTMENT OF CHEMICAL AND
BIOLOGICAL ENGINEERING

CBE Seminar Series – Fall 2022

Dr. Georges Belfort

Institute Professor, Chemical and Biological Engineering
Rensselaer Polytechnic Institute

Seminar: Wednesday, October 19, 2022

9:30 a.m. (Ricketts 203)

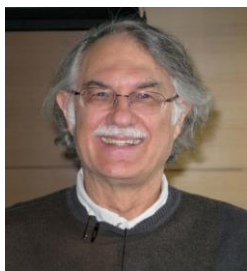
“Design and Synthesis of Polymer Membranes Based on Theoretical Principles”

Abstract:

To optimize the filtration performance of synthetic polymer membranes, their internal microstructure needs to be designed and synthesized based on theoretical principles and not empirically, as is done at present, using phase inversion and interfacial polymerization. Here we present a rational approach in which we develop an *in-silico* tool to (a) simulate separation of particles with different properties (i.e., chemistry, size, shape, flexibility, etc.), and (b) propose, test, and optimize novel microstructures. To validate these predictions, experiments are required. The *in-silico* tool comprises 2D computational fluid and particle drag mechanics combined with particle and membrane force measurements in ionic solutions, modeled by the DLVO and the extended DLVO (xDLVO) theories, to study particle intrusion and capture in and escape through microporous polymer membranes. We have previously demonstrated¹ that (a) the *in-silico* tool predictions for a commercial membrane show substantial flow channeling and qualitatively agree with experimental filtration measurements using scanning electron microscopy with particle tracking via energy dispersive X-ray spectroscopy, and (b) tear-drop microstructures of different orientation weakly separate particles that differ in size by a factor of 2.

In this work, we have conducted extensive intermolecular force measurements between streptavidin, a stable protein coated on a polystyrene sphere, and two commercial microfiltration poly(ether sulfone) and poly(vinylidene difluoride) membranes and obtained requisite parameters such as the Hamaker constants, surface potentials, hydrogen-bonding free energies of cohesion between the water molecules and characteristic decay lengths of water ($\lambda=1.0$ nm at 20°C) from theoretical fits of DLVO and xDLVO theories² for 100s of experimental runs at various solution conditions (pH and ionic strength). We have also used the *in-silico* tool to obtain filtration performance predictions with membranes comprising a series of spherical microstructures of one size and in mixtures of different sizes to separate suspensions of particles that differ in size by a factor of 10 (i.e., the holy grail of membrane filtration). These microstructures allow adjustment of the tortuosity of the flow path and variation of the reactivity of the surface. Experiments are also underway testing these spherical particle microstructures. To our knowledge, this is the first attempt combining particle drag mechanics with intermolecular force measurements to design and synthesize microfiltration membranes based on theoretical principles. The *in-silico* tool can be used to characterize membranes for separation performance and guide improved design, synthesis, and testing of new microporous membranes.

Biography:



Dr. Georges Belfort holds the endowed “Institute Chair” at RPI since 2011. He was educated in Chemical Engineering, University of Cape Town, South Africa (BS degree) and the University of California at Irvine, CA (MS and PhD degrees in Engineering). He has held faculty positions at the Hebrew University (1973-1977) and RPI (1978-date). He designed the first water reuse system for NASA’s test spacecraft and worked on fuel cells and on reverse osmosis at Astropower Laboratory, McDonnell Douglas Corp. He was elected to the US National Academy of Engineering in 2003 and chosen as one of the “100 Chemical Engineers of the Modern Era” as part of the AIChE Centennial Celebration. In 2012, he was elected as a foreign member of the Bologna Academy of Sciences, Italy, and in 2019, he was awarded a Doctor of Science in Engineering (DSc (Eng.)) honoris causa. Dr Belfort currently chairs the managing board of the Society of Biological Engineers (SBE-AIChE), New York, 2014-date. He is a past

President and co-founder of The North American Membrane Society (NAMs). He has published over 250 peer-reviewed publications, 25 book chapters, and 10 assigned patents. He has won several US national scientific awards including the 2017

Food, Pharmaceutical and Bioengineering Division Distinguished Service Award in Chemical Engineering, AIChE, the 2016 Rensselaer Best Teacher Award in Engineering, RPI, Troy, NY, the 2014 NAMS Alan S. Michaels Award for Innovation in Membrane Science and Technology. Dr Belfort’s research uses fundamental concepts to solve important technical challenges in the areas of continuous bio-separations and purification of mRNA (vaccines), in vitro production and purification of biofuels and organic solvents. His expertise is in the fields of molecular separations, membranes for liquid filtration, affinity membrane separations, interfacial chemistry, intermolecular force measurements with xDLVO theory, protein aggregation (i.e., for Alzheimer’s disease) and transport phenomena including fluid and mass transport.

Refreshments will be available at 9:00 a.m. in the Ricketts Coonley Lounge (RI 120).

For more information, please contact Lisa Martin (swishl@rpi.edu)