New Paradigms in Chemical Engineering: Health, Climate Change and Energy, and Product Design

ARTICLE *in* INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · MAY 2010

Impact Factor: 2.59 · DOI: 10.1021/ie1002894

Dimitris Hatziavramidis
National Technical University of Athens

New Paradigms in Chemical Engineering: Health, Climate Change and Energy, and Product Design

Dimitris T. Hatziavramidis*

School of Chemical Engineering, National Technical University of Athens, Zografou Campus 15780, Athens, Greece

Chemical engineering originated from the need to design processes and equipment in the chemical industry; it evolved to encompass product design in other industry sectors, including (but not limited to) energy, consumer products, pharmaceuticals, and performance materials, and it has advanced to analysis and design of complex systems. It is believed that chemical engineering, in the near future, will focus on three areas: health, climate change and energy, and functional products. To support this belief, three unpublished paradigms—one from each of these areas—are presented. The first paradigm deals with encapsulation of pancreatic islet cells for transplantation in patients with Type 1 diabetes. The second paradigm presents an analysis of energy needs of Greece over the next 15 years, given the observed climate changes. Finally, the third paradigm is the design of a new material on which information is stored and recovered in replicated media optical discs.

Introduction

Chemical engineering, as a discipline, originated in the chemical industry (soda ash, sulfuric acid, organic dyes, ammonia) during the industrial revolution (1850−1900).[1,2] Its name and the term "unit operations" appeared first in 1901 in England[3] and, later, in 1923 in the United States.[4] Early on, it expanded its scope into the oil industry and synthetic fuels during the period between the two World Wars. By the end of World War II, the production of synthetic rubber from styrene and butadiene, and polymers from petrochemicals, opened new industrial sectors to chemical engineering. The production of antibiotics by fermentation in 1940−1950 opened a door to the pharmaceutical industry, to which more doors opened in the 1980s with the production of biopharmaceutical drugs (proteins and peptides) via biotechnology.

In the 1960s, the book *Transport Phenomena*[5] had a seminal effect on chemical engineering. This book, together with books on chemical reaction engineering,[6] applied mathematics, and process control provided the foundations for establishing a unique engineering science discipline.

For the most part, chemical engineering has dealt with the analysis and design of processes to convert raw materials into useful products. Polymers brought product design to the forefront, which is an area that was highlighted by the manufacture of semiconductors, microelectronics, and performance materials.[7] Every new discipline, from biotechnology to biomedical engineering, nanotechnology, and fuel cells, has benefited from the chemical engineering approach. It is this approach that moved from unit operations to transport phenomena to systems engineering[8] to analyze and design complex systems[9] in areas as diverse as health, environment, energy, and functional materials. The new paradigms that follow clearly demonstrate the diversity in theme and methodology, as well as the problem-solving power of current chemical engineering.

The Health Paradigm: Encapsulation of Pancreatic Islet Cells for Type 1 Diabetes Treatment

Type 1 diabetes is a chronic, autoimmune, metabolic disease in which the pancreatic beta cells loose their ability to produce insulin, thus, negatively affecting the glucose cycle. In this cycle, glucose enters the blood through the epithelium of the gastrointestinal tract and, from there, is supplied to cells, tissues, and organs, in amounts and rates controlled by the level of insulin in the blood. The disease requires continuous monitoring of the glucose level in the blood and administering exogenous insulin, primarily by injection (hypodermic needle) or infusion (pump), to maintain the appropriate glucose level. An indicator of the patient's state that is better than the glucose level in the blood is the glycemic level or the level of glucosylated hemoglobin.

The administration of exogenous insulin, with frequent monitoring and strict compliance, is the primary therapeutic modality for Type 1 diabetes. It corrects the insulin deficiency but does not restore the glycemic level to its normal state, and it is not effective in advanced stages of the disease (cardiovascular problems, retinopathy, pathologies of the extremities, etc.). Other therapeutic modalities for Type 1 diabetes include (1) transplantation of the entire pancreas organ and (2) replacement or regeneration of pancreatic beta cells. Transplantation of the pancreas is done when there is a need for kidney transplantation or at the end stage of renal disease. It has two serious disadvantages: (1) low supply of organs and (2) post-surgical complications from a difficult operation. Therapeutic methods based on the replacement or regeneration of pancreatic beta cells through reprogramming of embryonic or adult pluripotent stem cells[10,11] are far from becoming realizable modalities. This, then, leaves the transplantation of pancreatic cell or Langerhans islets as the only alternative treatment.

Transplantation of pancreatic cell islets, which originated in the 1960s in Edmonton, Canada, has evolved into an accepted treatment (known as the Edmonton Protocol[12]). Similar to the administration of exogenous insulin, it corrects the deficiency, but unlike the former, it also restores the glycemic level, because the islets, in addition to insulin, produce amylin and glucagon, which are the other components needed for a balanced level. It does not share in the disadvantages of pancreas transplantation, namely, low supply of organs, difficult surgery, and post-surgical complications. Instead, it involves an easy operation with no need for hospitalization and no major discomfort for the patient, which can be repeated as many times as needed.

The islets needed for effective transplantation, according to the Edmonton protocol, amount to 11 000 IEQ (where IEQ

* E-mail: dthatzia@central.ntua.gr.

10.1021/ie1002894
Published on Web 05/13/2010

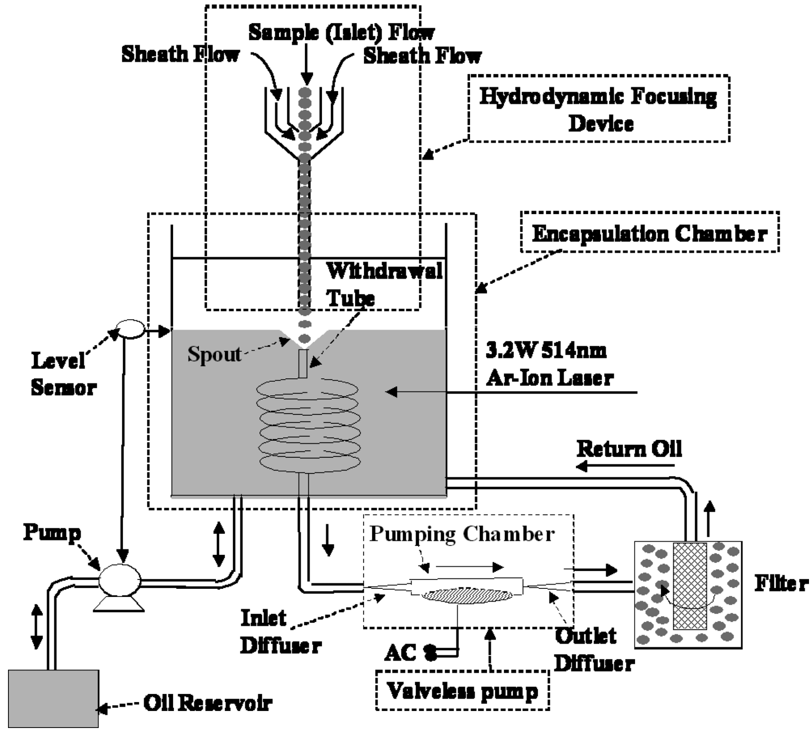

Figure 1. Schematic of the encapsulation apparatus.

denotes the islet equivalent, which is a mass of islets equal to the mass of an islet of average size, 150 μm) per kilogram of patient weight; this is clearly an example for personalized medicine. The transplanted islets, in a few cases only, come from the patients themselves. They can come from other individuals (allotransplantation) or even from animals (xenotransplantation) and cause a severe reaction of the patient's immune system for their rejection. The immunological reaction is addressed two ways: (1) through the administration of antirejection drugs, following transplantation and continuing for the patient's lifetime (immunosuppression), and (2) isolation of transplanted islets from the patient's immune system by mechanical means (immunoisolation). Immunoisolation is accomplished by encapsulating each individual islet by a membrane of a biocompatible, cross-linked polymer, which allows nutrients, insulin, and other metabolites but prevents moieties generated by the immune system (e.g., antibodies, cytokines, free radicals, and other toxic small molecules such as nitrous oxide) to pass through it.

Although the isolation and purification of islets for transplantation has been standardized,[13] the encapsulation of the islets, as practiced up to now, suffers from low rates and efficiencies, and it presents obstacles to this method reaching the stage of clinical trials and becoming a mainstream therapeutic modality.[14] Encapsulation techniques include droplet and emulsion formation, polyelectrolyte multilayering, and direct polymerization from a surface-adsorbed initiator. When applied to pancreatic islets, which are clusters of insulin-producing cells that must be kept alive and functional for as long as possible, these techniques become limited by constraints on chemical composition, uniformity, and thickness of the membrane, polymerization scheme, and maximum allowable shear stress.

Based on the principles of mechanics and cytotechnology, an apparatus has been designed to enclose individual islets in microcapsules, comprised of membranes of biocompatible, cross-linked polymer, at high enough rate and efficiency to

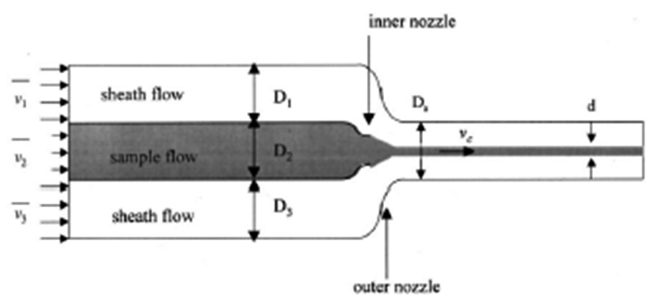

Figure 2. Schematic of the hydrodynamic focusing device.

supply insulin for clinical trials (initially) and patient treatment (later). The apparatus is shown in Figure 1.

For encapsulation, the apparatus utilizes the method of selective withdrawal from a two-layer system of two-immiscible liquids.[15] This technique was initially used in an apparatus for coating solid particles at a rate of 10 000 particles per hour;[15] however, when applied to a similar apparatus for encapsulating islets, the technique showed a low rate (100 islets a day) and efficiency (25%).[16] The low rate and efficiency resulted from the deficiencies in (1) feeding the pancreatic islets to be encapsulated, and (2) removing and isolating the encapsulated islets. In the encapsulation apparatus of Figure 1, the islets are fed by a two-nozzle device that utilizes hydrodynamic focusing as in cytometers[17] and removed by a valveless pump.[18]

The hydrodynamic focusing device (Figure 2) consists of two coaxial convergent nozzles, with its axis aligned with the axis of the encapsulation chamber and its outlet placed a distance h above the two-liquid interface. Islets in their culture medium are fed as a sample flow through the inner nozzle, and aqueous solution of PEG-DA, spiked with the initiator (0.09 mM eosin-Y), co-initiator (225 mM triethanolamine (TEA)), and accelerator (37 mM N-vinyl pyrrolidone (NVP)), are fed as sheath flow through the annular space between the two nozzles. The device aligns the islets, single file, in the center flow and focuses this flow on the center region of the two-liquid interface.

In the encapsulation chamber, the liquid of the upper layer is an aqueous solution of poly(ethylene glycol) diacrylate (PEG-DA), with a density of 1.18 g/cm^3, and the liquid of the lower layer is oil, a chlorinated hydrocarbon (paroil-152, Dover Chemical), with a density of 1.26 g/cm^3. A withdrawal tube of diameter equal to that of the outlet orifice of the hydrodynamic focusing device is placed in the lower liquid layer, with its axis aligned with the axis of the encapsulation chamber, at a distance h from the interface that is equal to that of the same outlet orifice. The rate of the withdrawal flow can be maintained by the valveless pump at a level equal to that of the feed rate from the hydrodynamic focusing device. If the distance from the interface (h) is smaller than a certain critical distance h_c, which can be estimated from a stability analysis of the flow in the interface region,[19] both the polymer solution with the islets and the oil enter the withdrawal tube. In a theoretical model,[20] the feed nozzle is modeled as a point source and the removal nozzle is modeled as a point sink. Small and large deformations of the interface are considered by analytical and boundary element methods and critical conditions for selective withdrawal are identified.

The polymer solution entering the withdrawal tube forms a liquid thread that contains an array of islets spaced apart along the centerline, surrounded by oil. A Rayleigh capillary instability causes the liquid thread to develop periodic disturbances of increasing amplitude and, eventually, to disintegrate into an array of drops. The size of the drops is such that a drop can engulf no more than one islet. From the analysis of the capillary instability, the islet coating thickness can be predicted.[21] The coating thickness for an islet of average size of 150 μm is 50 μm, which seems to agree with observations.[16]

The withdrawal tube starts as a straight vertical tube and ends into a coiled tube of specific length, helix diameter, and coil pitch. After the islets have been entrained into the coiled part of the withdrawal tube, they are exposed to a 514-nm light beam of an argon-ion laser, which excites Eosin-Y and initiates free-radical polymerization[22] to produce a poly(ethylene glycol) (PEG) hydrogel. Making the originally straight withdrawal tube into a coiled one provides sufficient time for polymer cross-linking and hydrogel formation. The thickness of the micro-capsule membrane enclosing an individual islet is controllable to within tens of a micrometer.

The encapsulated islets are removed from the encapsulation chamber at a rate equal to the feed rate and directed to a filter for recovery by a valveless nozzle-diffuser pump (see Figure 3) that has no interior mechanical parts and has been shown to transport mammalian cells without the slightest damage.[18] The valveless pump has a pumping chamber closed on the top by a diaphragm, two diffusers (as flow-directing elements), and a piezoelectric (PZT) patch bonded to the diaphragm with epoxy resin (as an actuator, to generate flow). An AC voltage is applied to set the three-layer (PZT-epoxy-diaphragm) plate into vibration at a frequency below the natural frequency of the diaphragm. The vibrating diaphragm drives fluid flow, and, at the same time, the flow increases the resistance to vibration (flow and vibration are coupled). If the action of the fluid is negligible, the plate will vibrate at the same frequency as the excitation force for small amplitude vibrations. The pump cycle (Figure 3) can be divided into a supply mode and a pump mode. In the supply mode, the fluid cavity volume increases; a larger amount of the fluid flows into the cavity through the input element, which acts as a diffuser, than through the output element, which acts as a

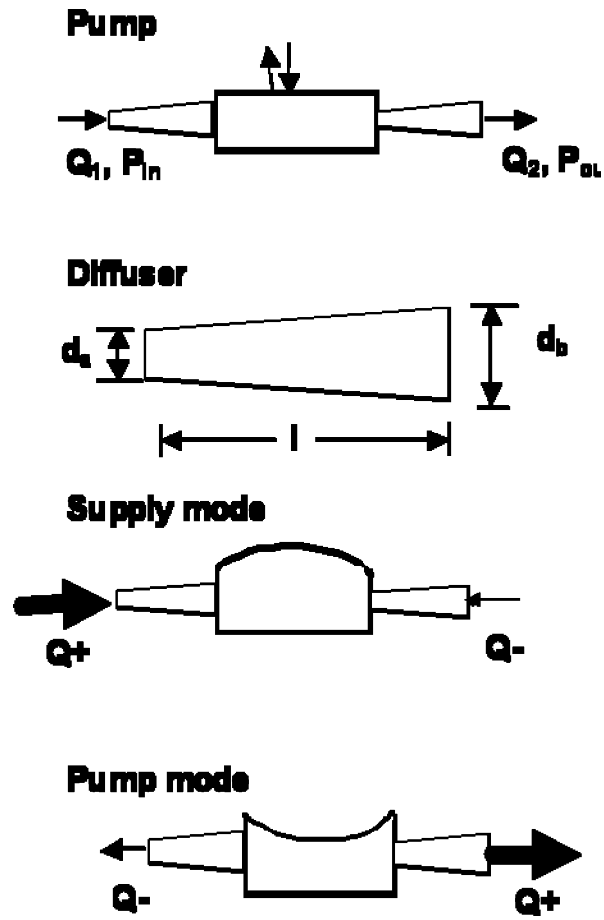

Figure 3. Schematic illustrations of the valveless pump and the diffuser, as well as depictions in pump and supply modes.

nozzle. In the pump mode, when the fluid cavity volume decreases, a larger amount of fluid flows out of the cavity through the output element, which acts as a diffuser, than the input element, which acts as a nozzle. The result for the complete pump cycle is that the net volume is transported from the input to the output side of the pump. The volumetric amplitude, which controls the flow rate, can be determined from the solution to the biharmonic equation for the deflection of the diaphragm,[23] which depends on the excitation force or the potential of the electric field applied.

Based on this design, a prototype of the encapsulation apparatus can be constructed. The two-nozzle hydrodynamic focusing device can be constructed by hot embossing. The tank of the encapsulation chamber, and the valveless pump diffusers and tank, with the exception of the diaphragm on the top, can be composed of poly(methyl methacrylate) (PMMA). The diaphragm of the valveless pump can be composed of poly-(dimethylsiloxane) (PDMS). It is expected that the rate will reach a value of 1 islet per second (~8 days are needed to produce ~700 000 encapsulated, viable, and functional islets that are needed for transplantation into a patient with a mass of 70 kg) and an efficiency of 83% (83% of the islets fed to the apparatus are encapsulated properly and are viable and functional).

Paradigm of Climate Change and Energy: Energy Policy for Greece

Sustenance of life on Earth is a result of a delicate balance of solar energy distribution between the atmosphere and the

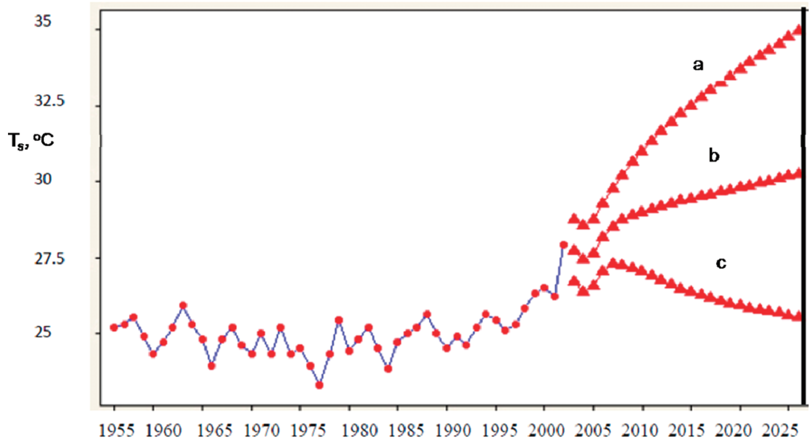

Figure 4. Average summer temperature (T_s). Data for the period from 1955 to 2001 (denoted by solid circles) have been taken from Feidas et al.;[25] predictions (denoted by solid triangles: (a) maximum, (b) mean, and (c) minimum (95% confidence limits)) are for the period from 2002 to 2025.

planet. This balance is facilitated by the so-called "greenhouse gases" (GHGs) (carbon dioxide (CO_2), methane (CH_4), nitrous oxide (NO_x), etc.), which, although existing as traces in the atmosphere (current level of CO_2 380 ppm), are believed to be responsible for global warming.[24]

Increased levels of GHGs—primarily, CO_2—resulting from primary energy production from combustion of fossil fuels in developed and developing countries alike, have caused climate changes, which is evident at most parts of the Earth. In Greece, climate changes manifest themselves in (1) summers becoming hotter, and winters becoming colder, than in the past, (2) an increase in the number of tropical days per year (a tropical day is defined as a day with temperatures of >30 °C), (3) reduced precipitation, and (4) land desertification.

Analysis of the average seasonal temperatures of surface air for Greece[25] from 1955 to 2001 showed that (1) there is a significant warming trend in the average summer temperature, (2) there is a slight cooling trend in the average winter temperature, and (3) differences from the corresponding temperatures in the northern hemisphere are explained by local atmospheric circulation (pressure) data.

Electricity is the largest portion of primary energy consumed in Greece (energy consumption for transportation amounts to 39% of the primary energy consumption). Electricity consumption shows a monotonic increase over the period from 1980 to 2005.[28]

The emissions of GHGs released in the atmosphere in Greece consist of (1) 79.9% CO_2, primarily from combustion of fossil fuels, (2) 8.1% CH_4, from the production, transportation, and combustion of fossil fuels, (3) 8.2% N_2O, and (4) 3.3% fluorinated compounds. When it comes to human activities as sources of CO_2 emissions, 54% comes from power (thermoelectrical energy) generation, 23% from transportation (motor vehicles), 11% from industry, 9% from buildings and houses, and 3% from oil production and refining. Greece, as a member of the European Union, is a signatory to the Kyoto Protocol,[26] and, in accordance with it, undertook the obligation to reduce its GHG emissions to levels that do not exceed the levels of the 1990s by more than 25%.

It is desirable to make predictions of the magnitude of climate changes and primary energy needs of Greece over the next 15 years, and devise a plan for providing for these needs, while, at the same time, fulfilling the country's obligations to the world community.

Two types of methods are used for making the predictions: (1) time series methods, where predictions are made based on previous history, and (2) correlative methods, where predictions are made by extrapolating previous correlations.

Depending on the assumptions made, one type of method or the other is used. For example, if one assumes that energy consumption is the independent variable, energy predictions are made using ARIMA, a time series method. Since energy consumption (or production) affects CO_2 emissions, predictions of CO_2 emissions are made using a correlative method from neural networks trained with previous data of energy consumption and CO_2 emissions. Average seasonal temperatures, in turn, are predicted using a correlative method from neural networks trained with previous data of CO_2 emissions and average seasonal temperatures. One can also assume that climate changes or their metrics, average seasonal temperatures, affect energy consumption, which, in turn, affects CO_2 emissions (and even close the loop) and repeat predictions of average seasonal temperatures using ARIMA, energy consumption using neural networks trained with previous data of average seasonal temperatures, and CO_2 emissions using neural networks trained with previous data of energy consumption and CO_2 emissions (and, in the case of closing the loop, average seasonal temperatures using neural networks trained with previous data of CO_2 emissions and average seasonal temperatures).

Data for the average seasonal temperatures,[25] together with predictions for the next 15 years, using ARIMA, are shown in Figures 4 and 5. The predictions of the average seasonal temperatures in Figures 4 and 5 confirm the warming and cooling trends in the summer and winter, respectively.

Data on electricity consumption from 1980 to 2005,[28] together with predictions up to 2025, using ARIMA and neural networks, are shown in Figure 6. The neural networks that enable the predictions are of the feed-forward type, with 1 hidden layer, 10 neurons, 2 neurons at the entrance, average seasonal temperatures of T_w and T_s, 1 neuron at the exit, and an electricity consumption of E_{lc}.

Finally, data regarding the CO_2 emissions from power (electricity) generation[27] for the period from 1960 to 2005, together with predictions up to the year 2025, using ARIMA, are shown in Figure 7.

To meet the increasing energy needs of Greece in the next 15 years, its people need to make behavioral changes to avoid waste and increase the efficiency of its use. As for the state, it must increase the generation of electricity to meet increasing demand, without compromising the state of the environment and the lives of future generations. A large portion of electricity in Greece (86%) is generated from lignite, which is an

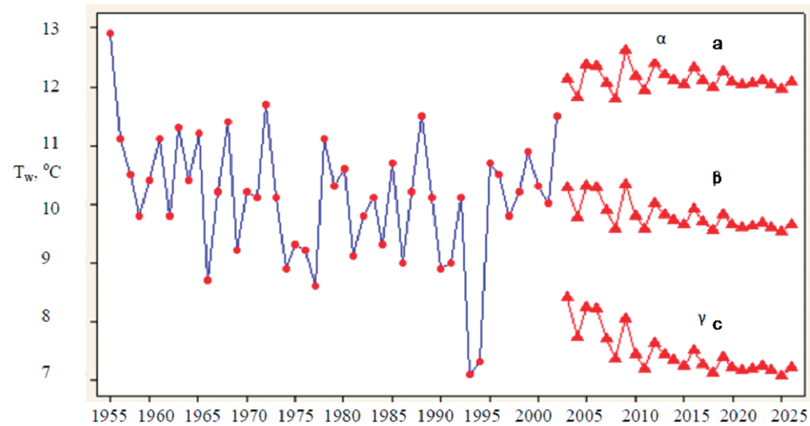

Figure 5. Average winter temperature (T_w). Data for the period from 1955 to 2001 (denoted by solid circles) have been taken from Feidas et al.;[25] predictions (denoted by solid triangles: (a) maximum, (b) mean, and (c) minimum (95% confidence limits)) are for the period from 2002 to 2025.

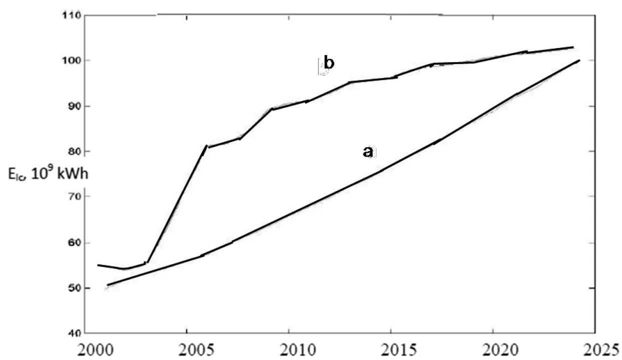

Figure 6. Electricity consumption. Energy data for the period from 1980 to 2005.[27] Average seasonal temperature data are taken from Feidas et al.[25] Predictions obtained using (a) ARIMA and (b) neural networks.

indigenous source of energy, and is associated with high amounts of CO_2 emissions. In accordance with its obligations to the Kyoto Protocol, the Greek state must reduce CO_2 emissions to levels that do not exceed the 1990s level by more than 25%. In compliance with the EU directives, part of the energy for the needs of the state members must be generated from renewable energy sources (RES). The additional energy that our predictions suggest is needed can come from RES (currently in practice), photovoltaic (PV) technology, and wind energy, as well as units of electricity generation from lignite with systems for capturing CO_2 emissions. The problem of distributing the additional electricity generation to PV, wind energy, and lignite units with zero emissions can be decided on the basis of solving the cost optimization problem:

$$\min(c_{ML} m_{ML,i} e_L + c_{PV} E_{PV,i} + c_w E_{w,i}) \qquad i = N + 1, N + 2, ..., NN \quad (2)$$

under the constraints (on the amounts of electricity needed and CO_2 released in the atmosphere)

$$m_{ML,i} e_L + E_{PV,i} + E_{W,i} = E_{lp,i} - E_{lp,N} \qquad i = N + 1, ..., NN \quad (3)$$

$$m_{ML,i} g_L + E_{PV,i} g_{PV} + E_{W,i} g_W = \alpha(G_i - G_{max}) \qquad i = N + 1, ..., NN \quad (4)$$

In eq 2, c_{ML} is the cost of electricity generation from lignite with a system for capturing CO_2 (20 €/T lignite),[29] $m_{ML,i}$ represents the mass of lignite for the lignite unit with CO_2 capturing in year i, e_L denotes the electricity generated from 1 ton of lignite (500 kWh/T),[29] c_{PV} is the cost of generating electricity from PV units (4.3−9.5 €/Wh),[30] $E_{PV,i}$ the electricity (in kWh) from PV units in year i, c_W is the cost of electricity generation from wind energy units (770−1000 €/kWh[30] electric), $E_{W,i}$ the electricity (in kWh) from wind energy units in year i, and N the last year for which predictions are made (e.g., 2025).

In eqs 3 and 4, $E_{lp,i}$ is the electricity (in kWh) in year i from the time series, g_L is the amount of CO_2 released per ton of lignite (0.56 T CO_2/Tt lignite),[31] g_{PV} the amount of reduction

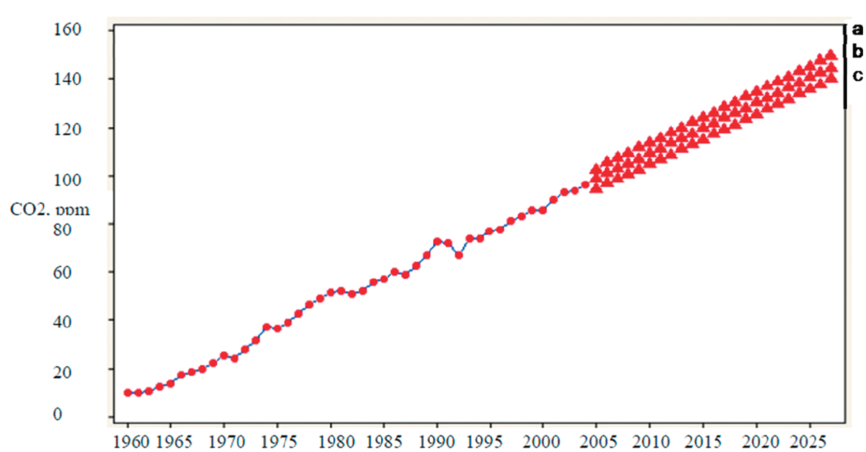

Figure 7. CO_2 emissions from power generation. Data for the period from 1960 to 2005.[27] Predictions ((a) maximum, (b) mean, and (c) minimum; 95% confidence limits) for the period from 2006 to 2025.

Table 1. Results of Solution to the Cost Optimization Problem for Electricity

year	$E_{PV,i}$ (kWh)	$E_{W,i}$ (kWh)	$m_{ML,i}$ (tn)	$E_{lp,i}$ (kWh)	$m_{L,i}$ (tn)
2005				5.61×10^{10}	1.12×10^{8}
2006		8.21×10^{6}	1.24×10^{6}	5.69×10^{10}	1.14×10^{8}
2007		7.60×10^{5}	5.00×10^{6}	5.93×10^{10}	1.19×10^{8}
2008		1.36×10^{6}	5.51×10^{6}	5.96×10^{10}	1.19×10^{8}
2009	2.11×10^{9}		6.00×10^{6}	6.20×10^{10}	1.24×10^{8}
2010	2.95×10^{9}		6.40×10^{6}	6.31×10^{10}	1.26×10^{8}
2011	4.52×10^{9}		6.52×10^{6}	6.48×10^{10}	1.30×10^{8}
2012	6.15×10^{9}		6.63×10^{6}	6.65×10^{10}	1.33×10^{8}
2013	7.56×10^{9}		6.82×10^{6}	6.80×10^{10}	1.36×10^{8}
2014	8.96×10^{9}		7.02×10^{6}	6.96×10^{10}	1.39×10^{8}
2015	1.04×10^{10}		7.21×10^{6}	7.11×10^{10}	1.42×10^{8}
2016	1.18×10^{10}		7.41×10^{6}	7.26×10^{10}	1.45×10^{8}
2017	1.32×10^{10}		7.60×10^{6}	7.41×10^{10}	1.48×10^{8}
2018	1.46×10^{10}		7.80×10^{6}	7.57×10^{10}	1.51×10^{8}
2019	1.60×10^{10}		8.00×10^{6}	7.72×10^{10}	1.54×10^{8}
2020	1.74×10^{10}		8.20×10^{6}	7.87×10^{10}	1.57×10^{8}
2021	1.88×10^{10}		8.39×10^{6}	8.03×10^{10}	1.61×10^{8}
2022	2.02×10^{10}		8.60×10^{6}	8.18×10^{10}	1.64×10^{8}
2023	2.16×10^{10}		8.78×10^{6}	8.33×10^{10}	1.67×10^{8}
2024	2.30×10^{10}		8.97×10^{6}	8.48×10^{10}	1.70×10^{8}
2025	2.44×10^{10}		9.17×10^{6}	8.64×10^{10}	1.73×10^{8}

in CO_2 emissions because of electricity generation by PV units (0.6 kg CO_2/kWh electricity),[40] g_W the amount of reduction in CO_2 emissions due to electricity generation by wind energy units (600 tn CO_2/GWh electricity),[30] α the fraction of electricity generated from fossil fuels (lignite, natural gas, oil) ($\alpha = 0.813$), G_i the mass (in tons) of CO_2 emissions in year i of the time series, and $G_{max} = \beta G_{1990}$ with $\beta = 1.25$ (this is the maximum multiple of CO_2 emissions for Greece in the 1990s, in compliance with the Kyoto protocol), and G_{1990} the CO_2 emissions (in tons) in the 1990s. The solution of the problem defined by eqs 2−4 determines the values of $m_{ML,i}$, $E_{PV,i}$, and $E_{W,i}$ in year i, from the last year of the data to the last year of the predictions. This problem is solved with differential evolution algorithms,[32] which are inspired by biological evolution and utilize its mechanisms, crossing, mutation, and natural selection. The set of solution candidates is called "population" and the solutions are called "individuals" or "elements". Population evolution is realized by repeated application of the aforementioned mechanisms. The main advantage of evolutionary algorithms is their ability to deal with optimization problems in which the objective conditions can neither be differentiated nor have discontinuities or many local extremes. The initial guesses of the values of the variables are random numbers in the domain of the problem. The results of the solution to the optimization problem are given in Table 1.

The year 2005 is the last year for which data exist. In the years after 2005, the amount of electricity needed from predictions is distributed for generation to PV technology, wind energy, and lignite with CO_2 emissions capture system units. In accordance with the solution to the optimization problem, starting in the year 2006 and advancing to the year 2025, for electricity generation, a portion of lignite must be processed in units with a CO_2 emissions capture system. In the first three years after 2005, a small portion of the electricity must be generated in wind energy units. Starting in 2009 and up to 2025, a portion of electricity must be generated in PV units. The solution to the optimization problem for electricity generation provides a blueprint for energy policy for Greece over the next 15 years or so. The technical challenge in this paradigm is the capture and sequestration of CO_2 from lignite units that generate electricity.[33]

Paradigm of Product Design: The Design of Material for Media Replication Discs

In the early 1980s, compact discs (CDs) revolutionized the sound recording industry. The new medium was more than a high-resolution, high-fidelity reproduction optical audio disc, a successor to the gramophone record for playing music; it was a medium to store digital data.[34] CD data are stored as a series of tiny indentations, known as "pits", encoded in a spiral tract on the top of a transparent polycarbonate layer. The pits have the same depth and width but variable length, and are separated by areas known as lands. For encoding purposes, a change from pit to land or vice versa indicates a binary "one", while no change indicates a series of binary "zeros", the number of which is defined by the pit length. Replicated CDs are mass-produced initially using a hydraulic press. Pellets of polycarbonate are

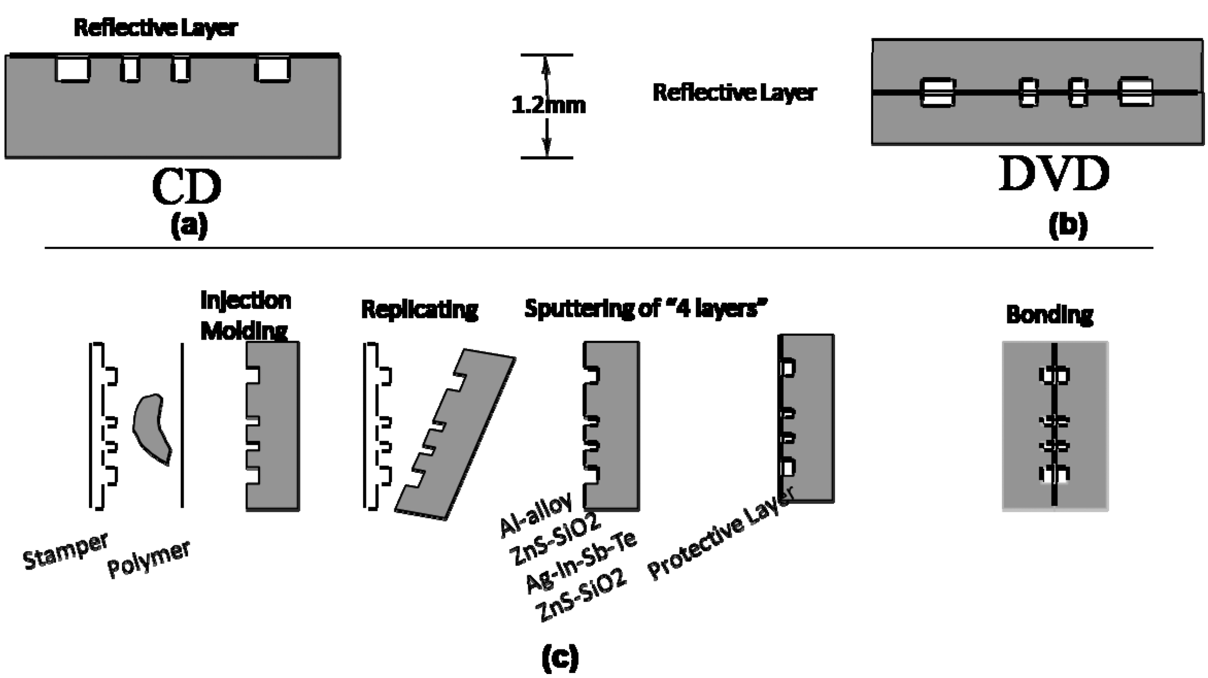

Figure 8. Schematics of (a) a compact disc (CD), (b) a digital versatile (video) disc (DVD), and (c) the manufacturing of optical discs.

Table 2. Design of Material for DVD Substrate: Customer Needs (Y = Optical Disc Performance), Measurable Characteristics (y), and Affecting Factors (x)

measurable characteristics, y	target	affecting factors, x
Disc Needs: Optical Properties		
birefrigence	<50 nm	monomers, polymerization
Disc Needs: Physical Properties		
tilt	0.7°	polymer processes
dimensional stability	0.7°	polymer processes
Disc Needs: Replication		
groove depth	95% stamper	polymer processes
Disc Needs: Cleanliness		
number of particulates	<10 000/g	raw materials, processes, equipment, room air

fed into the press while under heat. A screw forces the liquefied plastic into the mold cavity and the mold is closed with a stamper in contact with the molten plastic. After the plastic is cooled and hardened, a thin reflective layer of aluminum alloys is applied to the surface of the polycarbonate layer, followed by a protective layer of lacquer. A CD is read by focusing a 780-nm-wavelength (near-infrared) light beam of a semiconductor laser through the bottom of the polycarbonate layer.

In the early 1990s, the idea of storing digital data on an optical disk was extended to video by a new optical medium, known as the digital versatile disc or digital video disc (DVD).[34] DVDs have the same structure and dimensions as the CDs (Figure 8), but can store more than six times as much data. They operate on the same principles as CDs, but they use a different format and are read by laser light with a wavelength of 650 nm (red). Although polycarbonate is the same substrate (where data are stored) as that for CDs, this polycarbonate had stricter specifications and required appropriate design. Because, after 1980, chemical engineering focused its efforts more on products than processes, the design of the substrate material for DVDs was one of the very first examples of product design.[7] Product design starts with customer needs (designated here as Y), which are translated into measurable characteristics (denoted here as y), which, in turn, are correlated with the affecting factors (which are represented by x) (see Table 2).

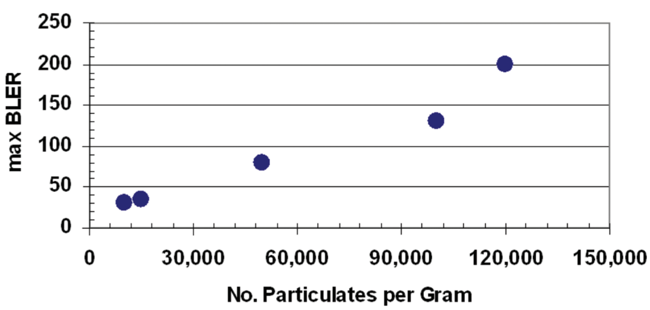

Figure 9. Effect of particulates on the block error rate (BLER).

The most critical requirements for the disc are structural stability and optical performance, which the latter being dependent on birefringence, which is the difference in refractive indices in directions parallel and perpendicular to the disk. Birefringence is a function of the orientation of the polymer molecule, hence, the stress during processing, the polarizability, and the dielectric capacity of the material. An adequate theory that relates this macroscopic optical property to microstructure currently does not exist,[35] and guidelines for this product design may be established through the design of experiments (DOE).[36] Structural stability and optical performance are compromised by the presence of impurities in the form of opaque particles in the material. Impurities include, but are not limited to, monomers, solvents, substances aiding polymerization (e.g., initiator, terminator, etc.), plasticizers, oligomers, carbonized polymer, metal fragments from piping and equipment, dust and airborne particles, etc. Hydrophilic particles under humid conditions swell and cause cracking of the disc. Impurity particles at levels higher than 10 000 per gram of resin cause an unacceptable increase in the Block Error Rate (BLER), which measures the error rate in extracting data frames from an optical disc (see Figure 9).

With the understanding that particulates can come from (1) raw materials, (2) processes (e.g., extrusion), (3) ambient air,

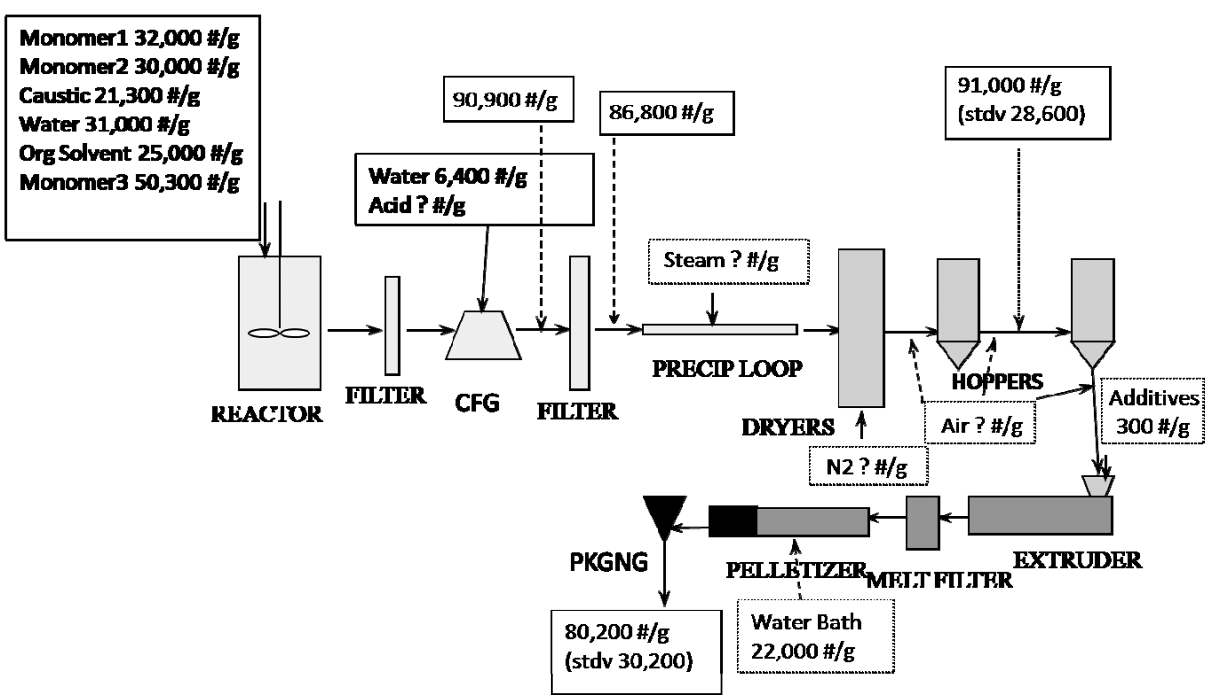

Figure 10. Balance of particulates throughout the flow diagram of polycarbonate material production.

and (4) piping and equipment, it was decided that a balance of particulates throughout the flow diagram would be performed (Figure 10), by measuring the size distribution of particulates before and after each process in the diagram. At this point, the problem of designing a new product (material) is reduced to process design.[37] For some processes, the number of particulates generated by the process can be estimated from simple models, e.g., a boundary-layer model can provide an estimate of 10 000 particles of carbonized polycarbonate material, with an average size of 1 μm, generated by extrusion.

Measurements of particulates before and after various processes in the flow diagram show that the best opportunities for removing impurity particulates from the polycarbonate material are solution and melt filtration. By the appropriate selection of filters, the number of particulates per gram of resin can be significantly reduced. If, in addition, other measures to improve cleanliness of the material are taken (e.g., selective removal of impurities from raw materials, coating of piping and equipment in contact with abrasive material, clean-room atmosphere for processes in contact with ambient air, etc.), the number of particulates per gram of resin can be kept below the upper specification limit of 10 000 per gram.

Conclusions

Over the years, chemical engineering has demonstrated its dynamic character through its involvement in solving technical problems in diverse areas of current interest, which impact the welfare of society. In doing so, its practitioners have learned to work in teams with others of diverse disciplines and utilize diverse methodologies and tools. It is believed that, in the near future, chemical engineering would become more involved in three areas: health, climate change and energy, and performance products. To support this belief, paradigms, one from each of the three areas, are presented.

The first paradigm is the design of a device for encapsulation of pancreatic cell islets for transplantation to treat Type 1 diabetes. Based on findings of clinical tests confirming that, for effective treatment of the disease ~10 000 islet equivalent (IEQ) per kilogram of body weight are needed, a device is designed to operate at a high rate and high efficiency of microencapsulation (one islet per capsule).

The second paradigm is from the area of climate change and energy. Climate changes in Greece manifest themselves, in addition to other effects, as an increase in the average summer temperature and a decrease in the average winter temperature, as data from 1955 to 2001 demonstrated. Predictions are made of average seasonal temperatures, CO_2 emissions, and electricity consumption from 2002 to 2025, using ARIMA and neural networks. A cost optimization scheme, using evolutionary algorithms, is employed for the additional power generation needed in the years to come, under the constraint of meeting Greece's self-assumed obligations to the Kyoto Protocol. The solution to the optimization problem shows how the additional power generation in the years to come must be distributed among lignite units equipped with systems for capturing CO_2 emissions, photovoltaic units, and wind energy units.

The third paradigm deals with the design of a new material for media replicated discs, on which information is stored and from which information is recovered by laser light. The most critical specification of this material pertains to its purity, which is measured by the number of submicrometer particles of foreign matter per gram of resin. The particles in the resin, which is sold to disc makers in pellets, originate from raw materials used in its synthesis (monomers, solvents, and initiators, accelerators and terminators of polymerization), airborne matter, equipment material, and processes. By delineating the sources of impurity particles, assessing the capabilities of reducing the number of particles in the resin downstream from their origin, and implementing the most effective capabilities along the flow diagram, pellets of material of desirable purity are produced.

Literature Cited

(1) Fogler, H. S. Chemical Engineering Perspectives for the Next Decade. Presented at the *8th World Congress of Chemical Engineering*, Montreal, Canada, Aug. 23−27, 2009.

(2) Stephanopoulos, G. Process Systems Engineering: From Solvay to the 21st Century. A History of Development, Successes and Prospects for the Future. *Comput.-Aided Chem. Eng.* **2009**, *27*, 149−155. (Presented at the 10th International Symposium on Process Systems Engineering, Salvador, Bahia, Brazil, Aug. 16−20, 2009.)

(3) Davis, G. E. *A Handbook of Chemical Engineering*; Davis Brothers: Manchester, U.K., 1901.

(4) Walker, W. H.; Lewis, W. K.; McAdams, W. H. *Principles of Chemical Engineering*; McGraw−Hill: New York, 1923.

(5) Bird, R. B.; Stewart, W. E.; Lightfoot, E. N. *Transport Phenomena*; Wiley: New York, 1960.

(6) Levenspiel, O. *Chemical Reaction Engineering*; Wiley: New York, 1962.

(7) Cussler, E. L.; Moggridge, G. D. *Chemical Product Design*; Cambridge University Press, 2001.

(8) Kwauk, M. Beyond transport phenomena and reaction engineering. *Chem. Eng. Sci.* **2004**, *59*, 1613.

(9) Ottino, J. M. New Tools, New Outlooks, New Opportunities. *AIChE J.* **2005**, *51*, 1840.

(10) Maehr, R.; Chen, S.; Snitow, M.; Ludwig, T.; Yagasaki, L.; Goland, R.; Leibel, R. L.; Melton, D. A. Generation of Pluripotent Stem Cells from Patients with Type Diabetes. *Proc. Natl. Acad. Sci., U.S.A.* **2009**, *106*, 15523.

(11) Takahashi, K.; Yamanaka, S. Induction of Pluripotent Stem Cells from Mouse Embryonic and Adult Fibroblast Cultures by Defined Factors. *Cell* **2006**, *126*, 663.

(12) Shapiro, A. M. J.; Ricordi, C.; Hering, B. J.; et al. International Trial of the Edmonton Protocol for Islet Transplantation. *New Engl. J. Med.* **2005**, *355*, 1318.

(13) Lacy, P. E.; Kostianovsky, M. Method for the Isolation of Intact Islets of Langerhans from the Rat Pancreas. *Diabetes* **1967**, *16*, 35.

(14) Orive, G.; Hernandez, R. M.; Garson, A. R.; Callafiore, R.; Chang, T. M. S.; Hortelano, G.; Hunkeler, D.; Lacik, I.; Shapiro, A. M. J.; Pedraz, J. L. Cell Encapsulation: Promise and Progress. *Nature Med.* **2003**, *9*, 104.

(15) Cohen, I.; Li, H.; Hougland, J. L.; Mrksich, M.; Nagel, S. R. Using Selective Withdrawal to Coat Microparticles. *Science* **2001**, *292*, 265.

(16) Wyman, J. L.; Kizilel, S.; Skarbek, R.; Zhao, X.; Connors, M.; Dillmore, W. S.; Murphy, W. L.; Mrksich, M.; Nagel, S. R.; Garfinkel, M. R. Immunoisolating Pancreatic Islets by Encapsulation with Selective Withdrawal. *Small* **2007**, *3*, 683.

(17) Lee, G. B.; Hung, C. I.; Ke, B. J.; Huang, G. R.; Hwei, B. H.; Lai, H. F. Hydrodynamic Focusing for a Micromachined Flow Cytometer. *J. Fluid Eng.* **2001**, *123*, 672.

(18) Yamahata, C.; Vandevyver, C.; Lacharme, F.; Izewska, P.; Vogel, H.; Freitag, R.; Gijs, M. A. M. Pumping of Mammalian Cells with a Nozzle-Diffuser Micropump. *Lab Chip* **2005**, *5*, 1083.

(19) Lister, J. R. Selective Withdrawal from Viscous Two-Layer System. *J. Fluid Mech.* **1989**, *198*, 231.

(20) Hatziavramidis, D.; Pozrikidis, C. Hydrodynamic Analysis of Pancreatic Islet Micro-Encapsulation by Selective Withdrawal. *Eng. Anal. Boundary Elem.* **2008**, *32*, 11.

(21) Blyth, M. G.; Pozrikidis, C. Particle Encapsulation due to Thread Breakup in Stokes Flow. *J. Fluid Mech.* **2008**, *617*, 141.

(22) Kizilel, S.; Perez-Luna, V. H.; Teymour, F. Photopolymerization of Poly(ethylene glycol) Diacrylate on Eosin-Functionalized Surfaces. *Langmuir* **2004**, *20*, 8652.

(23) Li, S.; Chen, S. Analysis of a circular PZT Actuator for a Valveless Micropump. *Sens. Actuators A* **2003**, *104*, 151.

(24) Hansen, J.; Sato, M.; Kharecha, P.; Russell, G.; Lea, D. W.; Siddall, M. Climate Change and Trace Gases. *Philos. Trans. R. Soc. A* **2007**, *365*, 1925.

(25) Feidas, H.; Makrogiannis, T.; Bora-Senta, E. Trend Analysis of Air Temperature Time Series in Greece and their Relationship with Circulation using Surface and Satellite Data: 1955−2001. *Theor. Appl. Climat.* **2004**, *79*, 185.

(26) *Kyoto Protocol to the United Nations Framework Convention on Climate Change*; UN, 1998.

(27) *EIA—International Energy Data and Analysis for Greece*, U.S. Energy Information Administration: Washington, DC, May 2009.

(28) Abdi, H.; Valentin, D.; Edelman, B. *Neural Networks*; Sage: Thousand Oaks, CA, 1999.

(29) Kaldellis, J. K.; Zafirakis, D.; Kondili, E. Contribution of Lignite in the Greek Electricity Generation: Review and Future Prospects. *Fuel* **2009**, *88*, 475.

(30) Tsoutsos, T.; Papadopoulou, E.; Katsiri, A.; Papadopoulos, A. Supporting Schemes for Renewable Energy Sources and their Impact on Reducing the Emissions of Greenhouse Gases in Greece. *Renew. Sustainable Energy Rev.* **2008**, *12*, 1767.

(31) Kaminaris, S. D.; Tsoutsos, T. D.; Agoris, D.; Machias, A. V. Assessing Renewables-to-Electricity Systems: A Fuzzy Expert System Model. *Energy Policy* **2006**, *34*, 1357.

(32) Homaifar, A.; Lai, A. H.; Qi, X. Constrained optimization via genetic algorithms. *Simulation* **1994**, *2*, 242.

(33) Herzog, H. What Future for Carbon Capture and Sequestration. *Environ. Sci. Technol.* **2001**, *35*, 148A.

(34) Tominaga, J.; Nakano, T. *Near-Field Recording: Science and Technology*; Springer: Berlin, 2004.

(35) Edwards, S. F.; Doi, M. *The Theory of Polymer Dynamics*; Clarendon Press: Oxford, U.K., 1992.

(36) Montgomery, D. C. *Design and Analysis of Experiments*; Wiley: New York, 2001.

(37) Seider, W. D.; Seader, J. D.; Lewin, D. R. *Product and Process Design Principles: Synthesis, Analysis and Evaluation*; Wiley: New York, 2009.

Received for review February 5, 2010
Revised manuscript received April 20, 2010
Accepted April 22, 2010

IE1002894