New Paradigms in Chemical Engineering: Health, Clima Change and Energy, Design of New Materials

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Symposium on New Frontiers in Chemical & Biochemical Engineering, CERTH, Thessaloniki, Greece
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New Frontiers in Chemical Engineering

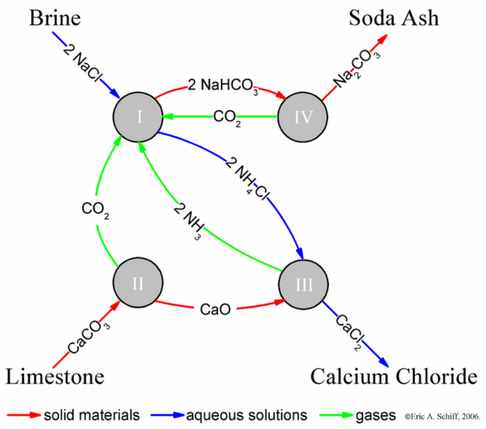
Scott Fogler, AIChE President (2009) ***"…where we are and where we want to go"***

Defining Forces: Industry & Academia

Industry

1850 – 1900	***Industrial Revolution***	***Sulfuric Acid, Organic Dyes, Ammonia Catalytic Cracking***

Solvay process (1861 – 1864) (beginning of Process Engineering according to George Stephanopoulos)



New Frontiers in Chemical Engineering

Industry

1900 – 1950	*2-World War Period*	*Syn-fuels, Syn-Rubber, Penicillin*
1942	*1st plant of synthetic rubber from styrene and butadiene (Goodyear)*	
1950 - 2000	*Reconstruction & Growth*	*Plastics, syn-fibers, herbicides, insecticides, electronic materials*

New Frontiers in Chemical Engineering

Industry

2000 – present	*Globalization Era*	*Biotechnology, Nanotechnology*

Academia

1901	*Unit Operations*	*Davis, G.E. "A Handbook of Chemical Engineering", Davis Bros., Manchester, GB*
1923	*Unit Operations*	*Walker, W.H., Lewis, W.K., McAdams, W.H. "Principles of Chemical Engineering", McGraw-Hill, New York, USA*
1958	*Transport Phenomena*	*Bird, R.B., Stewart, W.E., Lightfoot, E.N. "Notes on Transport Phenomena", Wiley, New York*
1962	*Chemical Reaction Engineering*	*Levenspiel, O. "Chemical Reaction Engineering", Wiley, New York*
1970 – 1990	*Process Control & Optimization*	
1990 – present	*Complex Systems*	*Composite, multi-component, multi-scale, non-linear, non-equilibrium*

Symposium on New Frontiers in Chemical & Biochemical Engineering, CERTH, Thessaloniki (2009):

Thematic Areas

- ***Functional Materials***
- ***Environmental Physical & Chemical Processes***
- ***Energy***
- ***Chemical Engineering Fundamentals***
- ***New Paradigms in Chemical/Biochemical Engineering***
- ***Process Systems Engineering***
- ***Biomedical Advances***

Personalized Medicine

The use of a person's clinical, genetic, genomic, and environmental information to select a medication, its dose, or to choose a therapy, or recommend preventive health measures. The goal of personalized medicine is optimize the health care and medical outcomes for each individual

Medicine: natural or synthetic substances, living (cells) or non-living (chemicals), micro- or macro-molecular, utilized for treatment (therapy) and prevention (prophylaxis) of diseases

Encapsulation of pancreatic islet cells for diabetes type 1 treatment

- ***Therapeutic modalities for type 1 diabetes, an autoimmune metabolic disease that affects 171 million people worldwide : (1) exogenous insulin therapy, (2) transplantation of pancreatic islet cells, and (3) transplantation of pancreas***
- ***Exogenous insulin treatment corrects the insulin deficiency but does not reinstate the normal glycaemic level. It is also not effective when circulatory problems and other complications arise***
- ***Therapies based on transformation of embryonic or adult stem cells or reprogramming of cells into pancreatic beta cells that secrete insulin, far from being guaranteed***

Encapsulation of pancreatic islet cells for diabetes type 1 treatment

- *Transplantation of islet cells, which seems to offer a feasible solution with many advantages, i.e., can control type 1 diabetes, restore normal glycemic control, does not require major surgical procedures, and can be repeated several times without discomfort to the patient, has been refined into a procedure known as the Edmonton protocol. Protocol makes use of immunosuppressive (anti-rejection) drugs to prevent the immune system from destroying transplanted islets*
- *A major obstacle to widespread use of islet transplantation is the shortage of islets. Researchers are pursuing various approaches to solve this problem, such as transplanting islets from a single donated pancreas, from a portion of the pancreas of a living donor, or from animals, e.g., swine*

Needed: 10,000 – 20,000 β-cells per kg of body weight

- *An alternative to immunosuppression is immunomodulation which is achieved through encapsulation by biocompatible and crosslinked polymer semipermeable membranes. Process time is an important factor in obtaining viable and functional islets for transplantation.*

Aim : design and build an encapsulation apparatus for pancreatic islets, which has a high yield and high rate, for animal model studies, and scale it up to meet the demands of clinical trials in humans

New Paradigms in Chemical Engineering: Health

Encapsulation of pancreatic islet cells for diabetes type 1 treatment

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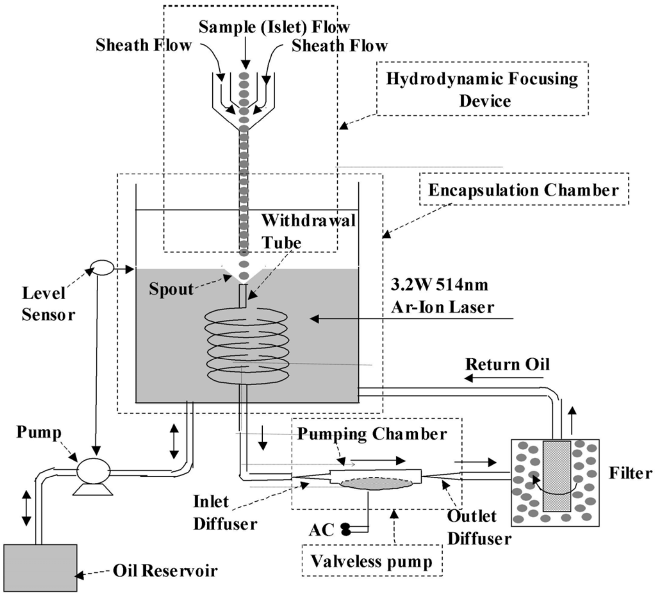
New Paradigms in Chemical Engineering: Health

Encapsulation of pancreatic islet cells for diabetes type 1 treatment



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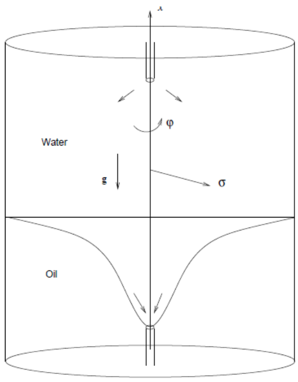
New Paradigms in Chemical Engineering: Health

Encapsulation of pancreatic islet cells for diabetes type 1 treatment

- ***Encapsulation technique** used here is based on **selective withdrawal** from a **two-fluid layer system**, the **upper layer** consisting of the **polymer solution and the islets with the culture medium**, the **lower layer** consisting of **heavy oil** not miscible with the aqueous polymer solution. In the selective withdrawal technique the **shear stress** is **small** and does not harm the islets. **Particles not caught in the selective withdrawal spout** lost and **not coated**.*



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New Paradigms in Chemical Engineering: Health

Encapsulation of pancreatic islet cells for diabetes type 1 treatment

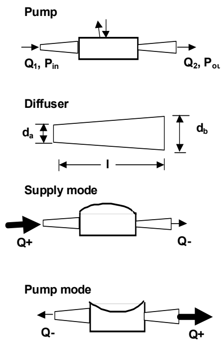
- ***Feeder** of the harvested islets is a **hydrodynamic focusing device** used in **cytometers**. Its main purpose to **align islets** in single file and ensure **encapsulation of individual islets**. A **theory for the hydrodynamic focusing device** has been reported in the literature (Lee et al, 2001), where **sheath and sample flows** consist of **homogeneous liquids** and the **volumetric fraction of the cells in the sample flow** is **small** enough to make **fluid-cell interactions negligible**. Here, the **sheath flow** consists of **aqueous solution of poly (ethylene glycol) diacrylate** spiked with **photoinitiator** and the **sample flow** consists of the **culture medium** with the **harvested islets***
- ***Islets coated with precursor solution** of poly (ethylene glycol) or PEG diacrylate **enter** the **withdrawal tube** through the **spout**. Upon **exposure** to **argon ion laser light**, polymer becomes **crosslinked** and **coating hardens** to form a **semipermeable membrane**. The photopolymerization requires an **initiator**, **eosin Y**, a **co-initiator**, **triethanolamine (TEA)**, and a **terminator**, **pyrrolidone**. The **degree of crosslinking** determines the characteristics of the membrane, e.g., **porosity**, **permeability***

New Paradigms in Chemical Engineering: Health

Encapsulation of pancreatic islet cells for diabetes type 1 treatment

- ***Successful encapsulation** of islet cells **isolates donor tissue** from the **host immune system**, thus assuring **long-term viability and functionality of the islet cell transplant**. **Membrane** acts as a **barrier** against **passage of immunologically active moieties**, e.g., antibodies, while **allowing passage of essential molecules**, e.g., oxygen, glucose, nutrients, insulin, and metabolites. For **survival**, **islets** need to be **close to sources of oxygen and nutrients**, and be **protected** against **local inflammation**, **fibrosis**, and **oxidative stress**. This is achieved by **incorporating** in the **polymeric material** of the encapsulating membrane **vascularization, anti-inflammatory, anticoagulant and antioxidant agents**. Some of these functional molecules added to the polymeric material act as **scavengers** for small molecules including **cytokines**, **NO**, and **free radicals**, which are known to be **toxic to the islets***
- *A **valveless pump**, with **no interior mechanical parts**, and shown to **transport mammalian cells** without the **slightest damage** (Yamahata, C. et al, 2005), is used to generate "selective withdrawal" flow and remove the encapsulated islets. It is a **diaphragm pump** that uses two **diffusers** as **flow directing elements** and a **pump chamber**, the **top** of which is made out of **flexible material**. An actuator, piezoelectric (**PZT**) patch or an **electromagnet**, bonded to the top of the pumping chamber with epoxy resin, is used in connection with applied AC voltage to set the **top plate into vibration** at a frequency, **below the natural frequency of the material the plate***

New Paradigms in Chemical Engineering: Health
Encapsulation of pancreatic islet cells for diabetes type 1 treatment



- ***Encapsulated islets are separated from oil by filtration***

New Paradigms in Chemical Engineering: Health
Encapsulation of pancreatic islet cells for diabetes type 1 treatment

An apparatus for encapsulating pancreatic cell islets for transplantation into patients with diabetes type 1 has been designed. Operation of this device is as follows:

1. ***Pancreatic cell islets in a culture medium and an aqueous solution of a biocompatible polymer are fed by a hydrodynamic focusing device from cytometry, which ensures alignment of the islets in a single file and focusing into a specific area on the interface of a two-layer water-oil system,***
2. ***The method of selective withdrawal in a two-layer water-oil system is utilized to coat each individual islet with the same aqueous solution of a biocompatible polymer as in the feed,***
3. ***The polymer solution coat of the islet is hardened or gelled by photo-initiated crosslinking of the polymer, to produce a uniform-thickness, semipermeable membrane (allows passage of insulin, oxygen, nutrients, and other metabolites, but not immunologically active molecules and cells)***
4. ***Encapsulated islets are removed from the encapsulation chamber by a valveless micropump and recovered by filtration***

New Paradigms in Chemical Engineering: Clima Change & Energy

Global Warming

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New Paradigms in Chemical Engineering: Clima Change & Energy

Clima Change

- *Clima change: a result of unbalanced development*
- *Clima change in combination with human activities hostile to environment and natural disasters leads to desertfication and deforestation impacting water supply, agriculture, and food chain*
- *Model of development based on market only leads to behaviors of over-consumption, and over-production without any regard for natural and human resources*

Sustainable Development

- *According to Brundtland Commission, "Sustainable development is the development that satisfiew the needs of the present, without downgrading the ability of the future generations to satisfy their needs"*

  For rational Sustainable Development ("Green Development" not "Green Horses"), one needs to keep in mind:

1. *Fuel based on chemistry of an element other than carbon, e.g., hydrogen, is beyond technological reach at present,*
2. *If a country has reserves of fossil fuel, it is bound to use them,*
3. *1 gal of gasoline has the same energy content with 5 acres of crops for food*
4. *Laws of Thermodynamics govern the direction of change and the efficiency of transformation*

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New Paradigms in Chemical Engineering: Clima Change & Energy

The Atmosphere

Life on earth depends on: (1) existence of the atmosphere, and (2) a delicate balance of solar radiation between earth and atmosphere

Absorption + Trapping – Emission = Surplus or Deficit

Atmosphre : 72 + 150 - 330 = - 108 W/m^2

92 (Evaporation) + 16 (Thermal Convection) W/m^2

Earth : 168 + 330 - 390 = 108 W/m^2

Pure dry air	(% vol.)
N_2	78,08
O_2	20.95
Ar	0.93
CO_2	0.035
Ne	1.8×10^{-3}
He	5×10^{-4}
Kr	1×10^{-4}
Xe	1×10^{-5}
CH_4	2×10^{-4}
N_2O	3×10^{-5}
CO	1×10^{-5}

New Paradigms in Chemical Engineering: Clima Change & Energy

Ozon & Greenhouse Gases

- O_3 in the atmosphere **ultraviolet radiation** and prevents it from reaching the earth to cause destructive **mutations** to living cells
- **Greenhouse gases,** primarily CO_2 trap **infrared radiation** and keep temperature on earth's surface at levels that allow maintenance of life

Time	Atmospheric CO2 , ppm	Characterization
130.000 – 12.000 BCE	180	ice age
12.000 πκη – 1800	280	warm age
2000*	380	warm age
???	480	superheated age**

* Ρυθμός αύξησης CO_2 = 2 ppm / έτος

** Earth an entirely different planet than it has been for the last 10,000,000 years

New Paradigms in Chemical Engineering: Clima Change & Energy

Clima Change in Greece

Observations of clima change in Greece

1. Unusually warm summers
2. Unusually warm winters
3. Decrease in rainfall
4. Increase in number of annual tropical days (days with temperature > 30°C)
5. Increase of desertification
6. Warming observed in Greece by far exceeds that in Northern Hemisphere.

This difference is due to differences in local atmospheric circulation

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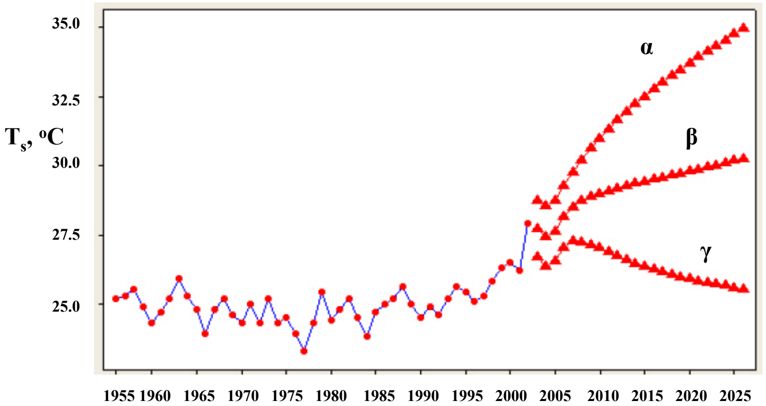
Predictions of average summer temperature in Greece from 2001 – 2025 (ARIMA)



(α) Max, (β) average, and (γ) min. Confidence Interval 95%

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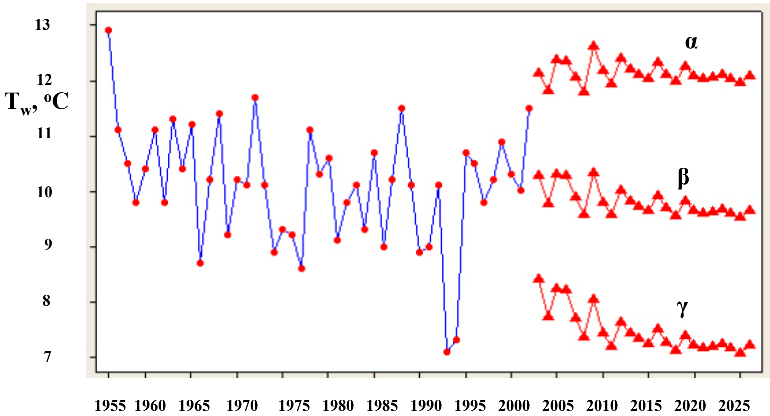
Predictions of average winter temperature in Greece from 2001 – 2025 (ARIMA)



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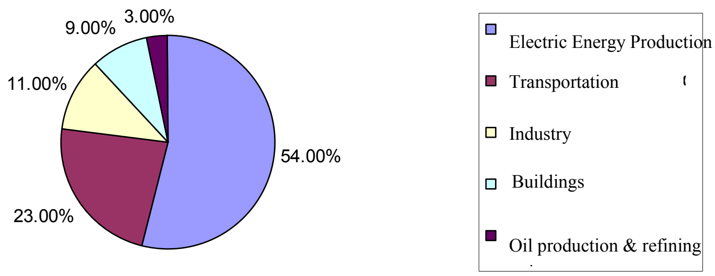
New Paradigms in Chemical Engineering: Clima Change & Energy

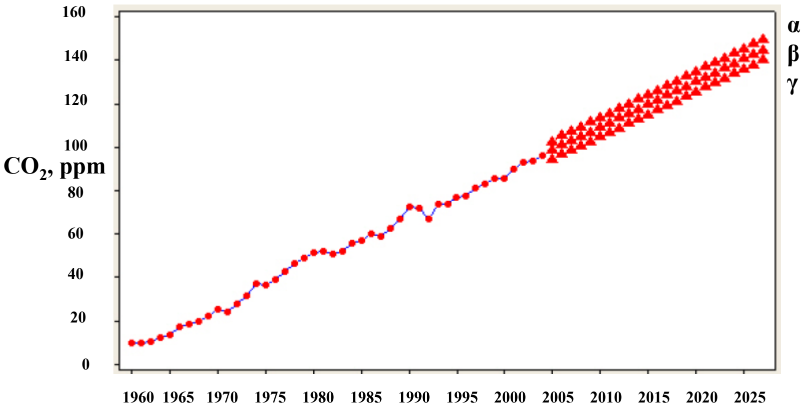
Composition of greenhouse gas emissions in Greece

Gas	%, vol	Source
CO2	79.9	combustion of fossil fuels
CH4	8.1	production, transport,combustion fossil fuels
N2O	8.2	
Fluorinated	3.3	

CO_2 from human activities



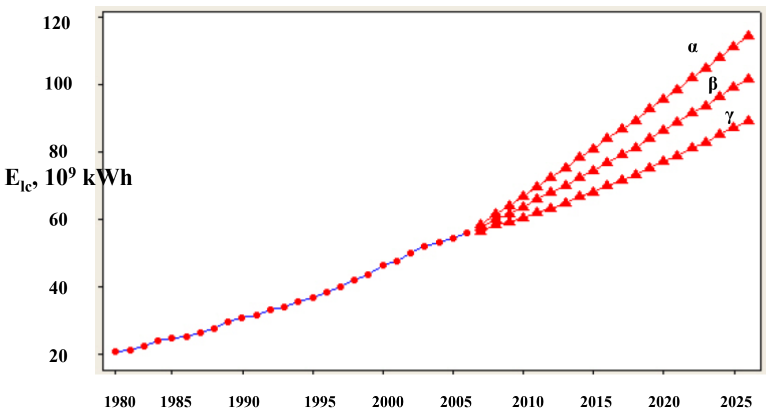
Predictions of CO_2 emissions from electric & thermal energy production



(α) Max, (β) average, and (γ) min. Confidence Interval 95%

New Paradigms in Chemical Engineering: Clima Change & Energy

Prediction of average annual consumption of electric energy, E_{lc}, in Greece (ARIMA)



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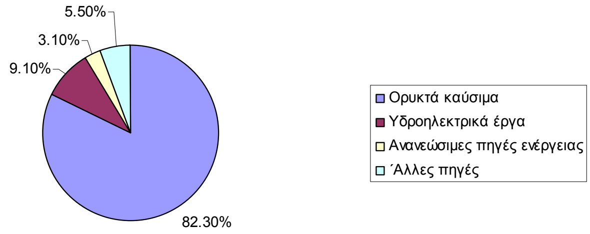
New Paradigms in Chemical Engineering: Clima Change & Energy

Electric Energy Sources in Greece

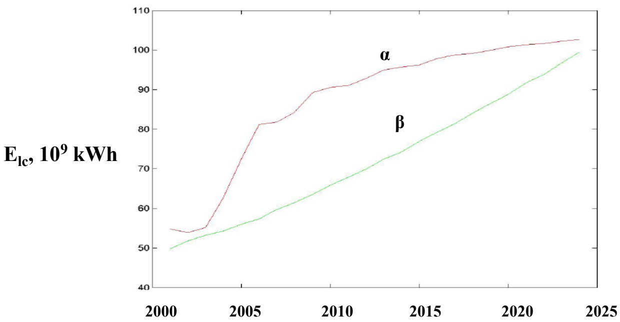


Electric Energy from Fossil Fuels in Greece

Lignite	***55.9%***
Oil	***13.5%***
Natural Gas	***12.9%***

New Paradigms in Chemical Engineering: Clima Change & Energy

Prediction of annual consumption of electric energy, E_{lc}, in Greece



(α) ARIMA , (β) Neural networks (front feedback, 1 hidden level, 10 neurons, 2 inlet, T_w και T_s, και 1 outlet, E_{lc})

New Paradigms in Chemical Engineering: Clima Change & Energy

An Energy Plan for Greece

Basis: to apply principles of sustainable development to construct production units for future energy needs ==> Greece needs to provide for

energy needs of its citizens, and, at the same time, as a signatory to Kyoto Protocol, fulfill state obligations to world community according to the protocol

Greece's obligations to Kyoto Protocol : CO_2 emissions should not exceed those of the 1990s more than 25%

How to provide for Energy Needs & comply with Kyoto Protocol

- *Transportation (23% of CO_2 emissions)*
  Car technology with fuel different than gasoline not yet developed. Hybrid cars costly
  Need programs to change behaviors
  1. *Replacement of driving own car by walking, biking, using mass transportation,*
  2. *Disencourage driving with taxes and other charges ,*
  3. *Replace air trips with railway trips*
- *Buildings (11% of CO_2 emissions)*
  1. *Energy insulation,*
  2. *Glass on south side,*
  3. *"Passive" houses (without heating or air conditioning)*

New Paradigms in Chemical Engineering: Clima Change & Energy

Energy Plan for Greece

How to provide for Energy Needs & comply with Kyoto Protocol

- *Industry (9% of CO_2 emissions)*
  1. *Increase efficiency,*
  2. *Monitor environmental behaviors by state regulatory agencies together with rewards for good environmental practices and fines for violations*
- *Electric energy production (54% of CO_2 emissions)*
  Encounter increase in electric energy production with production from
  1. *Lignite with systems for zero exhaust gas emissions (absorption of CO2 by triethanolamine, storage underground, etc) ,*
  2. *Wind energy, and*
  3. *Solar energy (photovoltaics)*

Energy Plan for Greece

Optimization Problem

To produce with the lowest cost additional energy needed from three sources, lignite with zero emissions, wind and solar energy, and, at the same time, keep CO_2 emissions at levels that do not exceed more than 25% the levels of the 1990's

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

$$m_{ML,i} e_L + E_{PV,i} + E_{W,i} = E_{lp,i} - E_{lp,N} \qquad i = N+1, \ldots\ldots, NN$$

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

Optimization Problem

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

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

c_{ML} = cost of producing electric energy from lignite with CO2 trapping, 20 € / tn lignite

e_L = electric energy produced from 1 tn λιγνίτη, 500 kWh / tn

c_{PV} = cost of producing electric energy with phtovoltaics (PV), 4.3 – 9.5 € /Wh

$E_{PV,i}$ = kWh electric energy produced from PV in year i

$E_{W,i}$ = kWh electric energy produced from wind in year i

$E_{lp,i}$ = electric energy in kWh produced in year I

g_L = 0.56 tn CO_2 / tn lignite

g_{PV} = 0.6 kg CO_2 / kWh emissions decrease because of PV production

g_W = 600 tn CO_2 / GWh emissions decrease because of wind energy production

α = percentage of electric energy produced from fossil fuels (lignite,oil, natural gas), 0.813

G_{max}= β G_{1990} , β = 1.25 (Greece's obligations in compliance with Kyoto Protocol)

G_{1990} = emissions tn CO_2 in the 1990's

G_i = tn CO_2 emitted in year i

New Paradigms in Chemical Engineering: Clima Change & Energy

Solution with differential evolutionary algorithm (Homaifar et al, 1994)

Table shows:

1. *Lignite quantity in year i, in tn, $m_{L,i} = E_{lp,i} / e_L$, and*
2. *Only a fraction ($m_{ML,i} / m_{L,i} < 1$) of production units from lignite needs to be upgraded for trapping of CO_2*

Year	$E_{PV,i}$ kWh	$E_{W,i}$ kWh	$m_{ML,i}$ tn	$E_{lp,i}$ kWh	$m_{L,i}$ tn
2006		8.21E+06	1.24E+06	5.69E+10	1.14E+08
2007		7.60E+05	5.00E+06	5.93E+10	1.19E+08
2008		1.36E+06	5.51E+06	5.96E+10	1.19E+08
2009	2.11E+09		6.00E+06	6.20E+10	1.24E+08
2010	2.95E+09		6.40E+06	6.31E+10	1.26E+08
2011	4.52E+09		6.52E+06	6.48E+10	1.30E+08
2012	6.15E+09		6.63E+06	6.65E+10	1.33E+08
2013	7.56E+09		6.82E+06	6.80E+10	1.36E+08
2014	8.96E+09		7.02E+06	6.96E+10	1.39E+08
2015	1.04E+10		7.21E+06	7.11E+10	1.42E+08
2016	1.18E+10		7.41E+06	7.26E+10	1.45E+08
2017	1.32E+10		7.60E+06	7.41E+10	1.48E+08
2018	1.46E+10		7.80E+06	7.57E+10	1.51E+08
2019	1.60E+10		8.00E+06	7.72E+10	1.54E+08
2020	1.74E+10		8.20E+06	7.87E+10	1.57E+08
2021	1.88E+10		8.39E+06	8.03E+10	1.61E+08
2022	2.02E+10		8.60E+06	8.18E+10	1.64E+08
2023	2.16E+10		8.78E+06	8.33E+10	1.67E+08
2024	2.30E+10		8.97E+06	8.48E+10	1.70E+08
2025	2.44E+10		9.17E+06	8.64E+10	1.73E+08

New Paradigms in Chemical Engineering: Clima Change & Energy

Conclusions

- *Based on meteorological data, the clima change in Greece manifests itself, in addition to others, with (α) warmer summers and colder winters thasn those in previous years, and (β) increase of CO_2 emissions. Clima change imacts the energy needs of the population*
- *Based on data from 1955 – 2000, predictions needs are made of electric energy , which to the greatest percentage (84%) is produced from lignite, with high levels of CO_2 emissions*
- *To meet the needs in electric energy, a plan is suggested according to which the additional electric energy is produced at minimum cost and in compliance with the Kyoto Protocol regarding CO2 emissions*
- *According to this plan, which is based on the solution of an optimization problem, the additional energy can be produced as follows*
  - *(α) A fraction of the lignite units should be upgraded with systems for trapping of exhaust gas, and*
  - *(β) From 2006 – 2009, the remainder of the energy needed should have been produced from wind energy, while from 2009 up to 2025 the remainder should be produced from solar energy (photovoltaics)*

New Paradigms in Chemical Engineering: Design of New Materials

Materials

- *Inert Structural*
- *Specialty*
- *Functional*
- *Smart: respond to stimuli and changes in the environment and activate their functions accordingly*

Material Science

1960 – 80	Basics of Composite Materials
1980 – 90	Understanding limits of material failure
1990 – present	Scale, structure, design of materials

Requirements for New Materials

1. *Technical properties, e.g., stiffness, strength, plastic flow, damage tolerance, fire resistance*
2. *Technological properties, e.g., easy to work, easy to repair*
3. *Περιβαντολογικές ιδιότητες, e.g., toxicity, degradation*
4. *Economic criteria, e.g., availability and cost of raw materials,*
5. *Criteria of sustainable development, e.g., recycling, reuse*

New Paradigms in Chemical Engineering: Design of New Materials

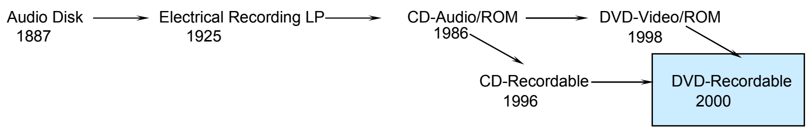
According to Ed Cussler, 8th World Congress of Chemical Engineering:

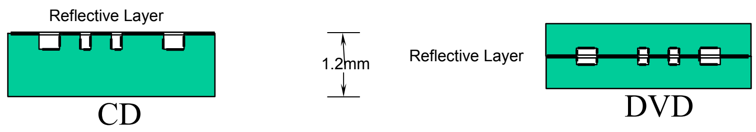
Process Design: How to make?	Product Design: What to make
batch vs. Continuous	customer need
input/output	idea generation
recycle	selection
separation/heat	manufacture

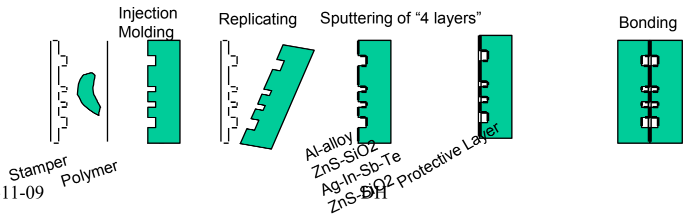
	Commodities	Molecules	Functional
Key	Cost	Speed	Function
Basis	Unit Ops	Chemistry	Microstructure
Risk	Feedstock	Discovery	Science

New Paradigms in Chemical Engineering: Design of New Materials

Design of Material for Media Replication Discs







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New Paradigms in Chemical Engineering: Design of New Materials

Design of Material for Media Replication Discs

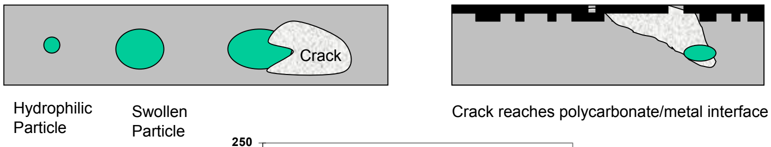
Fidelity in recovering information , Y →
Birefrigence, $n_{\square}$ - $n_{\square}$, y →
Structure & Purity, copolymer, particulate matter, ŷ

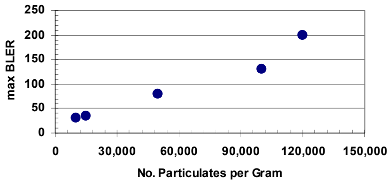
Customer CTQs	Y	y	Target
Optical Disk Performance	Optical Properties	Birefringence	<50nm
	Physical Properties	Tilt	.7 deg
		Dimensional Stability	.7 deg
	Replication	Groove Depth	95% of stamper
	Cleanliness	Particulate	10000/gm
Cost	Cycle Time	Cooling Time	< 10sec

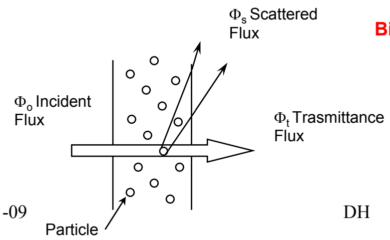
27-11-09 DH

New Paradigms in Chemical Engineering: Design of New Materials

Design of Material for Media Replication Discs



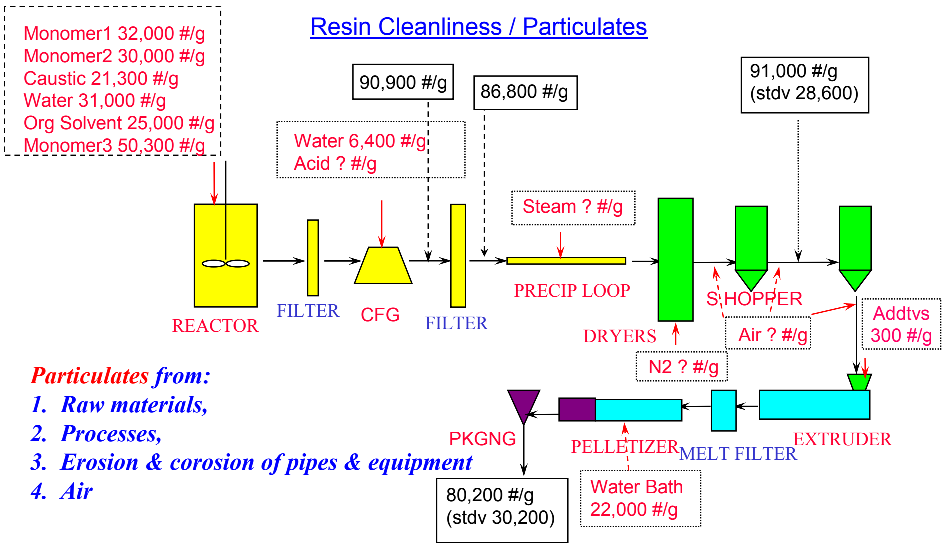




Birefrigence, Δn = Intrinsic BR
(mole orientation, polarizability)
+
Form BR
(polymer+impurities)

New Paradigms in Chemical Engineering: Design of New Materials

Design of Material for Media Replication Discs



Particulates from:

1. ***Raw materials,***
2. ***Processes,***
3. ***Erosion & corosion of pipes & equipment***
4. ***Air***

Conclusions

- ***Most-difficult-to-meet requirement on material for Media Replication Disks: Cleanliness < 10,000 particulates of size ~1mm per gr of resin (1 ppm weight)***
- ***Sources for particulates: raw materials (monomers, solvents, etc), ambient air, piping & equipment, processes***
- ***Biggest opportunities to remove particulates: solution filtration, melt filtration***
- ***Selectively reduce particulates in raw materials***
- ***Clean Rooms (air flows, air filters, clean practices) & electrostatic precipitators to reduce airborne particulates***
- ***Coat piping & equipment in contact with abrasive material***